



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 10:08 AM EDT

PDB ID : 9ZL9 / pdb_00009zl9
Title : Crystal structure of DCAF1 in complex with SDIPTAC C7
Authors : Mabanglo, M.F.; Srivastava, S.; Hoffer, L.; Ramnauth, J.; Vedadi, M.
Deposited on : 2025-12-08
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

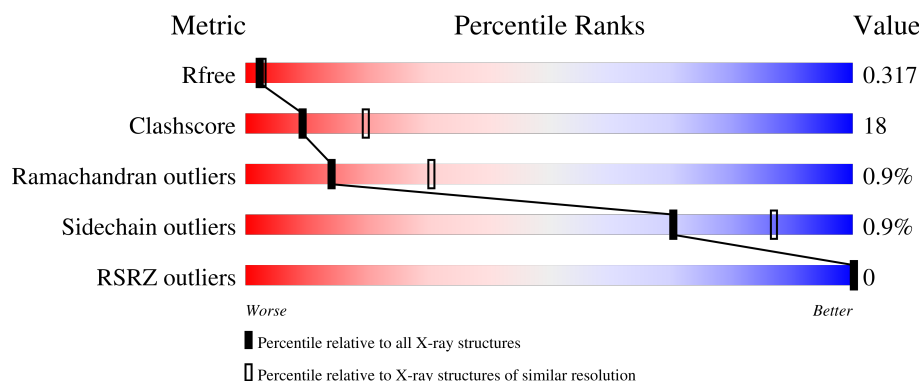
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	C	314	
1	D	314	
1	E	314	

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Mol	Chain	Length	Quality of chain
1	F	314	<div><div></div><div>60%</div><div>36%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14749 atoms, of which 126 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

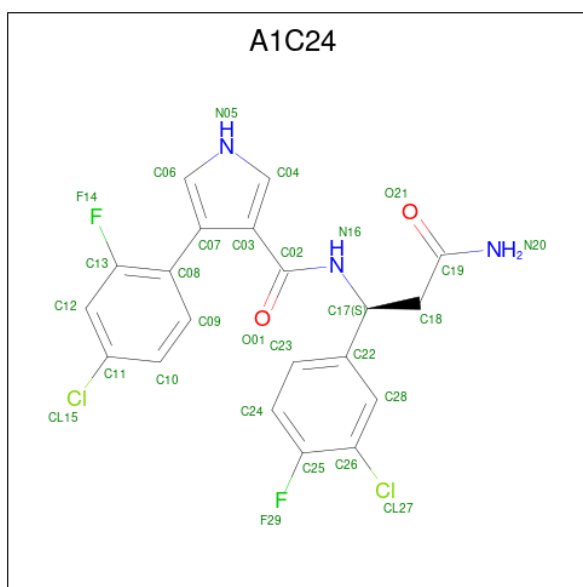
- Molecule 1 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	1	1
			2350	1488	401	445	16			
1	B	297	Total	C	N	O	S	0	1	1
			2369	1499	404	450	16			
1	C	296	Total	C	N	O	S	0	1	1
			2361	1495	404	446	16			
1	D	300	Total	C	N	O	S	0	1	1
			2388	1512	408	451	17			
1	E	295	Total	C	N	O	S	0	1	1
			2352	1489	402	445	16			
1	F	300	Total	C	N	O	S	0	1	1
			2394	1513	408	456	17			

There are 12 discrepancies between the modelled and reference sequences:

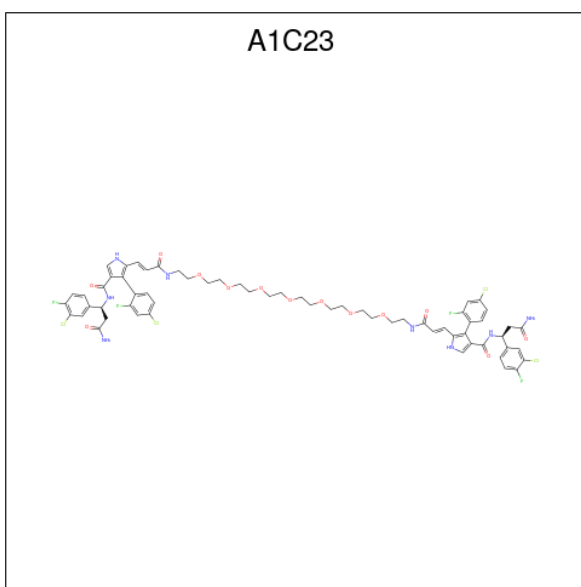
Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
A	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
B	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
B	1079	ALA	ARG	engineered mutation	UNP Q9Y4B6
C	1077	ALA	PHE	engineered mutation	UNP Q9Y4B6
C	1079	ALA	ARG	engineered 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: C₂₀H₁₅Cl₂F₂N₃O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is (4P,4'P)-5,5'-[(1E,30E)-3,29-dioxo-7,10,13,16,19,22,25-heptaoxa-4,28-diazah entriaconta-1,30-diene-1,31-diyl]bis{N-[(1S)-3-amino-1-(3-chloro-4-fluorophenyl)-3-oxopropyl]-4-(4-chloro-2-fluorophenyl)-1H-pyrrole-3-carboxamide} (CCD ID: A1C23) (formula: C₆₂H₆₆Cl₄F₄N₈O₁₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	F	1	Total	C	Cl	F	H	N	O	0	0
			157	62	4	4	66	8	13		

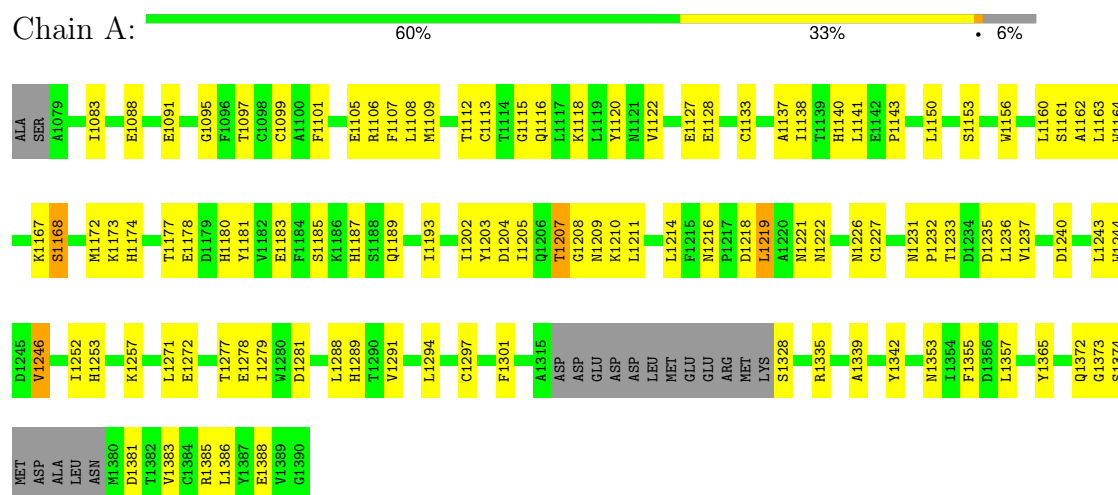
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	34	Total	O	0	0
			34	34		
4	C	32	Total	O	0	0
			32	32		
4	D	36	Total	O	0	0
			36	36		
4	E	29	Total	O	0	0
			29	29		
4	F	34	Total	O	0	0
			34	34		

3 Residue-property plots

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

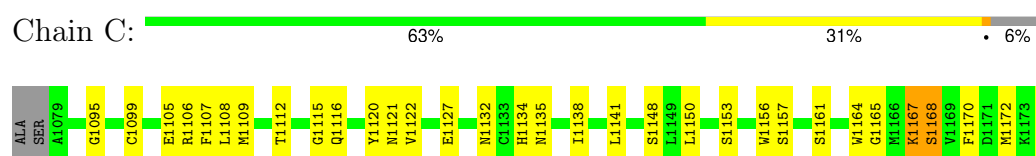
- Molecule 1: DDB1- and CUL4-associated factor 1

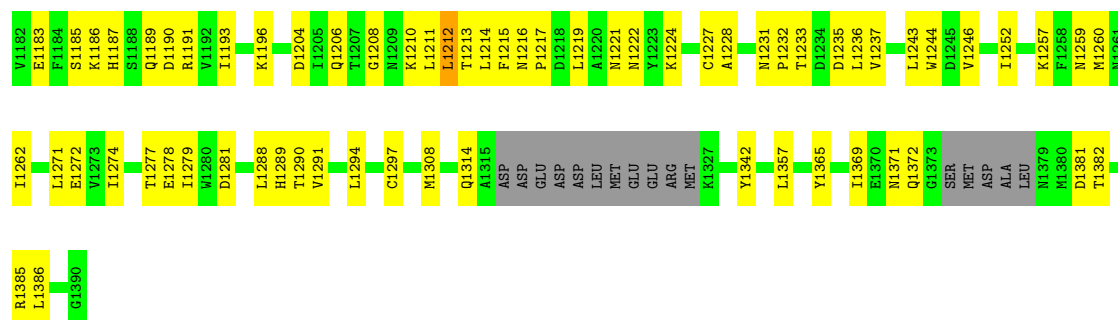


- Molecule 1: DDB1- and CUL4-associated factor 1

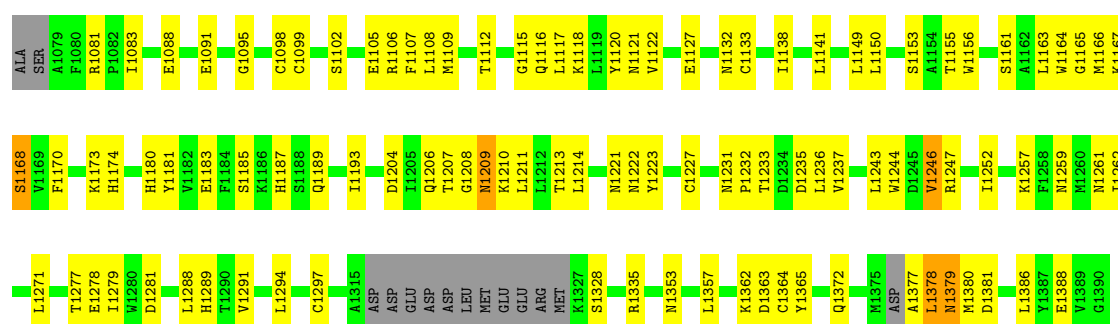


- Molecule 1: DDB1- and CUL4-associated factor 1

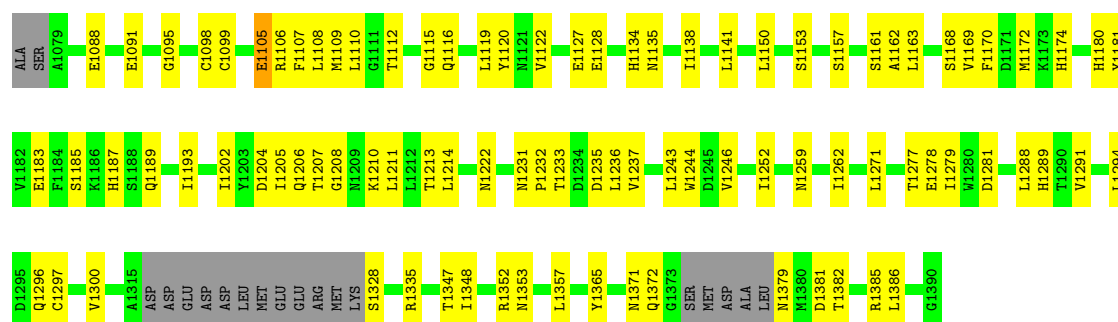




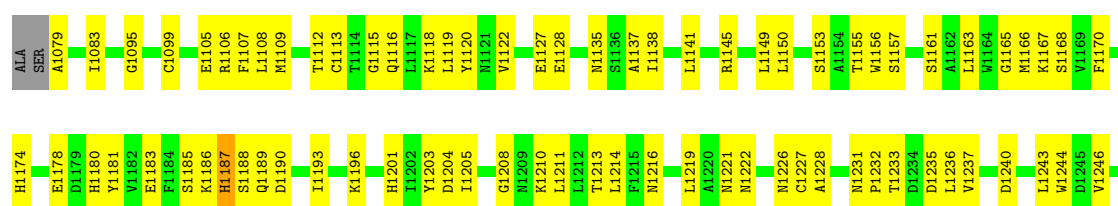
- Molecule 1: DDB1- and CUL4-associated factor 1

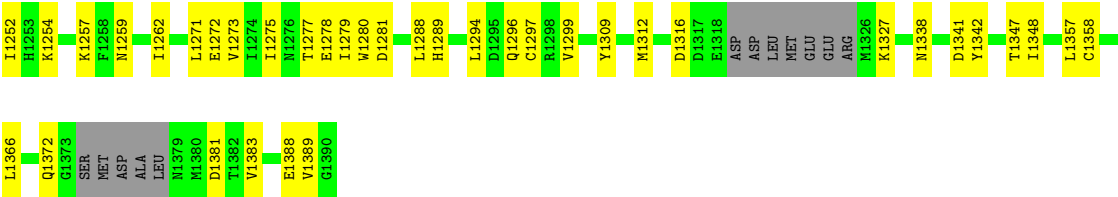


- Molecule 1: DDB1- and CUL4-associated factor 1



- 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, α , β , γ	147.30Å 85.13Å 222.55Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	30.75 – 2.60 30.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.75-2.60) 81.8 (30.75-2.60)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.269 , 0.317 0.268 , 0.317	Depositor DCC
R_{free} test set	1983 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.894	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.450 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.450 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.450 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.448 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.457 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14749	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1C24, A1C23

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	0.14	0/2405	0.37	0/3261
1	B	0.13	0/2424	0.38	0/3286
1	C	0.12	0/2416	0.35	0/3275
1	D	0.12	0/2443	0.34	0/3311
1	E	0.12	0/2407	0.34	0/3264
1	F	0.17	0/2449	0.38	0/3319
All	All	0.13	0/14544	0.36	0/19716

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	2350	0	2250	88	0
1	B	2369	0	2266	86	0
1	C	2361	0	2264	84	0
1	D	2388	0	2294	87	0
1	E	2352	0	2251	68	0
1	F	2394	0	2287	100	0
2	A	29	15	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	29	15	0	1	0
2	D	29	15	0	1	0
2	E	29	15	0	1	0
3	F	91	66	0	0	0
4	A	37	0	0	9	1
4	B	34	0	0	10	0
4	C	32	0	0	7	0
4	D	36	0	0	14	0
4	E	29	0	0	3	0
4	F	34	0	0	8	0
All	All	14623	126	13612	505	1

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 18.

All (505) 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:D:1204:ASP:HB2	1:D:1211:LEU:HD21	1.34	1.10
1:A:1204:ASP:HB2	1:A:1211:LEU:HD11	1.43	0.98
1:D:1163:LEU:HD12	1:D:1173:LYS:HB2	1.46	0.97
1:B:1083:ILE:HD11	1:B:1388:GLU:HB2	1.45	0.97
1:B:1204:ASP:HB2	1:B:1211:LEU:HD11	1.48	0.96
1:D:1081:ARG:NH2	1:D:1388:GLU:OE1	1.98	0.96
1:A:1181[A]:TYR:HE1	1:A:1183:GLU:HG3	1.34	0.93
1:A:1083:ILE:HD11	1:A:1388:GLU:HB2	1.51	0.91
1:B:1153:SER:HG	1:B:1161:SER:HG	1.18	0.91
1:B:1233:THR:OG1	1:B:1235:ASP:OD1	1.87	0.91
1:C:1204:ASP:HB2	1:C:1211:LEU:HD11	1.49	0.91
1:C:1148:SER:HB2	1:C:1167:LYS:HD2	1.53	0.88
1:A:1243:LEU:HB3	4:A:1502:HOH:O	1.74	0.88
1:F:1233:THR:OG1	1:F:1235:ASP:OD1	1.93	0.87
1:F:1083:ILE:HD11	1:F:1388:GLU:HB2	1.56	0.85
1:D:1233:THR:OG1	1:D:1235:ASP:OD1	1.94	0.85
1:F:1181[A]:TYR:HE1	1:F:1183:GLU:HG3	1.39	0.85
1:C:1181[B]:TYR:HE1	1:C:1183:GLU:HG3	1.43	0.84
1:A:1181[A]:TYR:CE1	1:A:1183:GLU:HG3	2.13	0.82
1:A:1253:HIS:N	4:A:1502:HOH:O	2.10	0.82
1:D:1362:LYS:O	4:D:1501:HOH:O	1.99	0.81
1:D:1181[A]:TYR:HE1	1:D:1183:GLU:HG3	1.47	0.80
1:F:1107:PHE:HE2	1:F:1128:GLU:HG2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1259:ASN:HD21	1:D:1262:ILE:H	1.30	0.80
1:D:1102:SER:HB3	1:D:1109:MET:HE3	1.61	0.80
1:B:1352:ARG:HH12	1:B:1385:ARG:HE	1.28	0.79
1:E:1259:ASN:HD21	1:E:1262:ILE:H	1.29	0.79
1:E:1109:MET:HE1	1:E:1150:LEU:HD13	1.63	0.79
1:F:1222:ASN:O	4:F:1501:HOH:O	2.02	0.78
1:F:1181[A]:TYR:CE1	1:F:1183:GLU:HG3	2.19	0.77
1:D:1156:TRP:HB2	4:D:1524:HOH:O	1.84	0.77
1:C:1233:THR:OG1	1:C:1235:ASP:OD1	2.03	0.76
1:A:1252:ILE:HG13	4:A:1502:HOH:O	1.84	0.76
1:E:1233:THR:OG1	1:E:1235:ASP:OD1	2.03	0.76
1:B:1107:PHE:HE2	1:B:1128:GLU:HG2	1.50	0.76
1:F:1155:THR:HG22	1:F:1156:TRP:CD1	2.22	0.75
1:F:1243:LEU:HD12	1:F:1252:ILE:CG1	2.17	0.75
1:D:1222:ASN:O	4:D:1502:HOH:O	2.04	0.75
1:D:1207:THR:HG23	4:D:1503:HOH:O	1.85	0.75
1:F:1243:LEU:HD12	1:F:1252:ILE:HG12	1.69	0.74
1:F:1153:SER:HG	1:F:1161:SER:HG	1.27	0.74
1:D:1174:HIS:HD2	1:D:1208:GLY:HA3	1.52	0.74
1:F:1214:LEU:HD22	1:F:1244:TRP:CE3	2.22	0.74
1:C:1259:ASN:HD21	1:C:1262:ILE:H	1.34	0.73
1:D:1153:SER:HG	1:D:1161:SER:HG	1.24	0.73
1:E:1206:GLN:HB2	4:E:1503:HOH:O	1.88	0.73
1:D:1102:SER:CB	1:D:1109:MET:HE3	2.18	0.73
1:D:1204:ASP:CB	1:D:1211:LEU:HD21	2.17	0.73
1:D:1107:PHE:HE1	1:D:1121:ASN:HD22	1.34	0.72
1:A:1109:MET:HE1	1:A:1150:LEU:HD13	1.72	0.72
1:A:1233:THR:HB	1:B:1271:LEU:HD11	1.71	0.72
1:E:1107:PHE:HE2	1:E:1128:GLU:HG2	1.55	0.72
1:A:1107:PHE:HE2	1:A:1128:GLU:HG2	1.53	0.71
1:B:1313:LEU:N	4:B:1403:HOH:O	2.22	0.71
1:D:1214:LEU:HD22	1:D:1244:TRP:CE3	2.25	0.71
1:B:1185:SER:O	1:B:1189:GLN:HG2	1.91	0.71
1:D:1206:GLN:HB2	4:D:1503:HOH:O	1.90	0.71
1:C:1385:ARG:NH1	4:C:1501:HOH:O	2.07	0.70
1:F:1211:LEU:HD12	1:F:1211:LEU:H	1.57	0.70
1:B:1116:GLN:NE2	1:B:1132:ASN:OD1	2.24	0.70
1:A:1162:ALA:HB1	1:A:1172:MET:HE2	1.73	0.70
1:C:1148:SER:HB2	1:C:1167:LYS:CD	2.21	0.70
1:E:1204:ASP:HB2	1:E:1211:LEU:HD21	1.73	0.69
1:A:1160:LEU:HD12	1:A:1178:GLU:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1107:PHE:HE1	1:C:1121:ASN:HD22	1.39	0.69
1:B:1139:THR:OG1	4:B:1401:HOH:O	2.11	0.69
1:B:1341:ASP:OD2	1:B:1343:LYS:NZ	2.24	0.69
1:D:1083:ILE:HD11	1:D:1388:GLU:HB2	1.75	0.69
1:A:1185:SER:O	1:A:1189:GLN:HG2	1.94	0.68
1:C:1214:LEU:HD22	1:C:1244:TRP:CE3	2.27	0.68
1:B:1109:MET:HG2	4:B:1427:HOH:O	1.94	0.67
1:D:1281:ASP:HB2	1:D:1288:LEU:HD11	1.74	0.67
1:D:1181[A]:TYR:HE1	1:D:1183:GLU:CG	2.08	0.67
1:F:1204:ASP:N	1:F:1211:LEU:HD11	2.09	0.67
1:F:1259:ASN:HD21	1:F:1262:ILE:H	1.42	0.67
1:B:1287:LEU:H	1:C:1372:GLN:NE2	1.92	0.67
1:C:1181[B]:TYR:HE1	1:C:1183:GLU:CG	2.08	0.67
1:E:1185:SER:O	1:E:1189:GLN:HG2	1.95	0.67
1:A:1109:MET:CE	1:A:1150:LEU:HD13	2.24	0.66
1:F:1109:MET:CE	1:F:1150:LEU:HD13	2.26	0.66
1:B:1212:LEU:HD23	1:B:1213:THR:H	1.61	0.66
1:E:1207:THR:HG23	4:E:1503:HOH:O	1.95	0.66
1:F:1185:SER:O	1:F:1189:GLN:HG2	1.96	0.66
1:E:1222:ASN:O	4:E:1501:HOH:O	2.14	0.66
1:C:1181[B]:TYR:CE1	1:C:1183:GLU:HG3	2.29	0.65
1:E:1109:MET:CE	1:E:1150:LEU:HD13	2.26	0.65
1:D:1204:ASP:OD1	4:D:1503:HOH:O	2.15	0.65
1:F:1338:ASN:HD22	1:F:1341:ASP:H	1.43	0.65
1:B:1214:LEU:HD22	1:B:1244:TRP:CE3	2.32	0.65
1:F:1079:ALA:O	4:F:1502:HOH:O	2.14	0.65
1:C:1222:ASN:O	4:C:1502:HOH:O	2.14	0.65
1:D:1174:HIS:CD2	1:D:1208:GLY:HA3	2.32	0.64
1:E:1235:ASP:O	1:E:1236:LEU:HD23	1.96	0.64
1:B:1107:PHE:CE2	1:B:1128:GLU:HG2	2.33	0.64
1:C:1372:GLN:HB2	1:C:1381:ASP:O	1.97	0.64
1:D:1163:LEU:HD12	1:D:1173:LYS:CB	2.24	0.64
1:E:1233:THR:HB	1:F:1271:LEU:HD11	1.78	0.64
1:A:1140:HIS:NE2	2:A:1401:A1C24:N20	2.46	0.64
1:D:1185:SER:O	1:D:1189:GLN:HG2	1.97	0.63
1:C:1185:SER:O	1:C:1189:GLN:HG2	1.97	0.63
1:B:1180:HIS:HB3	4:B:1424:HOH:O	1.98	0.63
1:E:1281:ASP:HB2	1:E:1288:LEU:HD11	1.81	0.62
1:F:1259:ASN:HD22	1:F:1296:GLN:HE22	1.47	0.62
1:D:1221:ASN:HD22	1:D:1257:LYS:HB2	1.65	0.62
1:F:1281:ASP:HB2	1:F:1288:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:LEU:HB2	1:A:1122:VAL:CG1	2.30	0.62
1:D:1181[A]:TYR:CE1	1:D:1183:GLU:HG3	2.33	0.61
1:D:1259:ASN:HD21	1:D:1262:ILE:N	1.97	0.61
1:C:1281:ASP:HB2	1:C:1288:LEU:HD11	1.82	0.61
1:A:1235:ASP:O	1:A:1236:LEU:HD23	2.01	0.61
1:B:1150:LEU:HB2	1:B:1166:MET:HE2	1.82	0.61
1:D:1378:LEU:O	1:D:1380:MET:N	2.33	0.61
1:B:1338:ASN:HD22	1:B:1341:ASP:H	1.48	0.61
1:C:1235:ASP:O	1:C:1236:LEU:HD23	2.01	0.61
1:E:1109:MET:HG3	1:E:1119:LEU:CD1	2.30	0.60
1:B:1277:THR:OG1	1:B:1278:GLU:OE2	2.19	0.60
1:A:1277:THR:OG1	1:A:1278:GLU:OE2	2.19	0.60
1:D:1328:SER:OG	1:D:1353:ASN:HB3	2.01	0.59
1:C:1237:VAL:HG23	1:C:1246:VAL:CG2	2.33	0.59
1:C:1274:ILE:HG12	4:C:1528:HOH:O	2.02	0.59
1:A:1173:LYS:C	1:A:1174:HIS:HD1	2.11	0.59
1:B:1243:LEU:HD23	1:B:1252:ILE:HD11	1.82	0.59
1:E:1107:PHE:CE2	1:E:1128:GLU:HG2	2.35	0.59
1:E:1365:TYR:HB3	1:E:1386:LEU:HD11	1.84	0.59
1:B:1287:LEU:H	1:C:1372:GLN:HE22	1.50	0.59
1:E:1328:SER:OG	1:E:1353:ASN:HB3	2.02	0.59
1:F:1109:MET:HG3	1:F:1119:LEU:CD1	2.33	0.59
1:B:1235:ASP:O	1:B:1246:VAL:HG12	2.02	0.58
1:A:1237:VAL:HG23	1:A:1246:VAL:CG2	2.34	0.58
1:B:1083:ILE:CD1	1:B:1388:GLU:HB2	2.27	0.58
1:B:1102:SER:HA	1:B:1109:MET:CE	2.32	0.58
1:A:1385:ARG:NH1	4:A:1501:HOH:O	2.05	0.58
1:F:1389:VAL:O	4:F:1502:HOH:O	2.17	0.58
1:A:1365:TYR:HB3	1:A:1386:LEU:HD11	1.84	0.58
1:C:1109:MET:CE	1:C:1150:LEU:HD13	2.34	0.58
1:A:1279:ILE:HB	1:A:1289:HIS:HB2	1.84	0.58
1:A:1281:ASP:HB2	1:A:1288:LEU:HD11	1.86	0.58
1:C:1237:VAL:HG23	1:C:1246:VAL:HG22	1.86	0.58
1:C:1148:SER:CB	1:C:1167:LYS:HD2	2.31	0.57
1:D:1221:ASN:ND2	1:D:1257:LYS:HB2	2.19	0.57
1:F:1235:ASP:O	1:F:1236:LEU:HD23	2.04	0.57
1:C:1099:CYS:HB3	1:C:1369:ILE:HD11	1.87	0.57
1:C:1271:LEU:HD11	1:D:1233:THR:HB	1.87	0.57
1:D:1120:TYR:CZ	1:D:1127:GLU:HB2	2.40	0.57
1:F:1180:HIS:HB3	4:F:1526:HOH:O	2.03	0.57
1:D:1237:VAL:HG23	1:D:1246:VAL:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:ASN:O	4:A:1503:HOH:O	2.18	0.57
1:E:1108:LEU:HB2	1:E:1122:VAL:CG1	2.35	0.56
1:C:1115:GLY:HA2	1:C:1138:ILE:HG13	1.87	0.56
1:F:1108:LEU:HB2	1:F:1122:VAL:CG1	2.35	0.56
1:F:1150:LEU:HB2	1:F:1166:MET:HE2	1.87	0.56
1:D:1235:ASP:O	1:D:1236:LEU:HD23	2.04	0.56
1:E:1237:VAL:HG23	1:E:1246:VAL:CG2	2.34	0.56
1:F:1181[A]:TYR:HE1	1:F:1183:GLU:CG	2.14	0.56
1:C:1206:GLN:HB2	4:C:1503:HOH:O	2.06	0.56
1:B:1243:LEU:CD2	1:B:1252:ILE:HD11	2.36	0.56
1:A:1372:GLN:HB2	1:A:1381:ASP:O	2.06	0.56
1:B:1235:ASP:O	1:B:1236:LEU:HD23	2.05	0.56
1:F:1107:PHE:CE2	1:F:1128:GLU:HG2	2.35	0.56
1:B:1352:ARG:NH1	1:B:1385:ARG:HE	2.02	0.55
1:F:1277:THR:OG1	1:F:1278:GLU:OE2	2.25	0.55
1:F:1312:MET:HE2	4:F:1510:HOH:O	2.04	0.55
1:D:1117:LEU:N	4:D:1504:HOH:O	2.39	0.55
1:E:1259:ASN:HD21	1:E:1262:ILE:N	2.00	0.55
1:E:1271:LEU:HD11	1:F:1233:THR:HB	1.88	0.55
1:A:1209:ASN:HB2	1:A:1211:LEU:CD2	2.35	0.55
1:F:1109:MET:HE1	1:F:1150:LEU:HD13	1.89	0.55
1:B:1313:LEU:HG	4:B:1403:HOH:O	2.05	0.55
1:C:1178:GLU:O	1:C:1196:LYS:HG3	2.07	0.55
1:E:1277:THR:OG1	1:E:1278:GLU:OE2	2.23	0.55
1:B:1212:LEU:HD23	1:B:1213:THR:N	2.22	0.55
1:B:1272:GLU:OE2	1:B:1342:TYR:OH	2.22	0.55
1:C:1365:TYR:HB3	1:C:1386:LEU:HD11	1.89	0.55
1:E:1204:ASP:HB2	1:E:1211:LEU:HD11	1.88	0.55
1:E:1347:THR:C	1:E:1348:ILE:HD12	2.31	0.54
1:A:1120:TYR:CZ	1:A:1127:GLU:HB2	2.43	0.54
1:C:1153:SER:HG	1:C:1161:SER:HG	1.34	0.54
1:C:1186:LYS:HE3	4:C:1508:HOH:O	2.07	0.54
1:D:1149:LEU:HD22	1:D:1163:LEU:HD11	1.89	0.54
1:B:1281:ASP:HB2	1:B:1288:LEU:HD11	1.90	0.54
1:C:1204:ASP:HB2	1:C:1211:LEU:HD21	1.89	0.54
1:D:1180:HIS:HB3	4:D:1531:HOH:O	2.07	0.54
1:A:1301:PHE:HD2	4:A:1507:HOH:O	1.90	0.54
1:D:1116:GLN:NE2	1:D:1132:ASN:OD1	2.41	0.54
1:D:1365:TYR:HB3	1:D:1386:LEU:HD11	1.88	0.54
1:A:1209:ASN:ND2	4:A:1504:HOH:O	2.19	0.53
1:C:1277:THR:OG1	1:C:1278:GLU:OE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:GLU:OE2	1:A:1342:TYR:OH	2.26	0.53
1:A:1209:ASN:HB2	1:A:1211:LEU:HD23	1.90	0.53
1:B:1105:GLU:O	1:B:1106:ARG:HB2	2.08	0.53
1:F:1236:LEU:HD13	1:F:1243:LEU:HD11	1.91	0.53
1:A:1271:LEU:HD21	1:B:1233:THR:HB	1.91	0.53
1:F:1272:GLU:OE2	1:F:1342:TYR:OH	2.23	0.53
1:B:1115:GLY:HA2	1:B:1138:ILE:HG13	1.91	0.53
1:A:1181[A]:TYR:HE1	1:A:1183:GLU:CG	2.15	0.53
1:A:1214:LEU:HD22	1:A:1244:TRP:CE3	2.44	0.53
1:B:1107:PHE:HE2	1:B:1128:GLU:CG	2.21	0.53
1:B:1292:PRO:HD2	4:B:1418:HOH:O	2.09	0.53
1:C:1135:ASN:OD1	1:C:1157:SER:HB3	2.09	0.53
1:F:1372:GLN:NE2	1:F:1383:VAL:HG11	2.24	0.53
1:C:1108:LEU:HB2	1:C:1122:VAL:CG1	2.39	0.53
1:C:1167:LYS:O	1:C:1168:SER:HB3	2.08	0.53
1:B:1210:LYS:HD3	1:B:1213:THR:OG1	2.09	0.52
1:E:1099:CYS:HA	1:E:1109:MET:O	2.09	0.52
1:A:1107:PHE:CE2	1:A:1128:GLU:HG2	2.39	0.52
1:A:1116:GLN:O	1:A:1138:ILE:HD12	2.08	0.52
1:C:1190:ASP:OD1	1:C:1191:ARG:HD3	2.09	0.52
1:D:1210:LYS:HD3	1:D:1213:THR:OG1	2.09	0.52
1:A:1372:GLN:NE2	1:A:1383:VAL:HG11	2.25	0.52
1:D:1279:ILE:HB	1:D:1289:HIS:HB2	1.91	0.52
1:B:1151:LEU:HG	1:B:1184:PHE:CZ	2.44	0.52
1:E:1372:GLN:HB2	1:E:1381:ASP:O	2.09	0.52
1:A:1219:LEU:HD12	1:A:1219:LEU:N	2.25	0.52
1:E:1105:GLU:O	1:E:1106:ARG:HB2	2.10	0.52
1:F:1237:VAL:HG23	1:F:1246:VAL:CG2	2.40	0.52
1:F:1178:GLU:N	4:F:1504:HOH:O	2.32	0.52
1:C:1109:MET:HE1	1:C:1150:LEU:HD13	1.90	0.52
1:D:1163:LEU:CD1	1:D:1173:LYS:HB2	2.30	0.52
1:C:1371:ASN:HA	1:C:1382:THR:HG22	1.92	0.52
1:C:1204:ASP:HB2	1:C:1211:LEU:CD1	2.32	0.52
1:C:1216:ASN:HD22	1:C:1219:LEU:HG	1.75	0.52
1:E:1214:LEU:HD22	1:E:1244:TRP:CE3	2.45	0.52
1:F:1099:CYS:HA	1:F:1109:MET:O	2.10	0.52
1:B:1365:TYR:HB3	1:B:1386:LEU:HD11	1.91	0.52
1:D:1095:GLY:O	1:D:1112:THR:HA	2.10	0.52
1:E:1120:TYR:CZ	1:E:1127:GLU:HB2	2.45	0.52
1:C:1120:TYR:CZ	1:C:1127:GLU:HB2	2.45	0.51
1:B:1120:TYR:CZ	1:B:1127:GLU:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1174:HIS:HD2	1:C:1208:GLY:HA3	1.75	0.51
1:D:1167:LYS:O	1:D:1168:SER:HB3	2.11	0.51
1:C:1357:LEU:C	1:C:1357:LEU:HD12	2.36	0.51
1:E:1243:LEU:HD23	1:E:1252:ILE:HD11	1.92	0.51
1:E:1348:ILE:HD12	1:E:1348:ILE:N	2.25	0.51
1:F:1174:HIS:CD2	1:F:1208:GLY:HA3	2.46	0.51
1:F:1109:MET:HG3	1:F:1119:LEU:HD12	1.92	0.51
1:A:1207:THR:OG1	1:A:1209:ASN:OD1	2.27	0.51
1:D:1105:GLU:O	1:D:1106:ARG:HB2	2.11	0.51
1:F:1279:ILE:HB	1:F:1289:HIS:HB2	1.92	0.51
1:F:1372:GLN:HB2	1:F:1381:ASP:O	2.10	0.51
1:C:1212:LEU:HD23	1:C:1213:THR:H	1.77	0.50
1:A:1140:HIS:CD2	2:A:1401:A1C24:N20	2.79	0.50
1:A:1204:ASP:CB	1:A:1211:LEU:HD11	2.28	0.50
1:B:1102:SER:HA	1:B:1109:MET:HE3	1.92	0.50
1:F:1357:LEU:HD12	1:F:1357:LEU:C	2.36	0.50
1:A:1097:THR:O	1:A:1355:PHE:HB3	2.12	0.50
1:B:1099:CYS:HA	1:B:1109:MET:O	2.11	0.50
1:C:1279:ILE:HD13	1:C:1342:TYR:CD2	2.46	0.50
1:F:1243:LEU:HD12	1:F:1252:ILE:CD1	2.41	0.50
1:A:1357:LEU:HD12	1:A:1357:LEU:C	2.37	0.50
1:D:1363:ASP:HB2	4:D:1501:HOH:O	2.12	0.50
1:A:1216:ASN:CG	1:A:1219:LEU:HD13	2.37	0.50
1:C:1174:HIS:CD2	1:C:1208:GLY:HA3	2.46	0.50
1:D:1118:LYS:NZ	1:D:1127:GLU:OE2	2.42	0.50
1:C:1095:GLY:O	1:C:1112:THR:HA	2.12	0.49
1:E:1352:ARG:HH22	1:E:1385:ARG:CZ	2.25	0.49
1:F:1174:HIS:HD2	1:F:1208:GLY:HA3	1.76	0.49
1:E:1259:ASN:ND2	1:E:1262:ILE:H	2.03	0.49
1:A:1113:CYS:HA	1:A:1137:ALA:HB1	1.94	0.49
1:E:1109:MET:HG3	1:E:1119:LEU:HD12	1.93	0.49
1:D:1181[A]:TYR:HE2	2:D:1401:A1C24:F14	1.85	0.49
1:D:1236:LEU:HD13	1:D:1243:LEU:HD11	1.95	0.49
1:E:1107:PHE:HE2	1:E:1128:GLU:CG	2.23	0.49
1:F:1178:GLU:O	1:F:1196:LYS:HG3	2.12	0.49
1:B:1108:LEU:HB2	1:B:1122:VAL:CG1	2.43	0.49
1:B:1235:ASP:C	1:B:1246:VAL:HG12	2.38	0.49
1:A:1203:TYR:HD1	1:A:1210:LYS:HA	1.77	0.49
1:D:1364:CYS:HA	4:D:1507:HOH:O	2.12	0.49
1:F:1294:LEU:O	1:F:1297:CYS:HB2	2.12	0.49
1:A:1216:ASN:ND2	1:A:1219:LEU:HD13	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:SER:OG	1:A:1353:ASN:HB3	2.12	0.49
1:D:1163:LEU:HD13	1:D:1163:LEU:C	2.38	0.49
1:B:1204:ASP:HB2	1:B:1211:LEU:HD21	1.94	0.49
1:C:1243:LEU:CD2	1:C:1252:ILE:HD11	2.43	0.49
1:E:1163:LEU:HD21	1:E:1205:ILE:HG23	1.93	0.49
1:A:1167:LYS:O	1:A:1168:SER:HB3	2.13	0.48
1:A:1233:THR:OG1	1:A:1235:ASP:OD1	2.28	0.48
1:D:1108:LEU:HB2	1:D:1122:VAL:CG1	2.43	0.48
1:F:1141:LEU:HD12	1:F:1141:LEU:C	2.38	0.48
1:A:1118:LYS:HD3	1:A:1120:TYR:HE1	1.78	0.48
1:C:1221:ASN:OD1	1:C:1257:LYS:HB2	2.13	0.48
1:C:1259:ASN:HD21	1:C:1262:ILE:N	2.07	0.48
1:E:1294:LEU:O	1:E:1297:CYS:HB2	2.13	0.48
1:C:1215:PHE:CE2	1:C:1217:PRO:HD3	2.48	0.48
1:D:1099:CYS:HA	1:D:1109:MET:O	2.13	0.48
1:F:1243:LEU:HD12	1:F:1252:ILE:HD11	1.95	0.48
1:B:1279:ILE:HB	1:B:1289:HIS:HB2	1.95	0.48
1:C:1099:CYS:HA	1:C:1109:MET:O	2.13	0.48
1:A:1204:ASP:HB2	1:A:1211:LEU:CD1	2.30	0.48
1:B:1357:LEU:HD12	1:B:1357:LEU:C	2.38	0.48
1:E:1135:ASN:OD1	1:E:1157:SER:HB3	2.14	0.48
1:B:1193:ILE:HD11	1:B:1228:ALA:HB1	1.95	0.48
1:F:1167:LYS:O	1:F:1168:SER:HB3	2.12	0.48
1:F:1275:ILE:HG22	4:F:1506:HOH:O	2.13	0.48
1:B:1227:CYS:O	4:B:1402:HOH:O	2.20	0.48
1:F:1105:GLU:O	1:F:1106:ARG:HB2	2.14	0.48
1:A:1181[A]:TYR:CD1	1:A:1227:CYS:SG	3.07	0.48
1:B:1099:CYS:HB3	1:B:1369:ILE:HD11	1.96	0.48
1:B:1106:ARG:O	1:B:1122:VAL:HG22	2.14	0.48
1:B:1117:LEU:HD21	4:B:1427:HOH:O	2.13	0.48
1:C:1279:ILE:HB	1:C:1289:HIS:HB2	1.96	0.48
1:B:1165:GLY:O	1:B:1170:PHE:HA	2.14	0.47
1:B:1174:HIS:CD2	1:B:1208:GLY:HA3	2.49	0.47
1:E:1162:ALA:HB1	1:E:1172:MET:CE	2.44	0.47
1:B:1095:GLY:O	1:B:1112:THR:HA	2.14	0.47
1:C:1116:GLN:O	1:C:1138:ILE:HD12	2.14	0.47
1:C:1243:LEU:HD23	1:C:1252:ILE:HD11	1.95	0.47
1:E:1115:GLY:HA2	1:E:1138:ILE:HG13	1.96	0.47
1:F:1115:GLY:HA2	1:F:1138:ILE:HG13	1.97	0.47
1:A:1101:PHE:HA	1:A:1108:LEU:HD12	1.96	0.47
1:A:1115:GLY:HA2	1:A:1138:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:LEU:HB2	1:A:1177:THR:O	2.14	0.47
1:D:1357:LEU:HD12	1:D:1357:LEU:C	2.39	0.47
1:E:1357:LEU:C	1:E:1357:LEU:HD12	2.40	0.47
1:B:1166:MET:HG2	1:B:1170:PHE:HD1	1.79	0.47
1:D:1116:GLN:O	1:D:1138:ILE:HD12	2.14	0.47
1:E:1116:GLN:O	1:E:1138:ILE:HD12	2.15	0.47
1:F:1118:LYS:HD3	1:F:1120:TYR:HE1	1.79	0.47
1:A:1088:GLU:CD	1:A:1091:GLU:HG3	2.39	0.47
1:A:1105:GLU:O	1:A:1106:ARG:HB2	2.14	0.47
1:A:1202:ILE:O	1:A:1211:LEU:N	2.47	0.47
1:D:1163:LEU:HD13	1:D:1164:TRP:N	2.29	0.47
1:E:1169:VAL:O	1:E:1170:PHE:C	2.57	0.47
1:E:1352:ARG:HH22	1:E:1385:ARG:NH1	2.12	0.47
1:F:1118:LYS:HE3	1:F:1127:GLU:OE2	2.15	0.47
1:C:1294:LEU:O	1:C:1297:CYS:HB2	2.14	0.47
1:D:1141:LEU:HD12	1:D:1141:LEU:C	2.39	0.47
1:A:1204:ASP:HB2	1:A:1211:LEU:HD21	1.97	0.47
1:B:1118:LYS:HD3	1:B:1120:TYR:HE1	1.80	0.46
1:F:1273:VAL:CG2	1:F:1280:TRP:HB2	2.45	0.46
1:C:1224:LYS:HE2	1:C:1260:MET:HB3	1.98	0.46
1:C:1236:LEU:HD13	1:C:1243:LEU:HD11	1.97	0.46
1:E:1279:ILE:HB	1:E:1289:HIS:HB2	1.97	0.46
1:F:1347:THR:C	1:F:1348:ILE:HD12	2.40	0.46
1:A:1180:HIS:CD2	1:A:1180:HIS:H	2.34	0.46
1:C:1156:TRP:HE3	1:C:1156:TRP:O	1.98	0.46
1:D:1156:TRP:HE3	4:D:1524:HOH:O	1.97	0.46
1:A:1193:ILE:O	1:A:1193:ILE:HG23	2.16	0.46
1:A:1335:ARG:HD3	4:A:1530:HOH:O	2.16	0.46
1:C:1105:GLU:O	1:C:1106:ARG:HB2	2.16	0.46
1:C:1294:LEU:HD21	1:C:1308:MET:CE	2.46	0.46
1:E:1115:GLY:HA3	1:E:1134:HIS:O	2.16	0.46
1:F:1216:ASN:HD22	1:F:1219:LEU:HG	1.80	0.46
1:B:1167:LYS:O	1:B:1168:SER:HB3	2.15	0.45
1:D:1281:ASP:HB2	1:D:1288:LEU:CD1	2.45	0.45
1:D:1088:GLU:CD	1:D:1091:GLU:HG3	2.40	0.45
1:D:1193:ILE:HG23	1:D:1193:ILE:O	2.17	0.45
1:D:1259:ASN:ND2	1:D:1262:ILE:H	2.06	0.45
1:F:1210:LYS:HD3	1:F:1213:THR:OG1	2.17	0.45
1:A:1203:TYR:CD1	1:A:1210:LYS:HA	2.51	0.45
1:C:1233:THR:HB	1:D:1271:LEU:HD11	1.99	0.45
1:B:1102:SER:HB3	1:B:1109:MET:HE2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1118:LYS:NZ	1:B:1127:GLU:OE2	2.47	0.45
1:E:1095:GLY:O	1:E:1112:THR:HA	2.16	0.45
1:F:1120:TYR:CZ	1:F:1127:GLU:HB2	2.52	0.45
1:C:1290:THR:HG23	4:C:1507:HOH:O	2.16	0.45
1:A:1294:LEU:O	1:A:1297:CYS:HB2	2.17	0.45
1:F:1201:HIS:HB2	1:F:1203:TYR:CE1	2.52	0.45
1:F:1201:HIS:HB2	1:F:1203:TYR:HE1	1.82	0.45
1:A:1181[A]:TYR:CE1	1:A:1183:GLU:CG	2.92	0.45
1:B:1116:GLN:O	1:B:1138:ILE:HD12	2.16	0.45
1:E:1181[B]:TYR:CE2	1:E:1183:GLU:HG3	2.52	0.45
1:B:1151:LEU:HG	1:B:1184:PHE:CE2	2.52	0.45
1:F:1135:ASN:OD1	1:F:1157:SER:HB3	2.16	0.45
1:F:1181[A]:TYR:CE1	1:F:1183:GLU:CG	2.95	0.45
1:B:1113:CYS:HA	1:B:1137:ALA:HB1	1.99	0.45
1:B:1193:ILE:HG23	1:B:1193:ILE:O	2.17	0.45
1:B:1303:HIS:CE1	1:B:1361:THR:HA	2.52	0.45
1:B:1352:ARG:HH12	1:B:1385:ARG:NE	2.07	0.45
1:D:1294:LEU:O	1:D:1297:CYS:HB2	2.17	0.44
1:E:1153:SER:OG	1:E:1161:SER:OG	2.26	0.44
1:F:1163:LEU:HD21	1:F:1205:ILE:HG23	1.98	0.44
1:F:1231:ASN:ND2	1:F:1236:LEU:HB2	2.32	0.44
1:C:1193:ILE:HG23	1:C:1193:ILE:O	2.18	0.44
1:D:1223:TYR:HA	4:D:1502:HOH:O	2.17	0.44
1:F:1095:GLY:O	1:F:1112:THR:HA	2.18	0.44
1:F:1193:ILE:O	1:F:1193:ILE:HG23	2.17	0.44
1:A:1099:CYS:HA	1:A:1109:MET:O	2.17	0.44
1:B:1102:SER:CB	1:B:1109:MET:HE2	2.47	0.44
1:B:1098:CYS:O	1:B:1110:LEU:HA	2.17	0.44
1:E:1106:ARG:O	1:E:1122:VAL:HG22	2.17	0.44
1:A:1083:ILE:CD1	1:A:1388:GLU:HB2	2.36	0.44
1:A:1221:ASN:OD1	1:A:1257:LYS:HB2	2.17	0.44
1:D:1204:ASP:O	1:D:1208:GLY:HA2	2.16	0.44
1:F:1279:ILE:HG12	1:F:1342:TYR:CZ	2.53	0.44
1:A:1141:LEU:HD12	1:A:1141:LEU:C	2.43	0.44
1:C:1164:TRP:CZ3	1:C:1172:MET:HB2	2.52	0.44
1:D:1098:CYS:SG	1:D:1138:ILE:HG22	2.58	0.44
1:F:1165:GLY:O	1:F:1170:PHE:HA	2.18	0.44
1:C:1204:ASP:O	1:C:1208:GLY:HA2	2.18	0.44
1:E:1141:LEU:C	1:E:1141:LEU:HD12	2.43	0.44
1:E:1202:ILE:O	1:E:1211:LEU:N	2.51	0.44
1:F:1149:LEU:CD1	1:F:1205:ILE:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LEU:C	1:B:1141:LEU:HD12	2.43	0.44
1:B:1204:ASP:CB	1:B:1211:LEU:HD11	2.34	0.44
1:D:1155:THR:HG22	1:D:1156:TRP:CE3	2.53	0.44
1:F:1358:CYS:O	1:F:1366:LEU:HD12	2.17	0.44
1:C:1231:ASN:HB2	1:C:1232:PRO:CD	2.48	0.43
1:D:1277:THR:OG1	1:D:1278:GLU:OE2	2.32	0.43
1:D:1372:GLN:HB2	1:D:1381:ASP:O	2.18	0.43
1:F:1204:ASP:HB2	1:F:1211:LEU:HD11	2.00	0.43
1:F:1259:ASN:ND2	1:F:1262:ILE:H	2.14	0.43
1:A:1133:CYS:HA	1:A:1164:TRP:CH2	2.53	0.43
1:A:1181[A]:TYR:CE1	1:A:1227:CYS:SG	3.11	0.43
1:E:1088:GLU:CD	1:E:1091:GLU:HG3	2.42	0.43
1:F:1236:LEU:HD13	1:F:1243:LEU:HD21	2.00	0.43
1:A:1107:PHE:HE2	1:A:1128:GLU:CG	2.24	0.43
1:B:1273:VAL:CG2	1:B:1280:TRP:HB2	2.48	0.43
1:B:1332:SER:HA	1:B:1352:ARG:O	2.18	0.43
1:C:1279:ILE:HD13	1:C:1342:TYR:CE2	2.53	0.43
1:D:1279:ILE:HD13	1:D:1291:VAL:HG23	2.00	0.43
1:E:1181[B]:TYR:HE2	1:E:1183:GLU:OE2	2.02	0.43
1:E:1379:ASN:ND2	1:E:1379:ASN:O	2.50	0.43
1:C:1116:GLN:NE2	1:C:1132:ASN:OD1	2.42	0.43
1:F:1181[A]:TYR:CD1	1:F:1227:CYS:SG	3.12	0.43
1:A:1373:GLY:O	1:A:1374:SER:C	2.60	0.43
1:B:1294:LEU:O	1:B:1297:CYS:HB2	2.17	0.43
1:B:1335:ARG:HD3	4:B:1419:HOH:O	2.18	0.43
1:C:1181[B]:TYR:HE2	2:C:1401:A1C24:F14	1.92	0.43
1:C:1210:LYS:HD3	1:C:1213:THR:OG1	2.17	0.43
1:E:1237:VAL:HG23	1:E:1246:VAL:HG23	2.00	0.43
1:F:1174:HIS:HD2	1:F:1208:GLY:CA	2.31	0.43
1:C:1141:LEU:C	1:C:1141:LEU:HD12	2.43	0.43
1:D:1377:ALA:O	1:D:1379:ASN:N	2.51	0.43
1:E:1335:ARG:HG2	1:E:1347:THR:OG1	2.19	0.43
1:F:1083:ILE:CD1	1:F:1388:GLU:HB2	2.39	0.43
1:A:1226:ASN:OD1	1:A:1240:ASP:N	2.47	0.43
1:E:1098:CYS:SG	1:E:1138:ILE:HG22	2.59	0.43
1:D:1259:ASN:ND2	1:D:1261:ASN:H	2.16	0.43
1:E:1210:LYS:HD3	1:E:1213:THR:OG1	2.19	0.43
1:F:1338:ASN:ND2	1:F:1341:ASP:H	2.12	0.43
1:B:1204:ASP:HB2	1:B:1211:LEU:CD1	2.33	0.43
1:D:1237:VAL:HG23	1:D:1246:VAL:HG23	2.01	0.43
1:A:1095:GLY:O	1:A:1112:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1209:ASN:O	1:D:1211:LEU:HD22	2.19	0.43
1:F:1204:ASP:N	1:F:1211:LEU:CD1	2.81	0.43
1:F:1221:ASN:N	1:F:1240:ASP:OD2	2.50	0.42
1:F:1149:LEU:HD11	1:F:1205:ILE:HG21	2.01	0.42
1:D:1150:LEU:HB2	1:D:1166:MET:HE2	2.02	0.42
1:A:1109:MET:HE1	1:A:1143:PRO:HB3	2.01	0.42
1:A:1279:ILE:HD13	1:A:1291:VAL:HG23	2.01	0.42
1:B:1185:SER:OG	1:B:1189:GLN:HA	2.20	0.42
1:B:1219:LEU:O	1:B:1254:LYS:HD2	2.20	0.42
1:B:1338:ASN:ND2	1:B:1340:THR:H	2.16	0.42
1:E:1098:CYS:O	1:E:1110:LEU:HA	2.20	0.42
1:C:1259:ASN:ND2	1:C:1262:ILE:H	2.09	0.42
1:A:1218:ASP:C	1:A:1219:LEU:HD12	2.45	0.42
1:D:1133:CYS:HB2	4:D:1504:HOH:O	2.19	0.42
1:D:1211:LEU:HD22	1:D:1211:LEU:H	1.84	0.42
1:F:1278:GLU:HG3	4:F:1507:HOH:O	2.20	0.42
1:A:1160:LEU:HD12	1:A:1178:GLU:CA	2.47	0.42
1:C:1294:LEU:HD21	1:C:1308:MET:HE1	2.00	0.42
1:D:1335:ARG:HD3	4:D:1519:HOH:O	2.19	0.42
1:F:1145:ARG:NH1	1:F:1186:LYS:O	2.53	0.42
1:F:1221:ASN:OD1	1:F:1257:LYS:HB2	2.20	0.42
1:A:1163:LEU:HD21	1:A:1205:ILE:HG23	2.01	0.41
1:D:1181[A]:TYR:CD1	1:D:1227:CYS:SG	3.12	0.41
1:D:1231:ASN:HB2	1:D:1232:PRO:CD	2.50	0.41
1:B:1372:GLN:HB2	1:B:1381:ASP:O	2.20	0.41
1:F:1116:GLN:O	1:F:1138:ILE:HD12	2.19	0.41
1:C:1193:ILE:HD11	1:C:1228:ALA:HB1	2.02	0.41
1:D:1165:GLY:O	1:D:1170:PHE:HA	2.19	0.41
1:A:1231:ASN:HB2	1:A:1232:PRO:CD	2.50	0.41
1:A:1365:TYR:CB	1:A:1386:LEU:HD11	2.50	0.41
1:C:1115:GLY:HA3	1:C:1134:HIS:O	2.21	0.41
1:D:1106:ARG:O	1:D:1122:VAL:HG22	2.20	0.41
1:F:1201:HIS:CB	1:F:1203:TYR:CE1	3.03	0.41
1:B:1279:ILE:HD13	1:B:1291:VAL:HG23	2.01	0.41
1:B:1290:THR:HG23	4:B:1411:HOH:O	2.20	0.41
1:E:1180:HIS:HD2	1:E:1181[A]:TYR:CD2	2.38	0.41
1:F:1226:ASN:OD1	1:F:1240:ASP:N	2.51	0.41
1:A:1153:SER:OG	1:A:1161:SER:OG	2.28	0.41
1:A:1339:ALA:HB2	4:A:1507:HOH:O	2.19	0.41
1:C:1204:ASP:CB	1:C:1211:LEU:HD11	2.36	0.41
1:F:1273:VAL:HG22	1:F:1280:TRP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1165:GLY:O	1:C:1170:PHE:HA	2.21	0.41
1:E:1259:ASN:HD22	1:E:1296:GLN:HE22	1.69	0.41
1:E:1300:VAL:HG12	2:E:1401:A1C24:C24	2.51	0.41
1:E:1371:ASN:HA	1:E:1382:THR:HG22	2.03	0.41
1:F:1243:LEU:HD13	1:F:1243:LEU:C	2.45	0.41
1:F:1281:ASP:HB2	1:F:1288:LEU:CD1	2.49	0.41
1:D:1118:LYS:HD3	1:D:1120:TYR:HE1	1.85	0.41
1:E:1193:ILE:O	1:E:1193:ILE:HG23	2.19	0.41
1:F:1237:VAL:HG23	1:F:1246:VAL:HG22	2.02	0.41
1:F:1299:VAL:HA	1:F:1309:TYR:O	2.20	0.41
1:B:1156:TRP:HE3	1:B:1156:TRP:O	2.03	0.41
1:F:1193:ILE:HD11	1:F:1228:ALA:HB1	2.03	0.41
1:F:1113:CYS:HA	1:F:1137:ALA:HB1	2.04	0.40
1:F:1145:ARG:NH2	1:F:1187:HIS:O	2.54	0.40
1:F:1219:LEU:O	1:F:1254:LYS:HD2	2.22	0.40
1:F:1231:ASN:HB2	1:F:1232:PRO:CD	2.51	0.40
1:C:1181[B]:TYR:CD1	1:C:1227:CYS:SG	3.14	0.40
1:C:1279:ILE:HD12	1:C:1291:VAL:HG23	2.03	0.40
1:E:1174:HIS:CD2	1:E:1208:GLY:HA3	2.56	0.40
1:E:1279:ILE:HD13	1:E:1291:VAL:HG23	2.03	0.40
1:D:1243:LEU:HD23	1:D:1252:ILE:HD11	2.03	0.40
1:A:1237:VAL:HG23	1:A:1246:VAL:HG23	2.01	0.40
1:B:1174:HIS:HD2	1:B:1208:GLY:HA3	1.86	0.40
1:C:1204:ASP:CB	1:C:1211:LEU:HD21	2.50	0.40
1:C:1272:GLU:OE2	1:C:1342:TYR:OH	2.31	0.40
1:D:1115:GLY:HA2	1:D:1138:ILE:HG13	2.03	0.40
1:F:1188:SER:O	1:F:1190:ASP:N	2.54	0.40
1:A:1174:HIS:CD2	1:A:1208:GLY:HA3	2.56	0.40
1:B:1174:HIS:HD2	1:B:1208:GLY:CA	2.35	0.40
1:C:1342:TYR:HE1	4:C:1528:HOH:O	2.03	0.40
1:E:1231:ASN:HB2	1:E:1232:PRO:CD	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1501:HOH:O	4:A:1526:HOH:O[4_455]	2.12	0.08

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%)	266 (92%)	22 (8%)	2 (1%)	18	38
1	B	292/314 (93%)	267 (91%)	22 (8%)	3 (1%)	12	28
1	C	291/314 (93%)	268 (92%)	20 (7%)	3 (1%)	12	28
1	D	295/314 (94%)	270 (92%)	21 (7%)	4 (1%)	9	19
1	E	290/314 (92%)	267 (92%)	21 (7%)	2 (1%)	18	38
1	F	295/314 (94%)	270 (92%)	24 (8%)	1 (0%)	36	58
All	All	1753/1884 (93%)	1608 (92%)	130 (7%)	15 (1%)	14	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1187	HIS
1	B	1187	HIS
1	B	1316	ASP
1	C	1187	HIS
1	D	1187	HIS
1	E	1187	HIS
1	F	1187	HIS
1	D	1378	LEU
1	D	1379	ASN
1	E	1168	SER
1	C	1167	LYS
1	A	1168	SER
1	C	1168	SER
1	B	1168	SER
1	D	1168	SER

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%)	256 (98%)	4 (2%)	57	80
1	B	262/276 (95%)	260 (99%)	2 (1%)	73	88
1	C	261/276 (95%)	259 (99%)	2 (1%)	73	88
1	D	264/276 (96%)	261 (99%)	3 (1%)	65	84
1	E	260/276 (94%)	259 (100%)	1 (0%)	84	93
1	F	265/276 (96%)	263 (99%)	2 (1%)	73	88
All	All	1572/1656 (95%)	1558 (99%)	14 (1%)	70	87

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1156	TRP
1	A	1207	THR
1	A	1219	LEU
1	A	1246	VAL
1	B	1212	LEU
1	B	1259	ASN
1	C	1212	LEU
1	C	1314	GLN
1	D	1209	ASN
1	D	1246	VAL
1	D	1247	ARG
1	E	1105	GLU
1	F	1316	ASP
1	F	1327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1116	GLN
1	A	1180	HIS
1	A	1187	HIS

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Mol	Chain	Res	Type
1	A	1372	GLN
1	B	1180	HIS
1	B	1216	ASN
1	B	1289	HIS
1	B	1314	GLN
1	B	1338	ASN
1	B	1353	ASN
1	C	1180	HIS
1	C	1187	HIS
1	C	1216	ASN
1	C	1259	ASN
1	C	1289	HIS
1	C	1314	GLN
1	C	1372	GLN
1	D	1180	HIS
1	D	1187	HIS
1	D	1201	HIS
1	D	1216	ASN
1	D	1221	ASN
1	D	1253	HIS
1	D	1259	ASN
1	D	1289	HIS
1	D	1314	GLN
1	E	1116	GLN
1	E	1158	GLN
1	E	1180	HIS
1	E	1187	HIS
1	E	1253	HIS
1	E	1259	ASN
1	E	1289	HIS
1	E	1379	ASN
1	F	1201	HIS
1	F	1216	ASN
1	F	1253	HIS
1	F	1259	ASN
1	F	1338	ASN
1	F	1372	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1C24	E	1401	-	31,31,31	1.67	5 (16%)	42,44,44	1.33	6 (14%)
2	A1C24	C	1401	-	31,31,31	1.67	5 (16%)	42,44,44	1.27	4 (9%)
2	A1C24	A	1401	-	31,31,31	2.13	5 (16%)	42,44,44	1.30	4 (9%)
3	A1C23	F	1401	-	94,96,96	1.03	3 (3%)	117,127,127	1.13	10 (8%)
2	A1C24	D	1401	-	31,31,31	1.70	5 (16%)	42,44,44	1.33	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1C24	E	1401	-	-	0/20/20/20	0/3/3/3
2	A1C24	C	1401	-	-	1/20/20/20	0/3/3/3
2	A1C24	A	1401	-	-	2/20/20/20	0/3/3/3
3	A1C23	F	1401	-	-	13/78/78/78	0/6/6/6
2	A1C24	D	1401	-	-	0/20/20/20	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1401	A1C24	C08-C07	-8.30	1.39	1.49
2	D	1401	A1C24	C02-N16	5.72	1.46	1.34
2	C	1401	A1C24	C02-N16	5.63	1.45	1.34
2	E	1401	A1C24	C02-N16	5.56	1.45	1.34
2	A	1401	A1C24	C02-N16	5.34	1.45	1.34
2	D	1401	A1C24	C19-N20	4.00	1.45	1.32
2	C	1401	A1C24	C19-N20	3.99	1.45	1.32
2	E	1401	A1C24	C19-N20	3.96	1.45	1.32
2	A	1401	A1C24	C19-N20	3.95	1.45	1.32
2	D	1401	A1C24	C08-C07	-3.67	1.44	1.49
2	C	1401	A1C24	C08-C07	-3.67	1.44	1.49
2	E	1401	A1C24	C08-C07	-3.50	1.44	1.49
2	E	1401	A1C24	O01-C02	-2.55	1.18	1.23
2	A	1401	A1C24	O01-C02	-2.47	1.18	1.23
2	D	1401	A1C24	O01-C02	-2.30	1.19	1.23
2	C	1401	A1C24	O01-C02	-2.25	1.19	1.23
2	D	1401	A1C24	C26-CL27	2.15	1.78	1.73
3	F	1401	A1C23	C14-C12	2.15	1.41	1.38
3	F	1401	A1C23	C76-C74	2.14	1.41	1.38
3	F	1401	A1C23	C55-C61	2.12	1.41	1.38
2	C	1401	A1C24	C26-CL27	2.12	1.78	1.73
2	E	1401	A1C24	C26-CL27	2.04	1.78	1.73
2	A	1401	A1C24	C26-CL27	2.03	1.78	1.73

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1401	A1C24	C06-C07-C03	4.11	109.37	106.93
2	C	1401	A1C24	C06-C07-C03	4.10	109.36	106.93
2	E	1401	A1C24	C06-C07-C03	3.77	109.17	106.93
2	A	1401	A1C24	C12-C13-C08	-3.16	119.99	123.48
2	A	1401	A1C24	C06-C07-C03	3.12	108.79	106.93
2	D	1401	A1C24	C12-C13-C08	-3.09	120.06	123.48
2	A	1401	A1C24	C09-C08-C13	3.04	120.08	116.70
3	F	1401	A1C23	C60-C61-C55	-3.02	120.15	123.48
3	F	1401	A1C23	C89-C90-C84	-2.99	120.17	123.48
2	C	1401	A1C24	C12-C13-C08	-2.94	120.23	123.48
2	D	1401	A1C24	C11-C12-C13	2.92	120.01	117.54
2	C	1401	A1C24	C11-C12-C13	2.84	119.94	117.54
2	E	1401	A1C24	C12-C13-C08	-2.84	120.34	123.48
2	E	1401	A1C24	C11-C12-C13	2.72	119.84	117.54
3	F	1401	A1C23	C85-C84-C90	2.72	119.72	116.70
2	D	1401	A1C24	C09-C08-C13	2.68	119.67	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1401	A1C24	C09-C08-C13	2.67	119.67	116.70
2	C	1401	A1C24	C09-C08-C13	2.65	119.64	116.70
2	A	1401	A1C24	C11-C12-C13	2.65	119.78	117.54
3	F	1401	A1C23	C56-C55-C61	2.63	119.62	116.70
3	F	1401	A1C23	C58-C60-C61	2.63	119.76	117.54
2	E	1401	A1C24	C18-C17-C22	-2.62	106.36	111.33
3	F	1401	A1C23	C87-C89-C90	2.60	119.73	117.54
3	F	1401	A1C23	C63-C64-N65	2.34	119.30	116.25
3	F	1401	A1C23	C67-C66-N65	2.27	113.05	108.94
3	F	1401	A1C23	C80-N81-C53	2.18	111.37	109.56
3	F	1401	A1C23	C18-N19-C20	2.16	111.36	109.56
2	D	1401	A1C24	C18-C17-C22	-2.16	107.24	111.33
2	E	1401	A1C24	C17-N16-C02	-2.01	119.40	122.21

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1401	A1C23	C36-C35-O34-C33
3	F	1401	A1C23	O28-C29-C30-O31
2	A	1401	A1C24	C17-C18-C19-O21
3	F	1401	A1C23	C66-C67-C68-N69
2	A	1401	A1C24	C17-C18-C19-N20
3	F	1401	A1C23	C66-C67-C68-O70
3	F	1401	A1C23	C39-C38-O37-C36
3	F	1401	A1C23	O34-C35-C36-O37
3	F	1401	A1C23	C35-C36-O37-C38
3	F	1401	A1C23	C26-C27-O28-C29
3	F	1401	A1C23	C33-C32-O31-C30
3	F	1401	A1C23	C48-C47-O46-C45
3	F	1401	A1C23	O46-C47-C48-N49
3	F	1401	A1C23	C83-C20-C21-C22
3	F	1401	A1C23	C51-C52-C53-C54
2	C	1401	A1C24	C06-C07-C08-C13

There are no ring outliers.

4 monomers are involved in 5 short contacts:

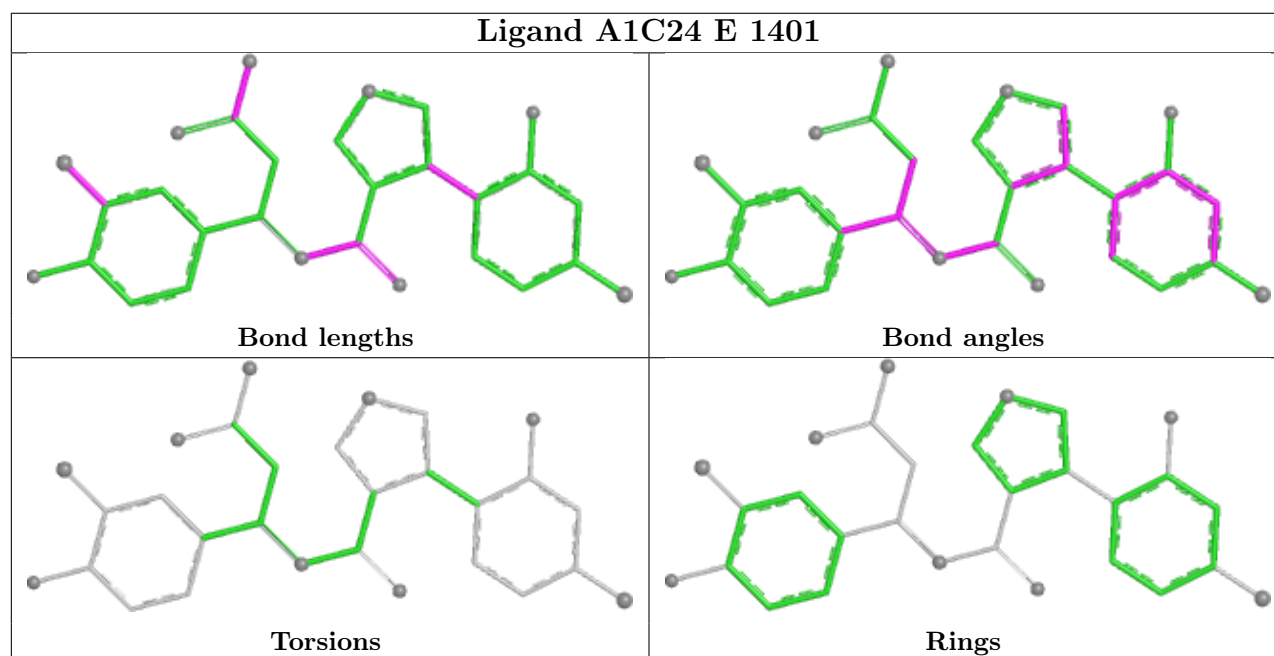
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1401	A1C24	1	0
2	C	1401	A1C24	1	0

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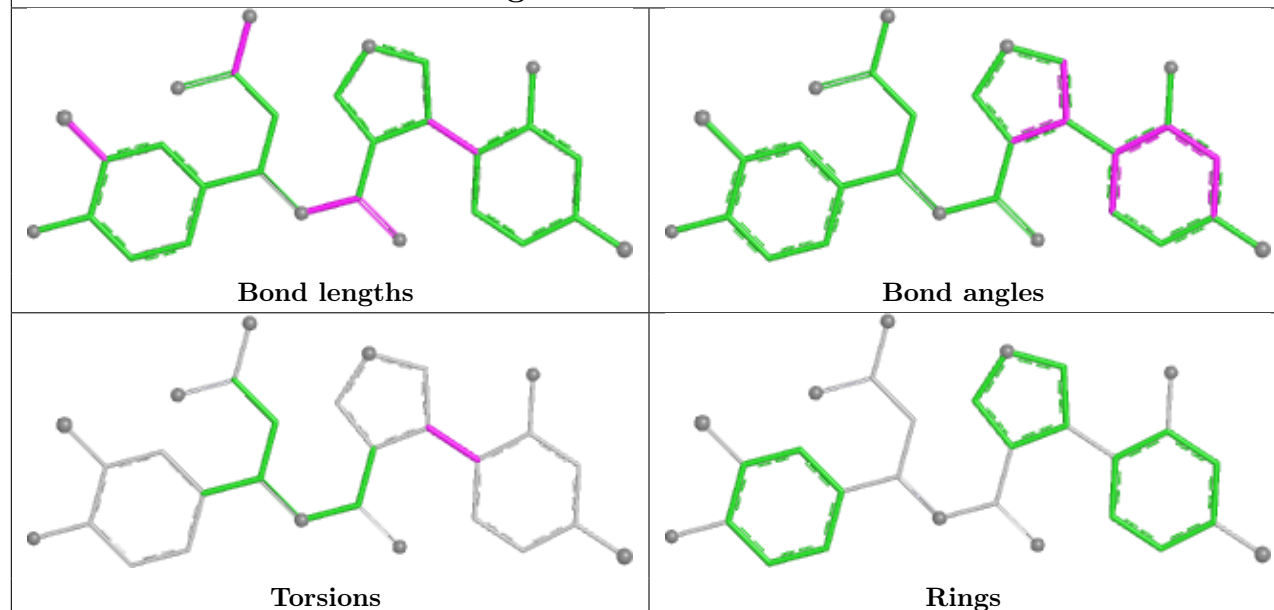
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	A1C24	2	0
2	D	1401	A1C24	1	0

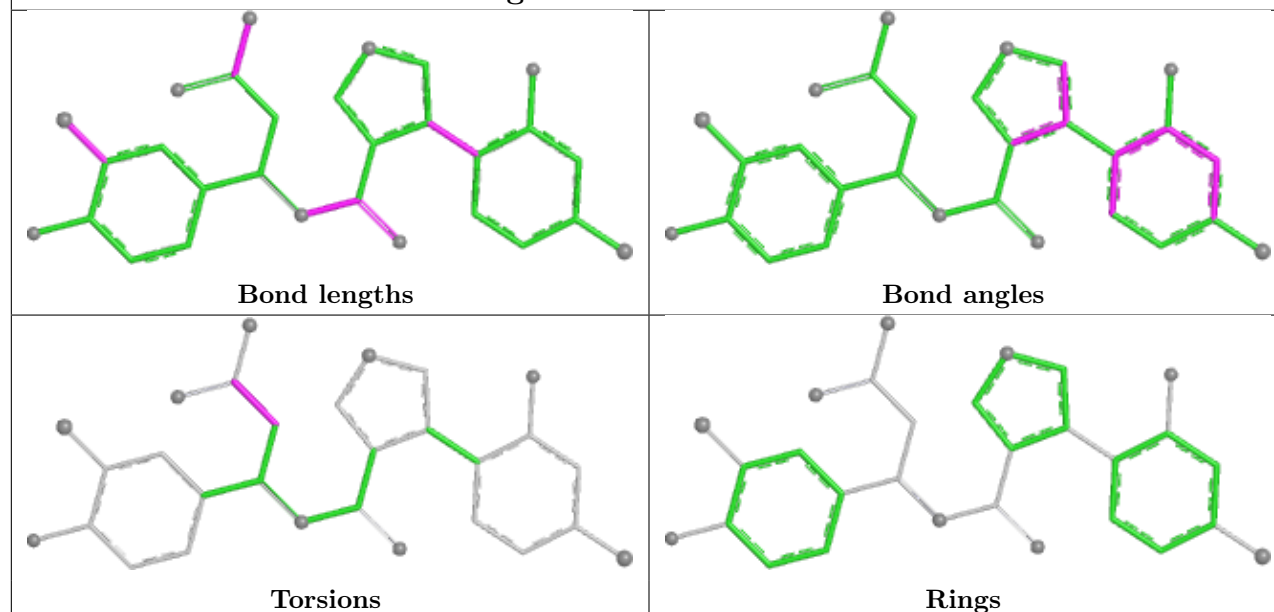
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



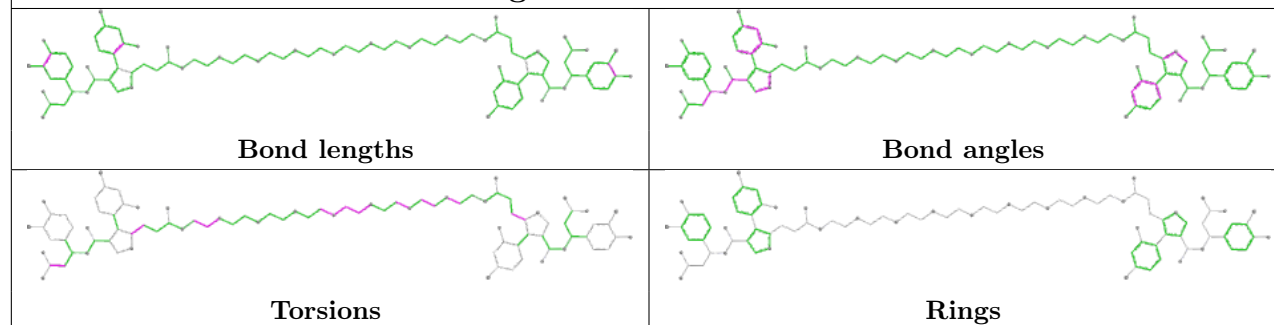
Ligand A1C24 C 1401

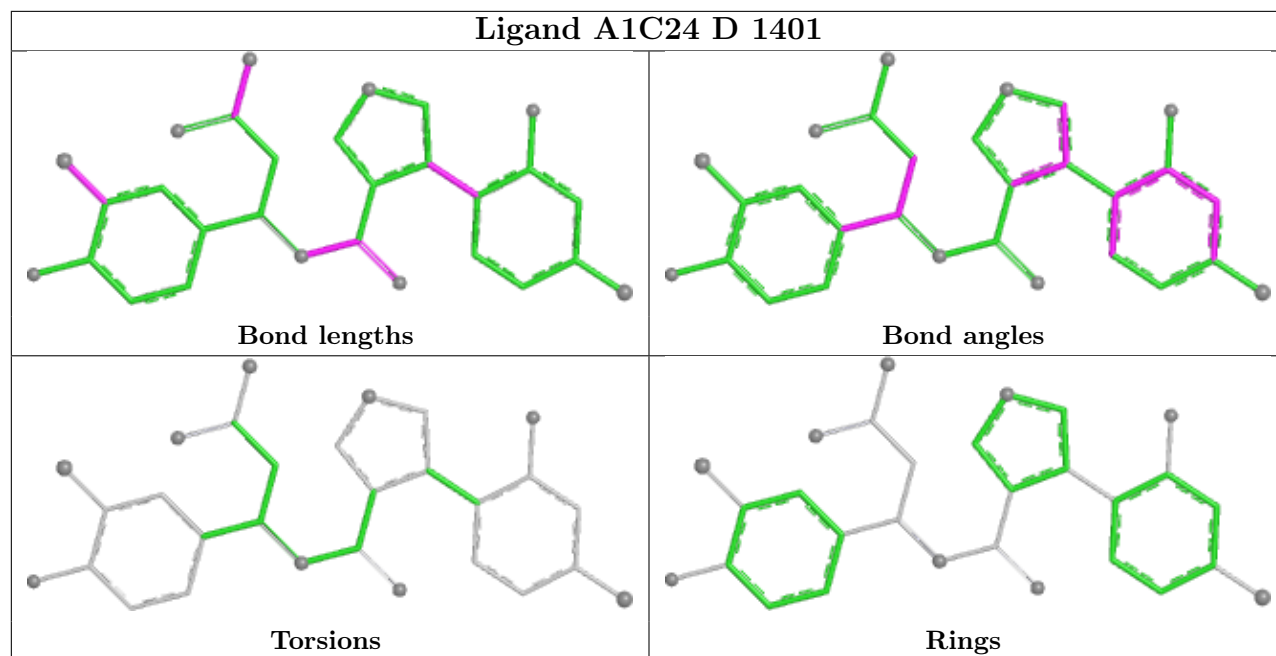


Ligand A1C24 A 1401



Ligand A1C23 F 1401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/314 (93%)	-1.23	0 100 100	23, 46, 62, 79	1 (0%)
1	B	297/314 (94%)	-1.22	0 100 100	23, 47, 64, 85	1 (0%)
1	C	296/314 (94%)	-1.21	0 100 100	23, 46, 62, 82	1 (0%)
1	D	300/314 (95%)	-1.20	0 100 100	24, 47, 65, 79	1 (0%)
1	E	295/314 (93%)	-1.24	0 100 100	24, 47, 63, 76	1 (0%)
1	F	300/314 (95%)	-1.22	0 100 100	24, 48, 64, 81	1 (0%)
All	All	1783/1884 (94%)	-1.22	0 100 100	23, 47, 63, 85	6 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1C24	E	1401	29/29	0.98	0.04	36,41,50,51	0

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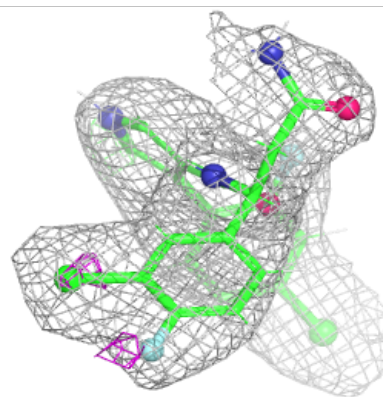
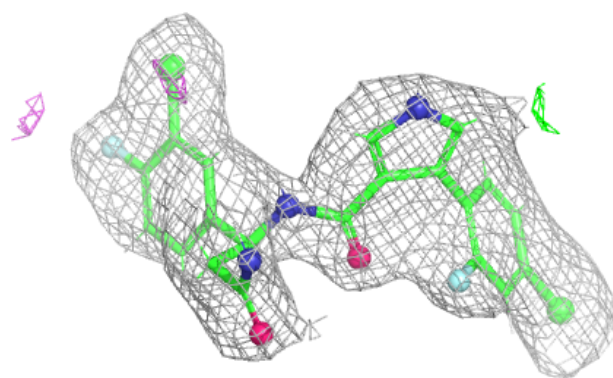
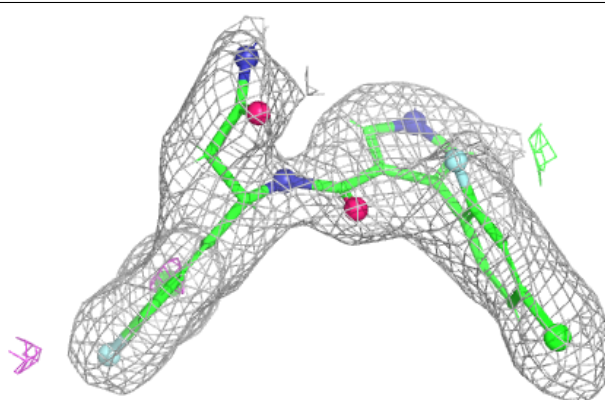
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1C23	F	1401	91/91	0.98	0.05	35,48,89,91	0
2	A1C24	D	1401	29/29	0.99	0.04	36,40,50,51	0
2	A1C24	A	1401	29/29	0.99	0.04	34,39,49,52	0
2	A1C24	C	1401	29/29	0.99	0.04	36,38,48,50	0

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.

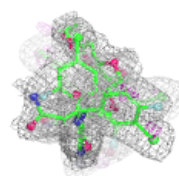
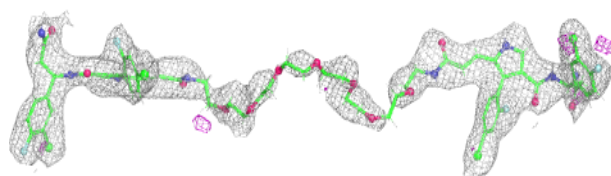
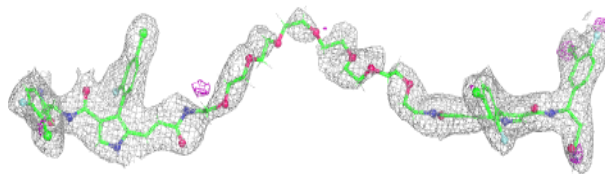
Electron density around A1C24 E 1401:

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



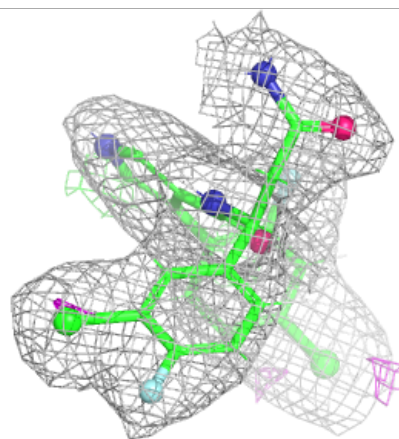
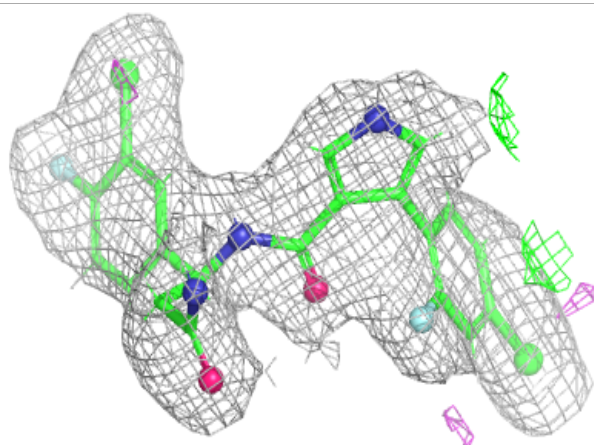
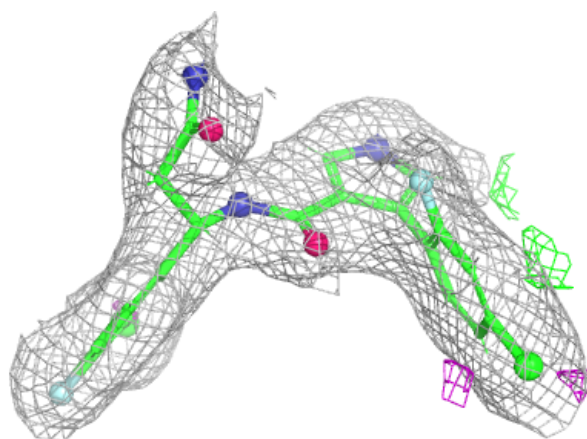
Electron density around A1C23 F 1401:

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



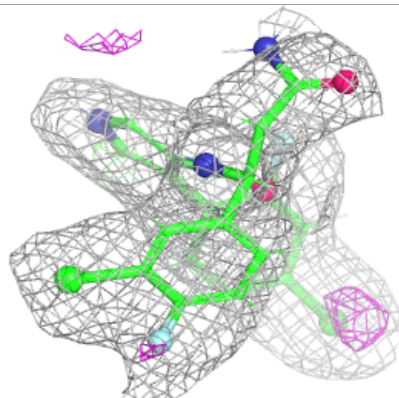
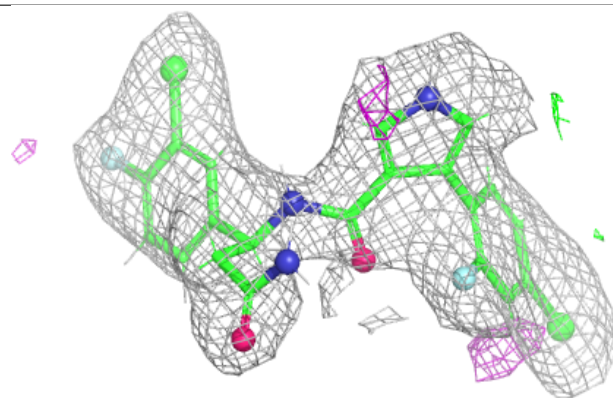
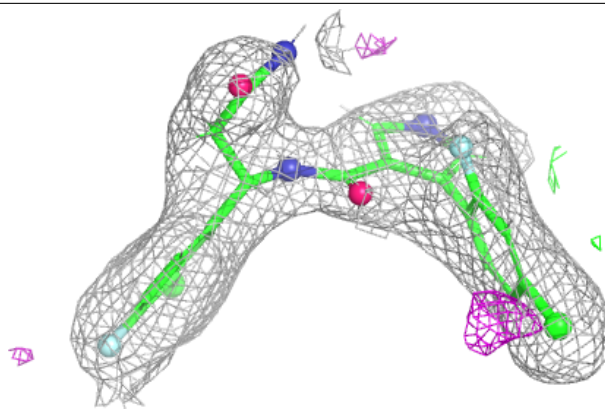
Electron density around A1C24 D 1401:

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



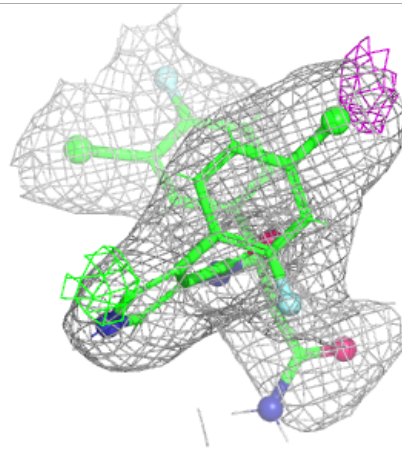
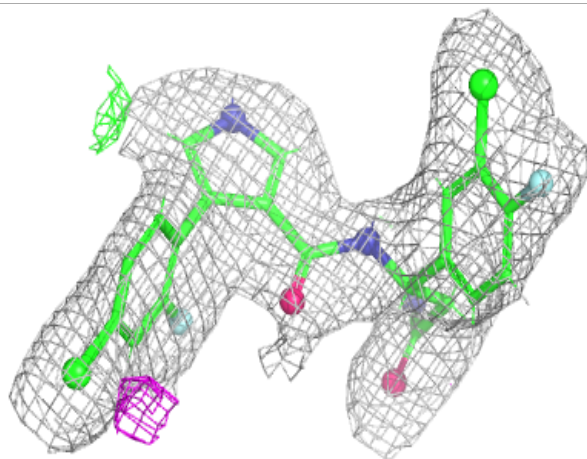
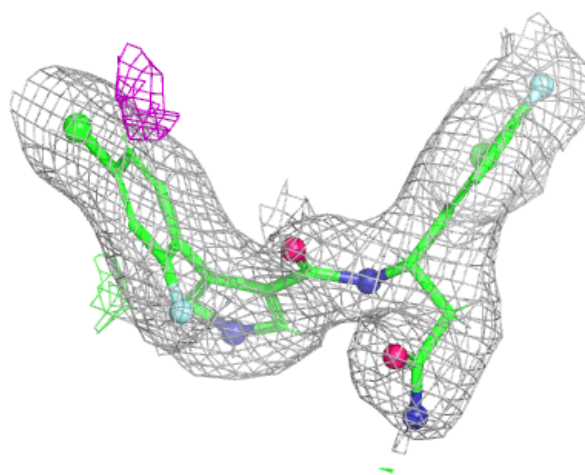
Electron density around A1C24 A 1401:

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



Electron density around A1C24 C 1401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.