



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:05 PM UTC

PDB ID : 7UW0 / pdb_00007uw0
Title : Crystal structure of human ClpP protease in complex with TR-133
Authors : Mabanglo, M.F.; Houry, W.A.
Deposited on : 2022-05-02
Resolution : 2.80 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

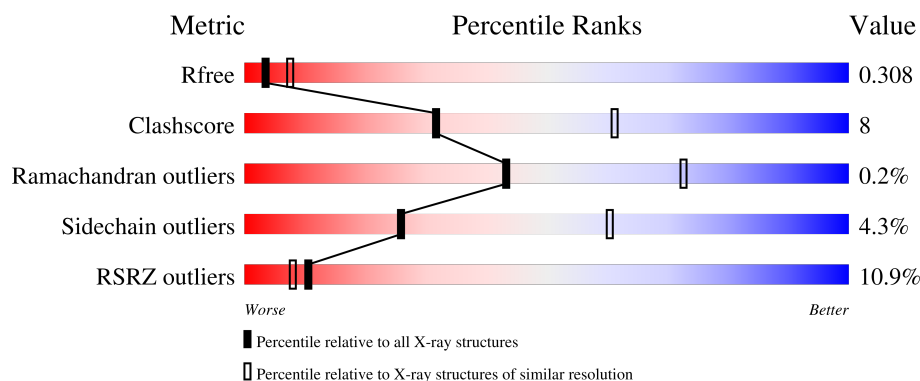
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	

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Mol	Chain	Length	Quality of chain
1	F	221	10% 63% 17% • 19%
1	G	221	7% 59% 21% • 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9959 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

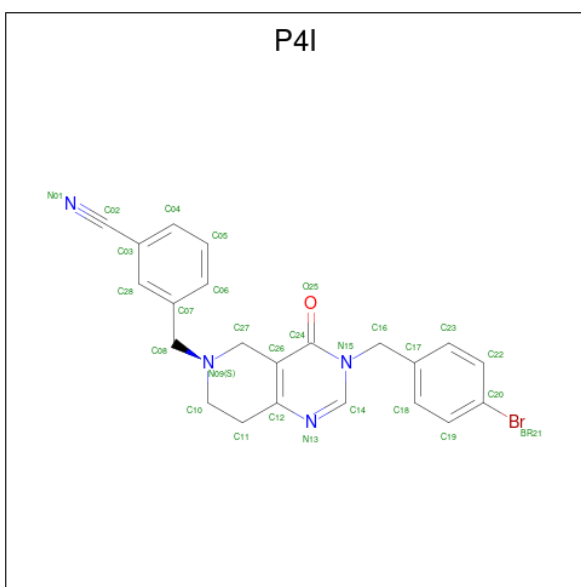
- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1403	895	238	257	13			
1	B	173	Total	C	N	O	S	0	0	0
			1346	862	228	243	13			
1	C	178	Total	C	N	O	S	0	0	0
			1381	884	233	251	13			
1	D	178	Total	C	N	O	S	0	0	0
			1383	884	233	253	13			
1	E	178	Total	C	N	O	S	0	0	0
			1381	884	233	251	13			
1	F	180	Total	C	N	O	S	0	1	0
			1401	894	239	254	14			
1	G	179	Total	C	N	O	S	0	0	0
			1398	892	237	256	13			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	SER	-	cloning artifact	UNP Q16740
B	57	SER	-	cloning artifact	UNP Q16740
C	57	SER	-	cloning artifact	UNP Q16740
D	57	SER	-	cloning artifact	UNP Q16740
E	57	SER	-	cloning artifact	UNP Q16740
F	57	SER	-	cloning artifact	UNP Q16740
G	57	SER	-	cloning artifact	UNP Q16740

- Molecule 2 is 3-({3-[(4-bromophenyl)methyl]-4-oxo-3,5,7,8-tetrahydropyrido[4,3-d]pyrimidin-6(4H)-yl}methyl)benzonitrile (CCD ID: P4I) (formula: C₂₂H₁₉BrN₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			28	1	22	4	1		
2	B	1	Total	Br	C	N	O	0	0
			28	1	22	4	1		
2	C	1	Total	Br	C	N	O	0	0
			28	1	22	4	1		
2	D	1	Total	Br	C	N	O	0	0
			28	1	22	4	1		
2	E	1	Total	Br	C	N	O	0	0
			28	1	22	4	1		
2	F	1	Total	Br	C	N	O	0	0
			28	1	22	4	1		
2	G	1	Total	Br	C	N	O	0	0
			28	1	22	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	10	Total	O	0	0
			10	10		
3	C	9	Total	O	0	0
			9	9		
3	D	9	Total	O	0	0
			9	9		
3	E	10	Total	O	0	0
			10	10		

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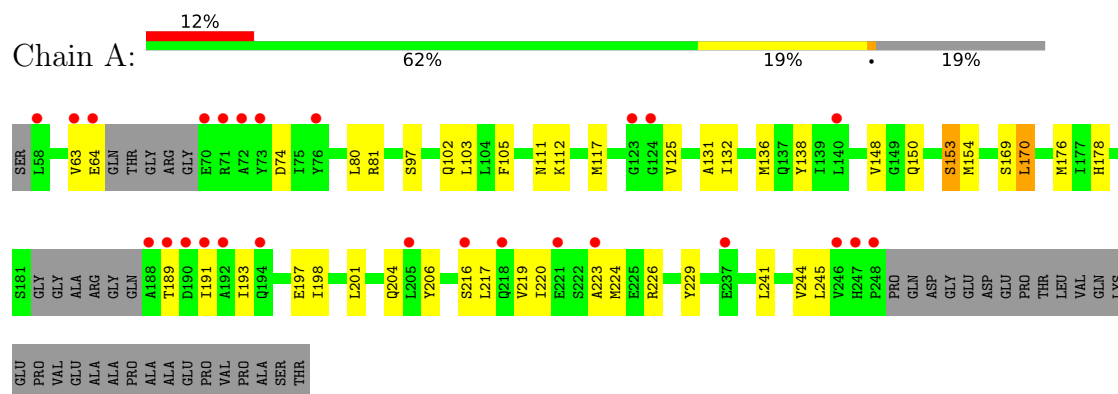
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	11	Total	O	0	0
			11	11		
3	G	11	Total	O	0	0
			11	11		

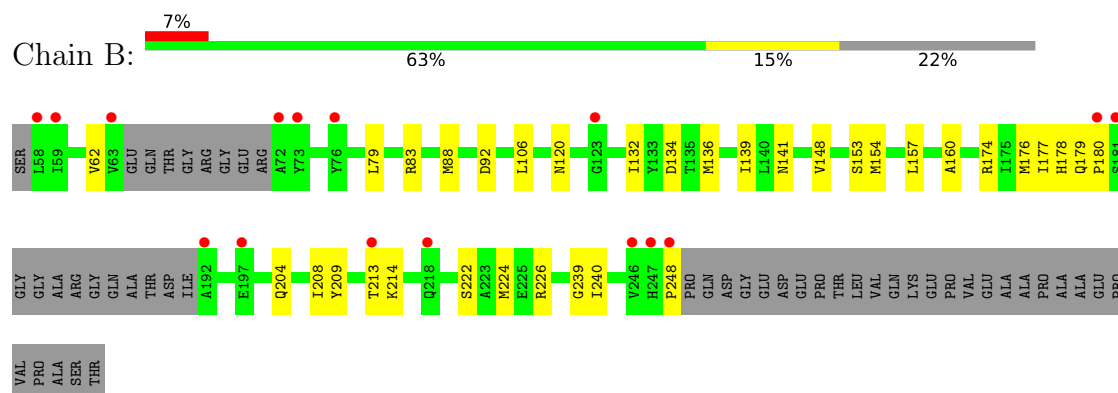
3 Residue-property plots

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: ATP-dependent Clp protease proteolytic subunit, mitochondrial



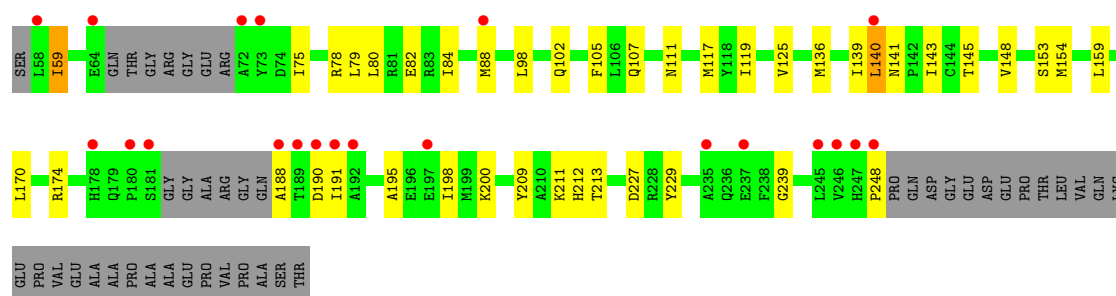
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial



SER
THR

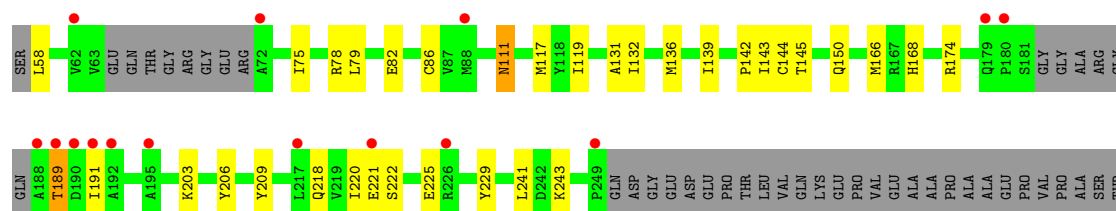
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain D:



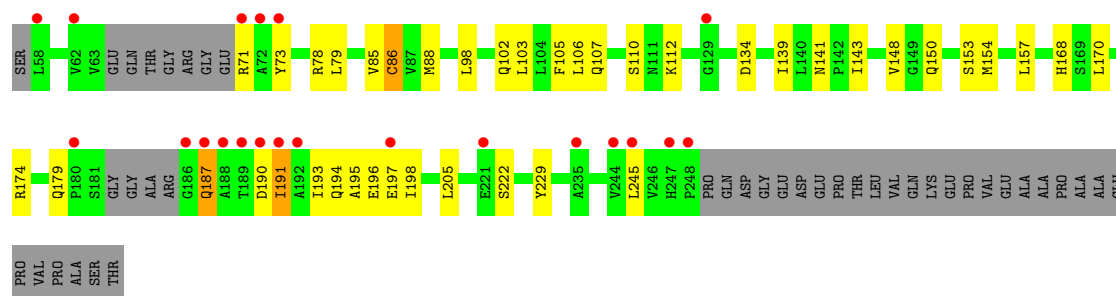
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain E:



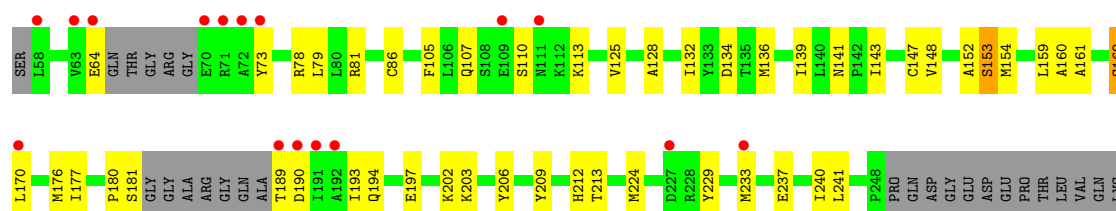
- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain F:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit, mitochondrial

Chain G:



GLU
PRO
VAL
GLU
ALA
ALA
PRO
ALA
GLU
PRO
VAL
PRO
ALA
SER
THR

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.66Å 153.80Å 133.21Å 90.00° 107.03° 90.00°	Depositor
Resolution (Å)	51.69 – 2.80 51.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (51.69-2.80) 94.1 (51.69-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.260 , 0.309 0.263 , 0.308	Depositor DCC
R_{free} test set	2000 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9959	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P4I

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/1427	0.28	0/1930
1	B	0.09	0/1370	0.26	0/1853
1	C	0.11	0/1406	0.32	0/1904
1	D	0.11	0/1407	0.30	0/1904
1	E	0.09	0/1406	0.30	0/1904
1	F	0.10	0/1428	0.27	0/1931
1	G	0.11	0/1422	0.29	0/1923
All	All	0.10	0/9866	0.29	0/13349

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

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	1403	0	1442	26	0
1	B	1346	0	1390	25	1
1	C	1381	0	1424	24	0
1	D	1383	0	1423	34	0
1	E	1381	0	1424	18	1
1	F	1401	0	1446	27	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1398	0	1437	27	1
2	A	28	0	0	2	0
2	B	28	0	0	3	0
2	C	28	0	0	0	0
2	D	28	0	0	2	0
2	E	28	0	0	1	0
2	F	28	0	0	4	0
2	G	28	0	0	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	9	0	0	1	0
3	D	9	0	0	0	0
3	E	10	0	0	0	0
3	F	11	0	0	2	0
3	G	11	0	0	1	0
All	All	9959	0	9986	161	2

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 8.

All (161) 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:C:134:ASP:HB3	1:D:170:LEU:HD23	1.66	0.76
1:D:139:ILE:HD11	1:D:143:ILE:HD11	1.69	0.74
1:C:193:ILE:HG12	1:C:198:ILE:HG23	1.71	0.72
1:F:197:GLU:OE1	1:G:229:TYR:N	2.21	0.69
1:B:88:MET:HG3	1:B:120:ASN:HB3	1.75	0.69
1:G:139:ILE:HD11	1:G:143:ILE:HD11	1.76	0.68
1:D:111:ASN:HB2	1:D:140:LEU:HD11	1.76	0.67
1:C:73:TYR:OH	1:C:81:ARG:NH1	2.28	0.67
1:E:139:ILE:HD11	1:E:143:ILE:HD11	1.78	0.66
1:G:209:TYR:O	1:G:213:THR:OG1	2.13	0.65
1:A:201:LEU:HD23	1:A:204:GLN:HE21	1.61	0.65
1:B:209:TYR:O	1:B:213:THR:OG1	2.13	0.65
1:F:139:ILE:HD11	1:F:143:ILE:HD11	1.79	0.65
1:D:125:VAL:HA	1:D:188:ALA:HA	1.78	0.65
1:A:223:ALA:HA	1:A:226:ARG:HG3	1.80	0.64
1:G:125:VAL:HG12	1:G:128:ALA:H	1.64	0.63
1:D:209:TYR:O	1:D:213:THR:OG1	2.17	0.62
1:G:64:GLU:HG3	1:G:78:ARG:HE	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:HD11	1:C:172:ASN:ND2	2.15	0.61
1:C:169:SER:HB3	1:C:241:LEU:HD21	1.83	0.61
1:C:147:CYS:HB3	1:C:169:SER:HB2	1.82	0.60
1:D:78:ARG:NH1	1:D:82:GLU:OE1	2.34	0.60
1:C:199:MET:O	1:C:203:LYS:HG3	2.02	0.60
1:D:145:THR:HB	1:D:159:LEU:HD12	1.84	0.59
1:A:125:VAL:HG13	1:A:189:THR:HA	1.84	0.59
1:A:193:ILE:HD13	1:A:198:ILE:HG13	1.85	0.59
1:C:112:LYS:NZ	3:C:403:HOH:O	2.35	0.59
1:F:194:GLN:HG3	1:F:195:ALA:H	1.68	0.58
1:B:83:ARG:HG2	1:B:106:LEU:HD22	1.84	0.58
1:G:153:SER:HB2	1:G:180:PRO:HD3	1.86	0.58
1:C:131:ALA:HB1	1:D:148:VAL:HG12	1.85	0.58
1:B:134:ASP:HB3	1:C:170:LEU:HD23	1.85	0.58
1:E:209:TYR:HB3	1:E:220:ILE:HD12	1.86	0.57
1:G:153:SER:OG	1:G:154:MET:N	2.36	0.57
1:G:194:GLN:NE2	3:G:401:HOH:O	2.38	0.56
1:F:148:VAL:HG13	1:F:170:LEU:HD12	1.86	0.56
1:B:208:ILE:HD11	1:C:172:ASN:HD21	1.71	0.56
1:G:160:ALA:HB2	1:G:240:ILE:HG23	1.86	0.56
1:F:105:PHE:HB2	2:G:301:P4I:BR21	2.61	0.56
1:C:209:TYR:O	1:C:213:THR:OG1	2.18	0.55
1:F:71:ARG:HE	1:F:73:TYR:HE1	1.54	0.55
1:A:132:ILE:O	1:A:136:MET:HG3	2.07	0.54
1:A:153:SER:OG	1:A:154:MET:N	2.39	0.54
1:A:148:VAL:HG22	1:A:170:LEU:HG	1.89	0.54
1:C:139:ILE:HD11	1:C:143:ILE:HD11	1.88	0.54
1:E:142:PRO:HB2	1:E:166:MET:HE1	1.89	0.54
1:C:132:ILE:O	1:C:136:MET:HG3	2.08	0.54
1:F:174:ARG:HB3	1:F:229:TYR:HD2	1.73	0.53
1:B:153:SER:HB2	1:B:180:PRO:HD3	1.91	0.52
1:G:148:VAL:HG12	1:G:170:LEU:HD13	1.91	0.52
1:B:160:ALA:HB2	1:B:240:ILE:HG23	1.92	0.52
1:C:98:LEU:HD11	1:D:59:ILE:HG23	1.91	0.52
1:G:107:GLN:HG3	1:G:141:ASN:OD1	2.09	0.52
1:E:144:CYS:SG	1:E:166:MET:HE3	2.50	0.51
1:E:174:ARG:HG3	1:E:229:TYR:HB3	1.92	0.51
1:A:80:LEU:HD13	1:A:102:GLN:HE21	1.76	0.51
1:A:204:GLN:HE22	1:B:174:ARG:HD3	1.75	0.51
1:A:148:VAL:HG21	2:A:301:P4I:C02	2.40	0.51
1:D:75:ILE:O	1:D:79:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:O	1:B:136:MET:HG3	2.10	0.50
1:B:153:SER:OG	1:B:154:MET:N	2.44	0.50
1:A:105:PHE:HB2	2:B:301:P4I:BR21	2.67	0.50
1:D:59:ILE:HG13	1:E:58:LEU:HD13	1.93	0.50
1:D:98:LEU:O	1:D:102:GLN:HG3	2.11	0.50
1:B:179:GLN:HG2	1:B:224:MET:HE3	1.92	0.49
1:C:217:LEU:O	1:C:221:GLU:HG3	2.12	0.49
1:F:174:ARG:HB3	1:F:229:TYR:CD2	2.47	0.49
1:C:189:THR:HG21	1:C:193:ILE:HD13	1.93	0.49
1:G:147:CYS:HB3	1:G:169:SER:HB2	1.93	0.49
1:B:213:THR:HG22	1:B:239:GLY:C	2.37	0.49
1:B:176:MET:HE2	1:B:178:HIS:HB3	1.95	0.49
1:E:218:GLN:NE2	1:E:221:GLU:OE1	2.45	0.49
1:B:139:ILE:HG12	1:B:141:ASN:H	1.78	0.48
1:D:211:LYS:HD3	1:D:212:HIS:CD2	2.48	0.48
1:A:169:SER:HB2	1:A:241:LEU:HD22	1.95	0.48
1:E:131:ALA:HB1	1:F:148:VAL:HG12	1.95	0.48
1:A:193:ILE:HD11	1:A:197:GLU:HG3	1.95	0.48
1:D:200:LYS:HD3	1:E:174:ARG:NH2	2.28	0.48
1:E:168:HIS:CE1	1:E:243:LYS:HG3	2.49	0.48
1:D:148:VAL:HG21	2:D:301:P4I:N01	2.29	0.48
1:D:59:ILE:HG22	1:D:75:ILE:HG22	1.96	0.47
1:G:159:LEU:HD21	1:G:241:LEU:HD21	1.96	0.47
1:A:216:SER:HB3	1:A:219:VAL:HG23	1.95	0.47
1:C:138:TYR:CZ	1:D:248:PRO:HG3	2.50	0.47
1:B:92:ASP:N	1:B:92:ASP:OD1	2.46	0.47
1:A:64:GLU:OE2	1:A:81:ARG:NH2	2.36	0.47
1:C:97:SER:OG	1:D:88:MET:HG2	2.15	0.47
1:G:233:MET:O	1:G:237:GLU:HG3	2.14	0.47
1:D:154:MET:HA	1:D:154:MET:HE2	1.97	0.46
1:B:204:GLN:O	1:B:208:ILE:HG13	2.16	0.46
1:E:203:LYS:HA	1:E:206:TYR:CD1	2.51	0.46
1:F:112:LYS:HA	1:F:112:LYS:HD3	1.78	0.46
1:F:86:CYS:SG	1:F:88:MET:HE2	2.56	0.46
1:D:80:LEU:HD12	1:D:80:LEU:HA	1.58	0.46
1:E:132:ILE:O	1:E:136:MET:HG3	2.15	0.46
1:F:148:VAL:HG21	2:F:301:P4I:N01	2.31	0.46
1:D:105:PHE:HB2	2:E:301:P4I:BR21	2.71	0.45
1:E:189:THR:HG22	1:E:191:ILE:O	2.16	0.45
1:D:153:SER:OG	1:D:154:MET:N	2.49	0.45
1:B:214:LYS:HB2	1:B:214:LYS:HE2	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:MET:HE2	1:E:119:ILE:HD11	1.99	0.45
1:F:193:ILE:HD11	1:F:198:ILE:HB	1.99	0.45
1:C:240:ILE:HG22	1:C:241:LEU:HD12	1.98	0.45
1:F:107:GLN:NE2	3:F:401:HOH:O	2.34	0.45
1:D:190:ASP:OD2	1:E:150:GLN:NE2	2.50	0.45
1:G:73:TYR:OH	1:G:81:ARG:NH1	2.50	0.45
1:A:131:ALA:HB1	1:B:148:VAL:HG12	1.98	0.45
1:D:79:LEU:HG	2:D:301:P4I:BR21	2.71	0.45
1:F:179:GLN:NE2	3:F:402:HOH:O	2.37	0.44
1:G:132:ILE:O	1:G:136:MET:HG3	2.17	0.44
1:F:78:ARG:HG3	2:F:301:P4I:BR21	2.73	0.44
1:C:152:ALA:HB1	1:C:176:MET:HE2	1.99	0.44
1:F:153:SER:OG	1:F:154:MET:N	2.42	0.44
1:D:195:ALA:O	1:D:198:ILE:HG22	2.18	0.44
1:D:213:THR:HG22	1:D:239:GLY:C	2.43	0.44
1:G:136:MET:HE3	1:G:143:ILE:HG21	1.99	0.44
1:E:111:ASN:HD22	1:E:111:ASN:H	1.64	0.44
1:C:169:SER:CB	1:C:241:LEU:HD21	2.47	0.43
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.91	0.43
1:D:174:ARG:HB3	1:D:229:TYR:HD2	1.82	0.43
1:F:79:LEU:HD23	2:F:301:P4I:BR21	2.72	0.43
1:F:148:VAL:HG21	2:F:301:P4I:C02	2.47	0.43
1:A:170:LEU:HD13	1:G:134:ASP:HB3	1.98	0.43
1:A:229:TYR:HB2	1:G:197:GLU:OE1	2.19	0.43
1:E:78:ARG:NH1	1:E:82:GLU:OE2	2.51	0.43
1:D:117:MET:HE3	1:D:117:MET:HB3	1.78	0.43
1:G:177:ILE:HD12	1:G:224:MET:HG2	2.00	0.43
1:C:194:GLN:NE2	1:D:227:ASP:OD2	2.45	0.43
1:G:152:ALA:HB1	1:G:176:MET:HE2	2.00	0.43
1:A:220:ILE:O	1:A:224:MET:HB2	2.19	0.43
1:G:79:LEU:HD23	1:G:79:LEU:HA	1.86	0.43
1:C:233:MET:O	1:C:237:GLU:HG3	2.19	0.42
1:D:136:MET:HE2	1:D:136:MET:HB3	1.76	0.42
1:D:82:GLU:HB3	1:D:84:ILE:HG13	2.01	0.42
1:F:134:ASP:HB3	1:G:170:LEU:HD23	2.01	0.42
1:A:154:MET:HE2	1:A:154:MET:HA	2.01	0.42
1:B:148:VAL:HG21	2:B:301:P4I:N01	2.35	0.42
1:G:110:SER:OG	1:G:113:LYS:HB2	2.19	0.42
2:A:301:P4I:BR21	1:G:105:PHE:HB2	2.74	0.42
1:A:103:LEU:HD21	1:A:117:MET:HE2	2.02	0.42
1:F:187:GLN:H	1:F:187:GLN:HG2	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:MET:HG2	1:A:178:HIS:H	1.85	0.41
1:B:148:VAL:HG21	2:B:301:P4I:C02	2.50	0.41
1:F:85:VAL:HG21	1:F:103:LEU:HD23	2.02	0.41
1:F:98:LEU:O	1:F:102:GLN:HG3	2.19	0.41
1:G:203:LYS:HA	1:G:206:TYR:CD2	2.55	0.41
1:F:168:HIS:CD2	1:F:245:LEU:HD11	2.55	0.41
1:B:157:LEU:HD21	1:B:208:ILE:HG21	2.01	0.41
1:E:203:LYS:HA	1:E:206:TYR:HD1	1.86	0.41
1:A:111:ASN:O	1:A:112:LYS:HD3	2.20	0.41
1:A:138:TYR:CZ	1:B:248:PRO:HG3	2.55	0.41
1:A:201:LEU:HD23	1:A:204:GLN:NE2	2.33	0.41
1:F:106:LEU:HD23	1:F:106:LEU:HA	1.85	0.41
1:A:206:TYR:HB3	1:A:217:LEU:HD11	2.03	0.41
1:D:136:MET:H	1:D:136:MET:HG2	1.72	0.41
1:F:157:LEU:HD13	1:F:205:LEU:HD22	2.03	0.41
1:D:107:GLN:HG3	1:D:141:ASN:OD1	2.21	0.41
1:G:161:ALA:HA	1:G:212:HIS:ND1	2.36	0.41
1:B:177:ILE:HD12	1:B:224:MET:HG3	2.03	0.40
1:D:198:ILE:HD12	1:D:198:ILE:HA	1.88	0.40
1:F:107:GLN:HG3	1:F:141:ASN:OD1	2.21	0.40

All (2) 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)
1:F:196:GLU:OE2	1:G:206:TYR:OH[2_555]	2.13	0.07
1:B:226:ARG:NH1	1:E:225:GLU:OE2[2_555]	2.18	0.02

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	174/221 (79%)	167 (96%)	7 (4%)	0	100	100
1	B	167/221 (76%)	163 (98%)	4 (2%)	0	100	100
1	C	172/221 (78%)	163 (95%)	7 (4%)	2 (1%)	10	34
1	D	172/221 (78%)	167 (97%)	5 (3%)	0	100	100
1	E	172/221 (78%)	168 (98%)	4 (2%)	0	100	100
1	F	175/221 (79%)	169 (97%)	5 (3%)	1 (1%)	21	51
1	G	173/221 (78%)	163 (94%)	10 (6%)	0	100	100
All	All	1205/1547 (78%)	1160 (96%)	42 (4%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	193	ILE
1	F	191	ILE
1	C	191	ILE

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	156/185 (84%)	147 (94%)	9 (6%)	18	49
1	B	150/185 (81%)	148 (99%)	2 (1%)	61	86
1	C	154/185 (83%)	146 (95%)	8 (5%)	21	53
1	D	154/185 (83%)	150 (97%)	4 (3%)	40	75
1	E	154/185 (83%)	146 (95%)	8 (5%)	21	53
1	F	156/185 (84%)	149 (96%)	7 (4%)	24	58
1	G	156/185 (84%)	148 (95%)	8 (5%)	21	54
All	All	1080/1295 (83%)	1034 (96%)	46 (4%)	26	60

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	VAL
1	A	74	ASP
1	A	97	SER
1	A	150	GLN
1	A	153	SER
1	A	170	LEU
1	A	191	ILE
1	A	244	VAL
1	A	245	LEU
1	B	62	VAL
1	B	222	SER
1	C	75	ILE
1	C	148	VAL
1	C	189	THR
1	C	191	ILE
1	C	198	ILE
1	C	219	VAL
1	C	241	LEU
1	C	246	VAL
1	D	59	ILE
1	D	119	ILE
1	D	140	LEU
1	D	191	ILE
1	E	75	ILE
1	E	79	LEU
1	E	86	CYS
1	E	111	ASN
1	E	145	THR
1	E	189	THR
1	E	222	SER
1	E	241	LEU
1	F	86	CYS
1	F	110	SER
1	F	150	GLN
1	F	187	GLN
1	F	190	ASP
1	F	191	ILE
1	F	222	SER
1	G	86	CYS
1	G	153	SER
1	G	169	SER
1	G	181	SER
1	G	189	THR

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Mol	Chain	Res	Type
1	G	190	ASP
1	G	193	ILE
1	G	202	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	107	GLN
1	A	168	HIS
1	A	178	HIS
1	A	204	GLN
1	A	207	ASN
1	A	236	GLN
1	B	172	ASN
1	B	207	ASN
1	C	137	GLN
1	C	150	GLN
1	C	218	GLN
1	D	107	GLN
1	E	111	ASN
1	E	179	GLN
1	E	218	GLN
1	F	137	GLN
1	F	168	HIS
1	F	207	ASN
1	G	137	GLN
1	G	168	HIS
1	G	179	GLN
1	G	194	GLN
1	G	204	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	P4I	D	301	-	31,31,31	3.45	14 (45%)	38,43,43	1.80	10 (26%)
2	P4I	A	301	-	31,31,31	3.43	15 (48%)	38,43,43	1.83	9 (23%)
2	P4I	E	301	-	31,31,31	3.44	15 (48%)	38,43,43	1.86	9 (23%)
2	P4I	G	301	-	31,31,31	3.43	15 (48%)	38,43,43	1.80	8 (21%)
2	P4I	C	301	-	31,31,31	3.45	15 (48%)	38,43,43	1.83	9 (23%)
2	P4I	B	301	-	31,31,31	3.44	15 (48%)	38,43,43	1.85	10 (26%)
2	P4I	F	301	-	31,31,31	3.43	15 (48%)	38,43,43	1.91	8 (21%)

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	P4I	D	301	-	-	0/10/19/19	0/4/4/4
2	P4I	A	301	-	-	0/10/19/19	0/4/4/4
2	P4I	E	301	-	-	1/10/19/19	0/4/4/4
2	P4I	G	301	-	-	0/10/19/19	0/4/4/4
2	P4I	C	301	-	-	1/10/19/19	0/4/4/4
2	P4I	B	301	-	-	2/10/19/19	0/4/4/4
2	P4I	F	301	-	-	0/10/19/19	0/4/4/4

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	P4I	C08-N09	-10.77	1.27	1.47
2	D	301	P4I	C08-N09	-10.75	1.27	1.47
2	E	301	P4I	C08-N09	-10.75	1.27	1.47
2	G	301	P4I	C08-N09	-10.73	1.27	1.47
2	A	301	P4I	C08-N09	-10.72	1.27	1.47
2	C	301	P4I	C08-N09	-10.72	1.27	1.47
2	F	301	P4I	C08-N09	-10.72	1.27	1.47
2	D	301	P4I	C27-N09	-9.29	1.38	1.46
2	F	301	P4I	C27-N09	-9.27	1.38	1.46
2	C	301	P4I	C27-N09	-9.26	1.38	1.46
2	B	301	P4I	C27-N09	-9.25	1.38	1.46
2	E	301	P4I	C27-N09	-9.22	1.38	1.46
2	G	301	P4I	C27-N09	-9.14	1.38	1.46
2	A	301	P4I	C27-N09	-9.10	1.38	1.46
2	D	301	P4I	C24-N15	-6.95	1.28	1.39
2	G	301	P4I	C24-N15	-6.89	1.29	1.39
2	B	301	P4I	C24-N15	-6.87	1.29	1.39
2	C	301	P4I	C24-N15	-6.87	1.29	1.39
2	A	301	P4I	C24-N15	-6.86	1.29	1.39
2	F	301	P4I	C24-N15	-6.86	1.29	1.39
2	E	301	P4I	C24-N15	-6.81	1.29	1.39
2	C	301	P4I	C03-C02	5.07	1.55	1.44
2	A	301	P4I	C03-C02	5.06	1.55	1.44
2	G	301	P4I	C03-C02	5.03	1.55	1.44
2	D	301	P4I	C03-C02	5.03	1.55	1.44
2	E	301	P4I	C03-C02	5.01	1.55	1.44
2	F	301	P4I	C03-C02	5.00	1.55	1.44
2	B	301	P4I	C03-C02	4.99	1.55	1.44
2	C	301	P4I	C08-C07	3.92	1.58	1.51
2	E	301	P4I	C08-C07	3.91	1.58	1.51
2	G	301	P4I	C08-C07	3.89	1.58	1.51
2	B	301	P4I	C08-C07	3.84	1.58	1.51
2	D	301	P4I	C08-C07	3.82	1.58	1.51
2	A	301	P4I	C08-C07	3.80	1.58	1.51
2	F	301	P4I	C08-C07	3.77	1.58	1.51
2	C	301	P4I	C10-C11	3.12	1.60	1.52
2	B	301	P4I	C10-C11	3.08	1.59	1.52
2	F	301	P4I	C10-C11	3.07	1.59	1.52
2	A	301	P4I	C10-C11	3.07	1.59	1.52
2	D	301	P4I	C10-C11	3.05	1.59	1.52
2	G	301	P4I	C10-C11	3.05	1.59	1.52
2	E	301	P4I	C10-C11	3.04	1.59	1.52
2	A	301	P4I	C16-N15	2.88	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	P4I	C16-N15	2.87	1.52	1.47
2	E	301	P4I	C16-N15	2.85	1.52	1.47
2	B	301	P4I	C16-N15	2.81	1.52	1.47
2	D	301	P4I	C16-N15	2.79	1.52	1.47
2	G	301	P4I	C16-N15	2.79	1.52	1.47
2	C	301	P4I	C11-C12	2.78	1.54	1.50
2	C	301	P4I	C28-C07	2.76	1.44	1.39
2	F	301	P4I	C16-N15	2.75	1.52	1.47
2	D	301	P4I	C11-C12	2.75	1.54	1.50
2	A	301	P4I	C14-N15	-2.70	1.33	1.36
2	F	301	P4I	C28-C07	2.70	1.43	1.39
2	G	301	P4I	C28-C07	2.70	1.43	1.39
2	D	301	P4I	C14-N15	-2.70	1.33	1.36
2	G	301	P4I	C11-C12	2.70	1.54	1.50
2	E	301	P4I	C28-C07	2.69	1.43	1.39
2	A	301	P4I	C11-C12	2.69	1.54	1.50
2	E	301	P4I	C11-C12	2.68	1.54	1.50
2	B	301	P4I	C14-N15	-2.68	1.33	1.36
2	A	301	P4I	C28-C07	2.68	1.43	1.39
2	B	301	P4I	C28-C07	2.67	1.43	1.39
2	F	301	P4I	C14-N15	-2.66	1.33	1.36
2	E	301	P4I	C14-N15	-2.65	1.33	1.36
2	F	301	P4I	C11-C12	2.64	1.54	1.50
2	B	301	P4I	C11-C12	2.64	1.54	1.50
2	C	301	P4I	C14-N15	-2.63	1.33	1.36
2	D	301	P4I	C28-C07	2.62	1.43	1.39
2	G	301	P4I	C14-N15	-2.53	1.33	1.36
2	E	301	P4I	BR21-C20	2.34	1.94	1.90
2	G	301	P4I	BR21-C20	2.27	1.94	1.90
2	D	301	P4I	BR21-C20	2.27	1.94	1.90
2	A	301	P4I	BR21-C20	2.26	1.94	1.90
2	C	301	P4I	BR21-C20	2.26	1.94	1.90
2	F	301	P4I	BR21-C20	2.26	1.94	1.90
2	B	301	P4I	BR21-C20	2.25	1.94	1.90
2	F	301	P4I	C26-C12	-2.18	1.33	1.37
2	E	301	P4I	C16-C17	2.16	1.55	1.51
2	D	301	P4I	C26-C12	-2.14	1.33	1.37
2	A	301	P4I	C16-C17	2.14	1.55	1.51
2	A	301	P4I	C26-C12	-2.12	1.33	1.37
2	E	301	P4I	C26-C12	-2.12	1.33	1.37
2	E	301	P4I	C05-C06	2.12	1.42	1.38
2	F	301	P4I	C05-C04	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	P4I	C05-C06	2.12	1.42	1.38
2	B	301	P4I	C05-C06	2.11	1.42	1.38
2	B	301	P4I	C05-C04	2.11	1.42	1.38
2	G	301	P4I	C05-C06	2.11	1.42	1.38
2	G	301	P4I	C05-C04	2.11	1.42	1.38
2	E	301	P4I	C05-C04	2.10	1.42	1.38
2	C	301	P4I	C16-C17	2.10	1.55	1.51
2	A	301	P4I	C05-C06	2.10	1.42	1.38
2	B	301	P4I	C26-C12	-2.10	1.33	1.37
2	A	301	P4I	C05-C04	2.10	1.42	1.38
2	D	301	P4I	C05-C04	2.09	1.42	1.38
2	C	301	P4I	C26-C12	-2.09	1.33	1.37
2	C	301	P4I	C05-C04	2.08	1.42	1.38
2	F	301	P4I	C05-C06	2.07	1.42	1.38
2	F	301	P4I	C16-C17	2.07	1.55	1.51
2	G	301	P4I	C16-C17	2.06	1.55	1.51
2	D	301	P4I	C05-C06	2.05	1.42	1.38
2	B	301	P4I	C16-C17	2.03	1.55	1.51
2	G	301	P4I	C26-C12	-2.01	1.33	1.37

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	P4I	N15-C14-N13	-5.59	121.00	126.45
2	F	301	P4I	N15-C14-N13	-5.58	121.00	126.45
2	E	301	P4I	N15-C14-N13	-5.57	121.02	126.45
2	C	301	P4I	N15-C14-N13	-5.53	121.05	126.45
2	F	301	P4I	C11-C10-N09	5.45	116.05	111.19
2	B	301	P4I	N15-C14-N13	-5.39	121.19	126.45
2	D	301	P4I	N15-C14-N13	-5.39	121.19	126.45
2	A	301	P4I	N15-C14-N13	-5.29	121.28	126.45
2	E	301	P4I	C11-C10-N09	4.80	115.48	111.19
2	C	301	P4I	C11-C10-N09	4.39	115.11	111.19
2	B	301	P4I	C11-C10-N09	4.33	115.05	111.19
2	G	301	P4I	C11-C10-N09	4.26	114.99	111.19
2	A	301	P4I	C11-C10-N09	4.21	114.95	111.19
2	D	301	P4I	C11-C10-N09	3.68	114.47	111.19
2	C	301	P4I	C11-C12-N13	3.60	120.07	114.57
2	E	301	P4I	C11-C12-N13	3.60	120.06	114.57
2	F	301	P4I	C11-C12-N13	3.58	120.04	114.57
2	D	301	P4I	C11-C12-N13	3.57	120.02	114.57
2	B	301	P4I	C11-C12-N13	3.56	120.01	114.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	P4I	C11-C12-N13	3.56	120.01	114.57
2	G	301	P4I	C11-C12-N13	3.56	120.01	114.57
2	A	301	P4I	C14-N15-C24	-3.42	120.62	123.06
2	B	301	P4I	C14-N15-C24	-3.24	120.74	123.06
2	C	301	P4I	C14-N15-C24	-3.16	120.80	123.06
2	G	301	P4I	C14-N15-C24	-3.13	120.82	123.06
2	D	301	P4I	C14-N15-C24	-3.12	120.83	123.06
2	E	301	P4I	C14-N15-C24	-3.11	120.84	123.06
2	D	301	P4I	C17-C16-N15	-3.03	108.14	112.84
2	A	301	P4I	C26-C12-N13	-3.03	119.38	123.68
2	B	301	P4I	C26-C12-N13	-3.01	119.41	123.68
2	D	301	P4I	C26-C12-N13	-3.00	119.42	123.68
2	C	301	P4I	C26-C12-N13	-3.00	119.42	123.68
2	G	301	P4I	C26-C12-N13	-2.98	119.45	123.68
2	F	301	P4I	C14-N15-C24	-2.97	120.94	123.06
2	E	301	P4I	C26-C12-N13	-2.94	119.51	123.68
2	F	301	P4I	C26-C12-N13	-2.91	119.55	123.68
2	F	301	P4I	C27-N09-C10	2.91	114.28	110.10
2	A	301	P4I	C27-N09-C10	2.86	114.21	110.10
2	B	301	P4I	C27-N09-C10	2.83	114.16	110.10
2	E	301	P4I	O25-C24-C26	-2.77	119.80	125.06
2	C	301	P4I	O25-C24-C26	-2.76	119.81	125.06
2	D	301	P4I	O25-C24-C26	-2.73	119.86	125.06
2	A	301	P4I	O25-C24-C26	-2.73	119.87	125.06
2	G	301	P4I	O25-C24-C26	-2.72	119.88	125.06
2	G	301	P4I	C26-C24-N15	2.70	120.27	115.15
2	F	301	P4I	O25-C24-C26	-2.68	119.96	125.06
2	B	301	P4I	O25-C24-C26	-2.67	119.98	125.06
2	C	301	P4I	C26-C24-N15	2.67	120.20	115.15
2	A	301	P4I	C26-C24-N15	2.67	120.20	115.15
2	E	301	P4I	C26-C24-N15	2.65	120.17	115.15
2	B	301	P4I	C26-C24-N15	2.64	120.15	115.15
2	D	301	P4I	C26-C24-N15	2.59	120.05	115.15
2	F	301	P4I	C26-C24-N15	2.58	120.05	115.15
2	E	301	P4I	C27-N09-C10	2.58	113.80	110.10
2	B	301	P4I	C17-C16-N15	-2.56	108.88	112.84
2	D	301	P4I	C27-N09-C10	2.50	113.68	110.10
2	C	301	P4I	C27-N09-C10	2.46	113.64	110.10
2	G	301	P4I	C27-N09-C10	2.33	113.44	110.10
2	A	301	P4I	C16-N15-C24	2.22	120.03	117.73
2	D	301	P4I	C16-N15-C24	2.18	119.99	117.73
2	B	301	P4I	C16-N15-C24	2.13	119.94	117.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	P4I	C17-C16-N15	-2.02	109.71	112.84
2	C	301	P4I	C16-N15-C24	2.02	119.82	117.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

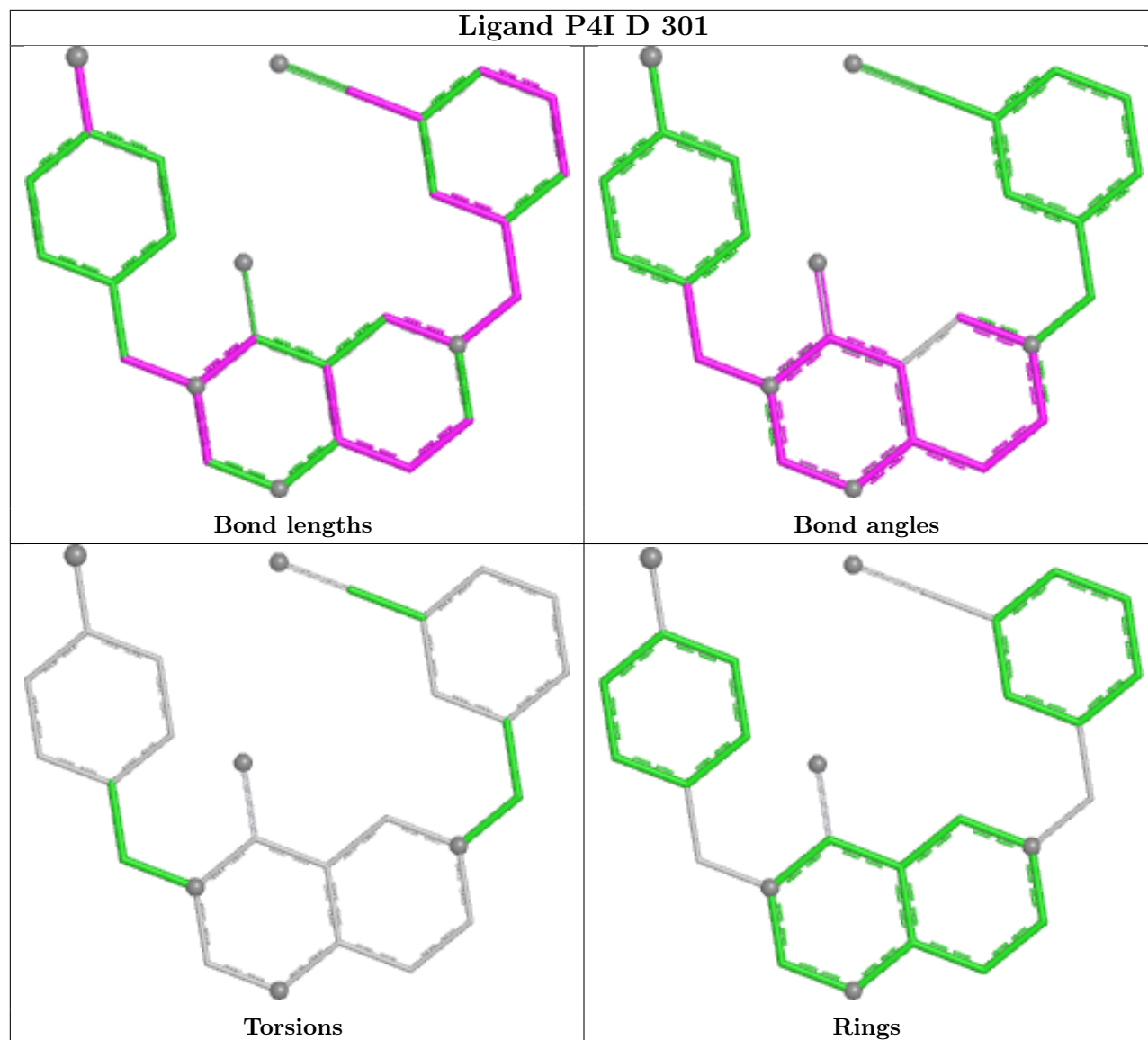
Mol	Chain	Res	Type	Atoms
2	B	301	P4I	C07-C08-N09-C10
2	B	301	P4I	C07-C08-N09-C27
2	E	301	P4I	C07-C08-N09-C10
2	C	301	P4I	C07-C08-N09-C10

There are no ring outliers.

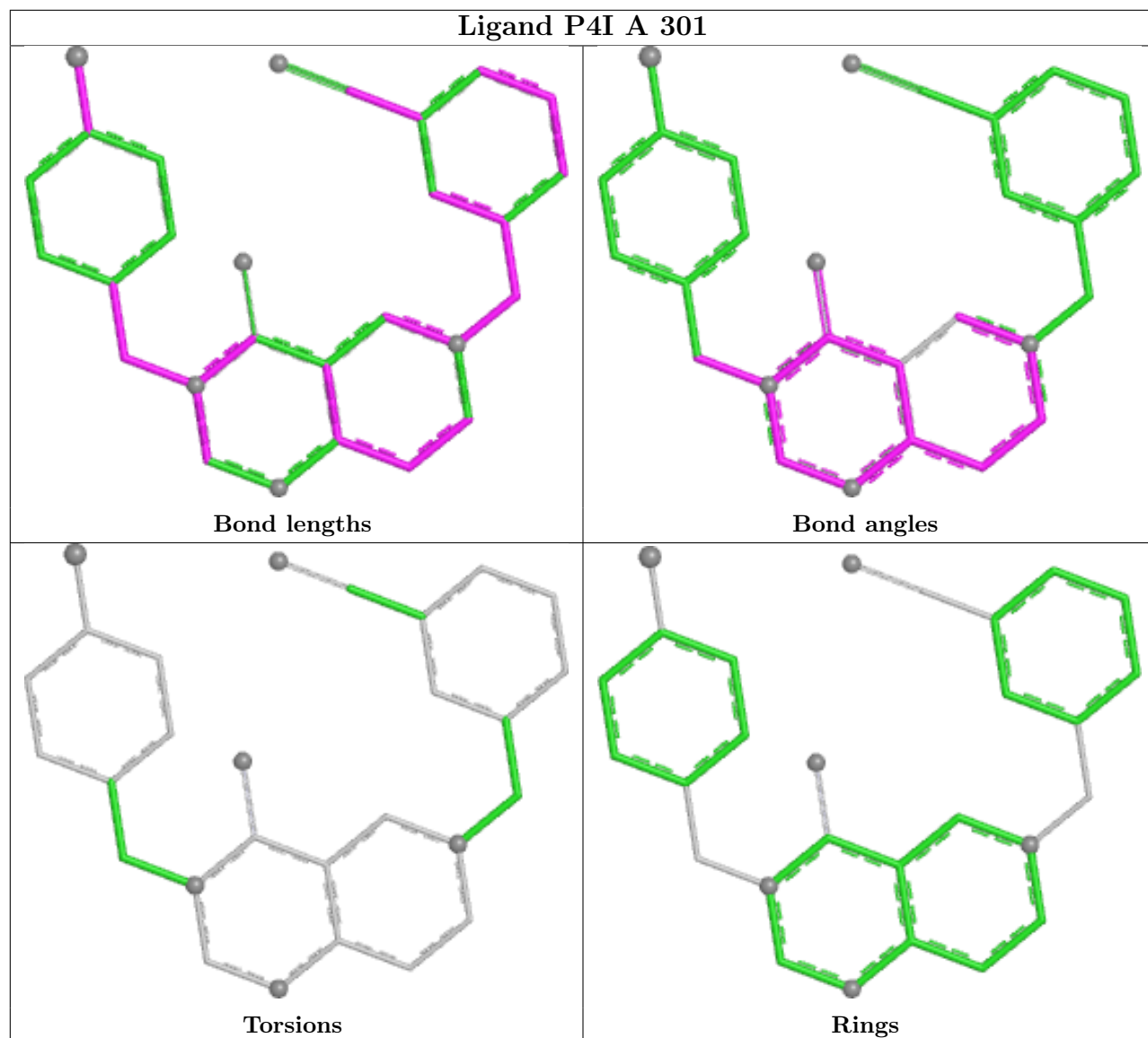
6 monomers are involved in 13 short contacts:

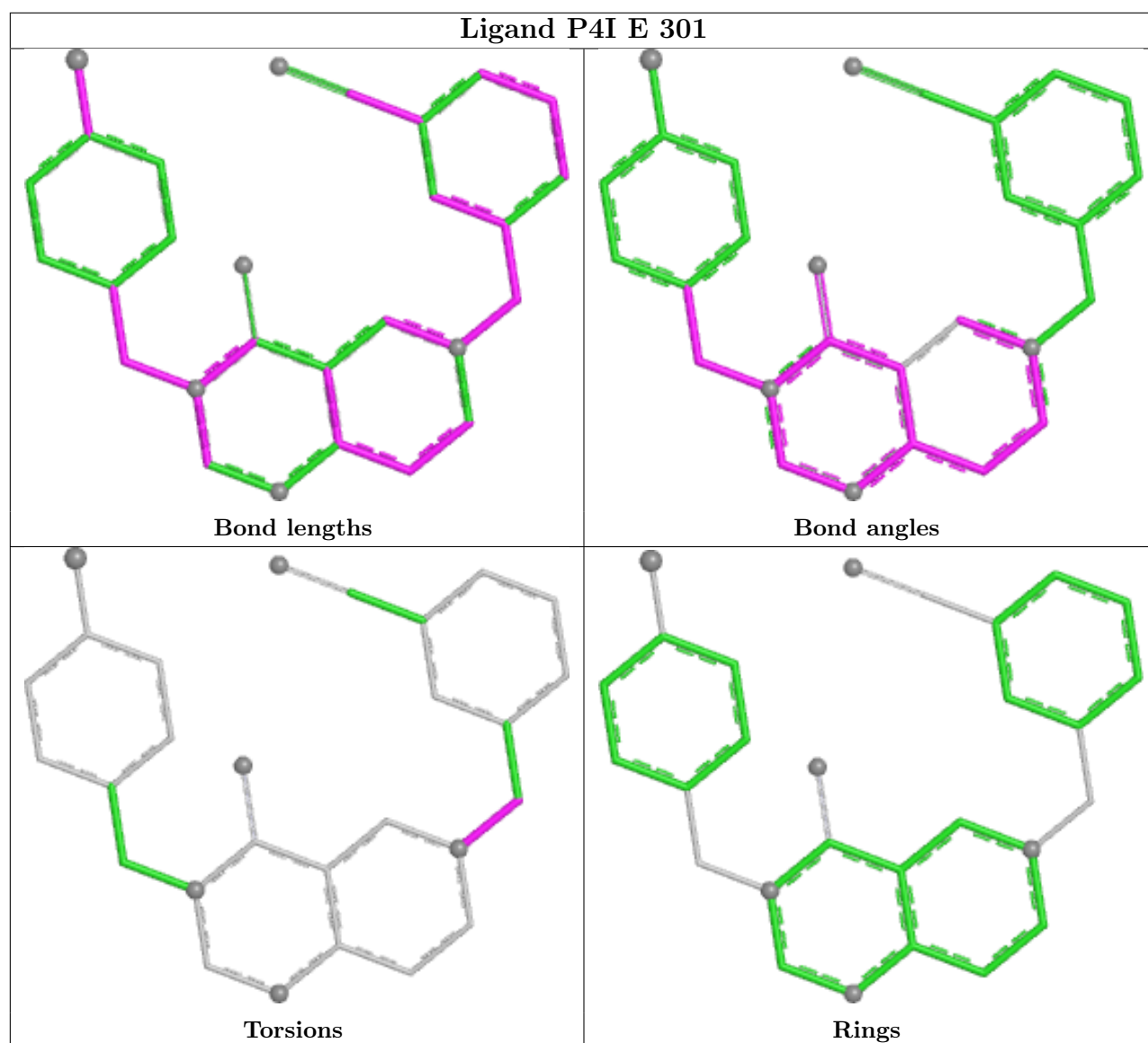
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	P4I	2	0
2	A	301	P4I	2	0
2	E	301	P4I	1	0
2	G	301	P4I	1	0
2	B	301	P4I	3	0
2	F	301	P4I	4	0

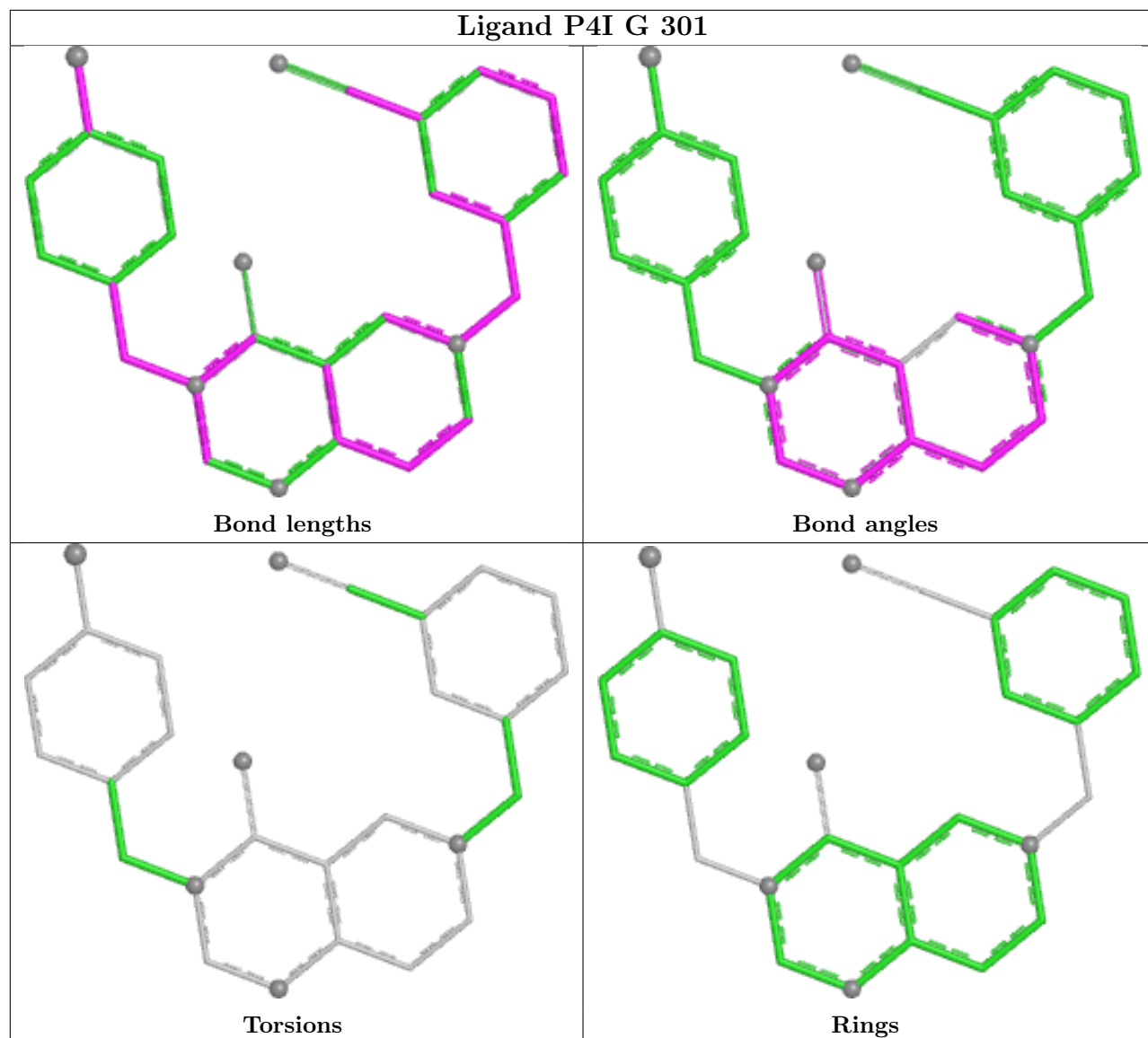
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

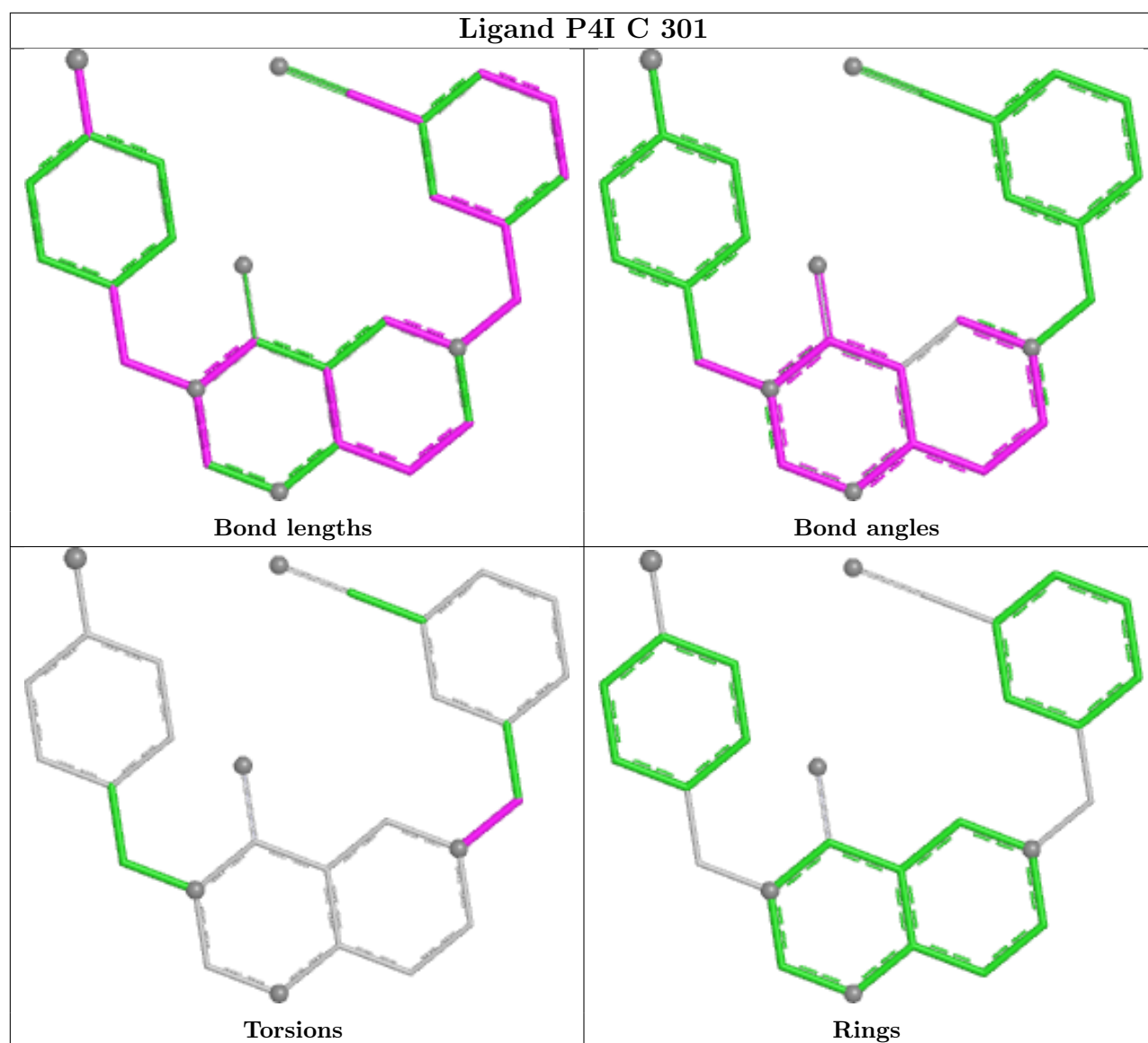


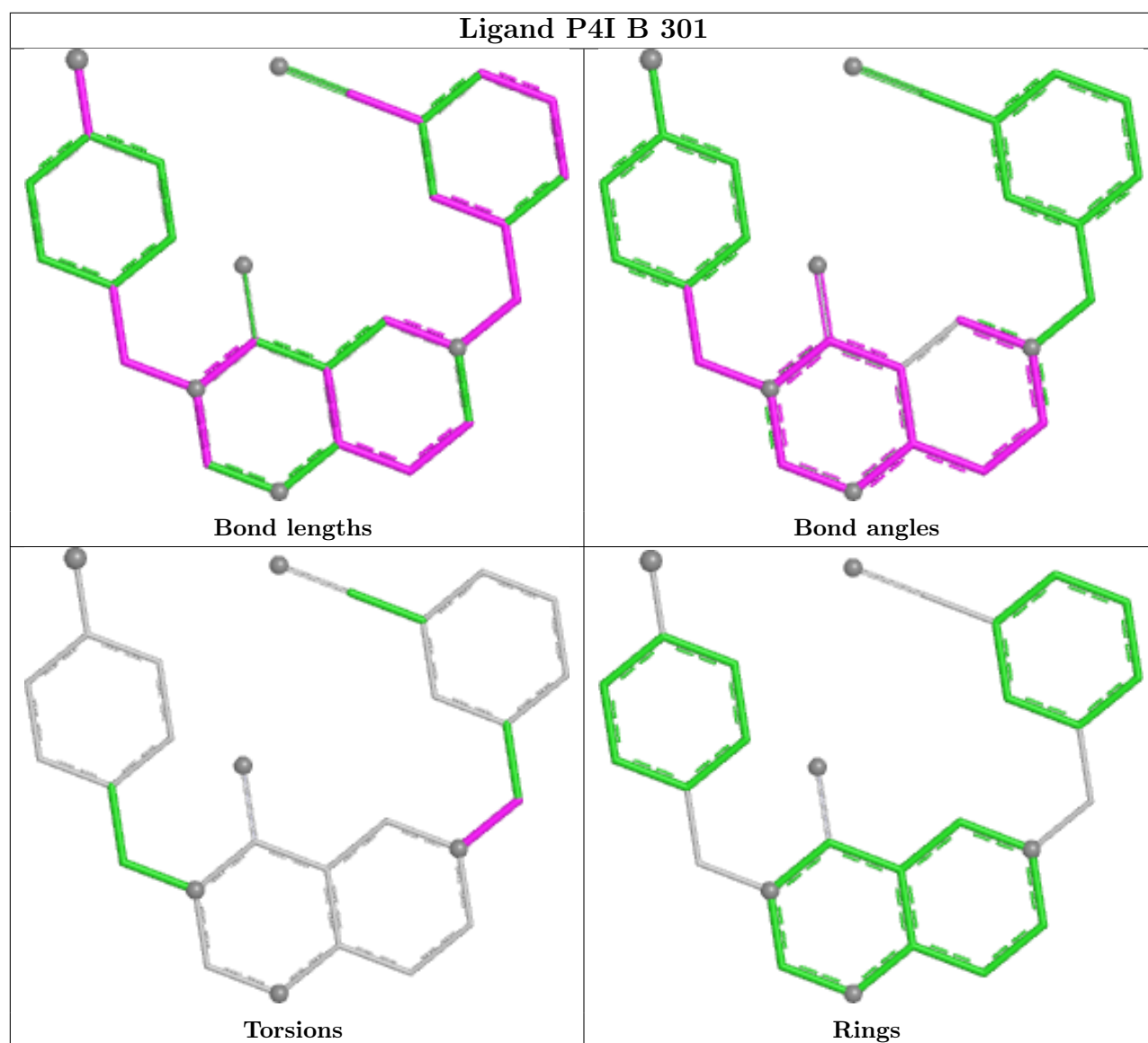
Ligand P4I A 301

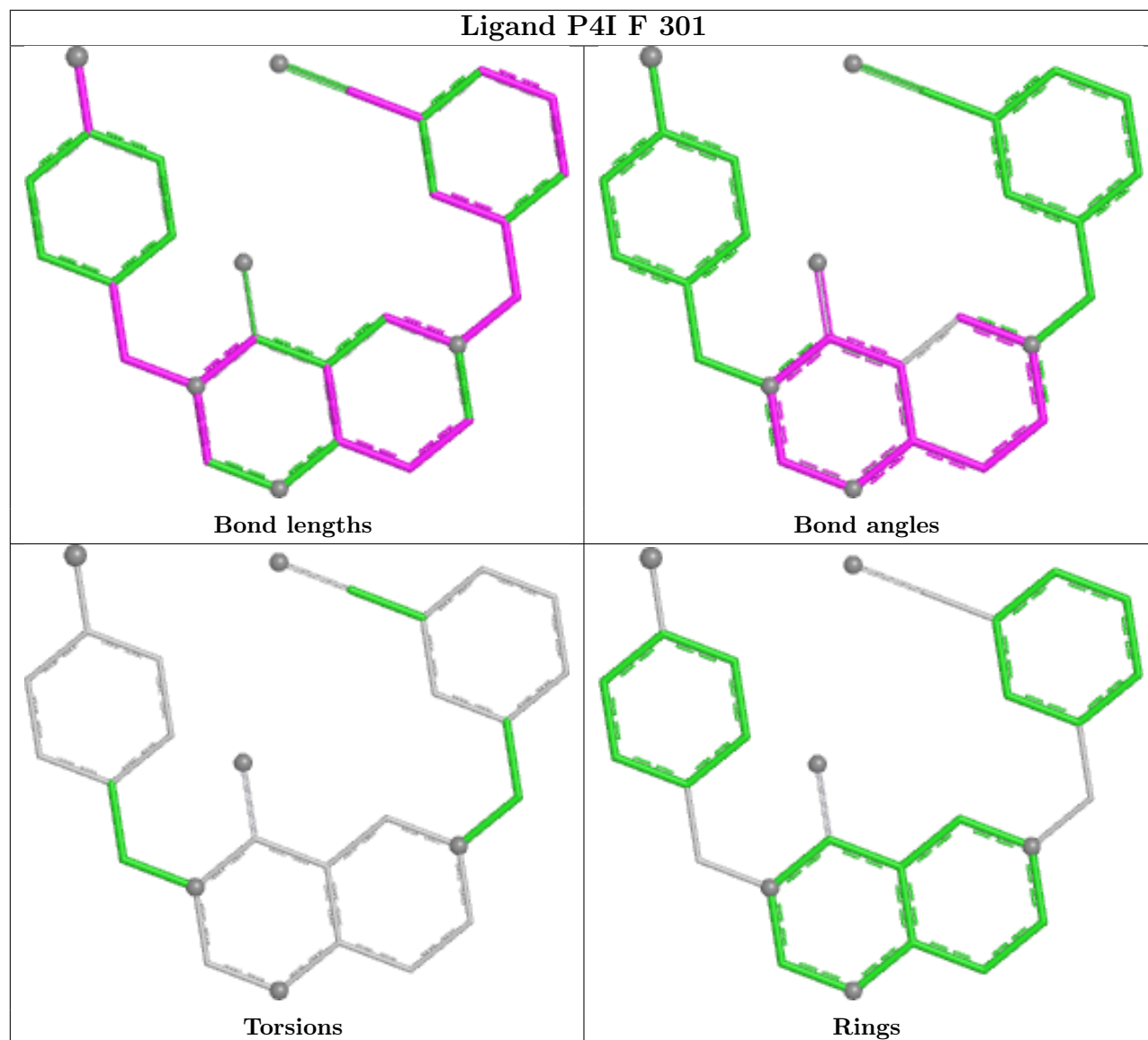












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	180/221 (81%)	1.05	26 (14%) 6 5	11, 23, 53, 77	0
1	B	173/221 (78%)	0.90	16 (9%) 14 10	11, 22, 39, 55	0
1	C	178/221 (80%)	0.85	21 (11%) 9 7	10, 19, 48, 75	0
1	D	178/221 (80%)	0.87	21 (11%) 9 7	10, 20, 48, 65	0
1	E	178/221 (80%)	0.84	15 (8%) 17 12	8, 18, 43, 66	0
1	F	180/221 (81%)	0.83	21 (11%) 9 7	10, 20, 51, 63	1 (0%)
1	G	179/221 (80%)	0.81	16 (8%) 15 11	10, 18, 50, 68	0
All	All	1246/1547 (80%)	0.88	136 (10%) 10 8	8, 20, 48, 77	1 (0%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	5.6
1	C	188	ALA	5.2
1	E	188	ALA	5.2
1	F	190	ASP	5.1
1	F	58	LEU	4.9
1	C	249	PRO	4.8
1	E	249	PRO	4.8
1	C	191	ILE	4.7
1	E	191	ILE	4.7
1	E	189	THR	4.6
1	F	247	HIS	4.6
1	A	72	ALA	4.6
1	A	64	GLU	4.6
1	G	189	THR	4.4
1	A	191	ILE	4.3
1	A	73	TYR	4.3
1	D	190	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	191	ILE	4.2
1	A	70	GLU	4.1
1	D	192	ALA	4.1
1	D	64	GLU	3.9
1	B	73	TYR	3.9
1	A	247	HIS	3.9
1	A	71	ARG	3.9
1	B	218	GLN	3.8
1	C	190	ASP	3.8
1	G	190	ASP	3.8
1	A	218	GLN	3.7
1	A	188	ALA	3.7
1	B	63	VAL	3.7
1	D	246	VAL	3.7
1	B	192	ALA	3.6
1	F	186	GLY	3.6
1	F	73	TYR	3.6
1	B	247	HIS	3.6
1	E	192	ALA	3.6
1	F	191	ILE	3.6
1	C	189	THR	3.6
1	A	58	LEU	3.6
1	B	248	PRO	3.5
1	C	73	TYR	3.5
1	D	58	LEU	3.5
1	F	248	PRO	3.4
1	A	192	ALA	3.4
1	D	189	THR	3.4
1	E	190	ASP	3.4
1	C	193	ILE	3.3
1	D	247	HIS	3.3
1	D	72	ALA	3.3
1	C	218	GLN	3.3
1	F	189	THR	3.2
1	D	73	TYR	3.2
1	G	73	TYR	3.1
1	G	192	ALA	3.1
1	G	71	ARG	3.1
1	E	180	PRO	3.0
1	F	245	LEU	3.0
1	A	190	ASP	3.0
1	C	248	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	216	SER	3.0
1	C	198	ILE	2.9
1	G	70	GLU	2.9
1	G	233	MET	2.9
1	A	223	ALA	2.9
1	G	63	VAL	2.9
1	C	58	LEU	2.8
1	F	197	GLU	2.8
1	B	197	GLU	2.8
1	D	197	GLU	2.8
1	G	191	ILE	2.8
1	F	71	ARG	2.7
1	F	72	ALA	2.7
1	G	64	GLU	2.7
1	B	181	SER	2.7
1	A	140	LEU	2.7
1	A	189	THR	2.7
1	C	181	SER	2.7
1	C	235	ALA	2.6
1	A	124	GLY	2.6
1	A	248	PRO	2.6
1	E	195	ALA	2.6
1	A	63	VAL	2.6
1	F	180	PRO	2.6
1	G	58	LEU	2.5
1	B	180	PRO	2.5
1	F	244	VAL	2.5
1	D	180	PRO	2.4
1	C	239	GLY	2.4
1	D	237	GLU	2.4
1	E	221	GLU	2.4
1	C	180	PRO	2.4
1	G	109	GLU	2.4
1	F	187	GLN	2.4
1	D	140	LEU	2.4
1	B	246	VAL	2.3
1	A	237	GLU	2.3
1	C	192	ALA	2.3
1	A	76	TYR	2.3
1	F	221	GLU	2.3
1	D	181	SER	2.3
1	A	123	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLY	2.3
1	F	188	ALA	2.3
1	E	72	ALA	2.3
1	G	227	ASP	2.3
1	C	177	ILE	2.3
1	F	129	GLY	2.3
1	E	88	MET	2.2
1	G	170	LEU	2.2
1	D	245	LEU	2.2
1	C	172	ASN	2.2
1	A	194	GLN	2.2
1	A	221	GLU	2.2
1	F	192	ALA	2.2
1	D	248	PRO	2.2
1	D	88	MET	2.2
1	B	76	TYR	2.2
1	A	205	LEU	2.2
1	E	62	VAL	2.1
1	F	62	VAL	2.1
1	E	217	LEU	2.1
1	G	72	ALA	2.1
1	C	237	GLU	2.1
1	D	178	HIS	2.1
1	D	235	ALA	2.1
1	F	235	ALA	2.1
1	C	234	GLU	2.1
1	B	72	ALA	2.0
1	C	72	ALA	2.0
1	D	188	ALA	2.0
1	A	246	VAL	2.0
1	E	179	GLN	2.0
1	E	226	ARG	2.0
1	G	111	ASN	2.0
1	B	59	ILE	2.0
1	B	213	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

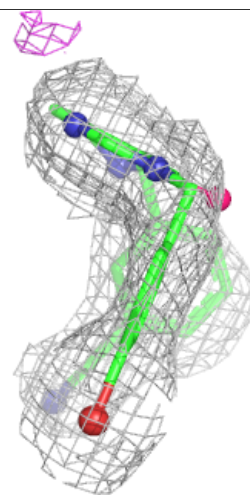
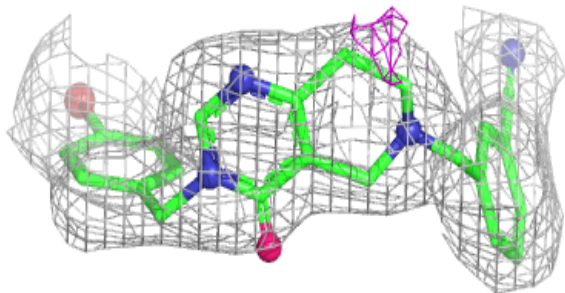
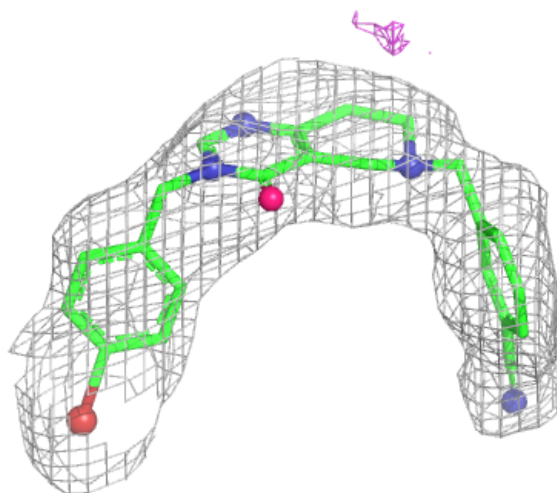
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P4I	B	301	28/28	0.93	0.13	12,23,31,53	0
2	P4I	A	301	28/28	0.94	0.12	15,25,34,49	0
2	P4I	D	301	28/28	0.94	0.12	17,24,32,42	0
2	P4I	E	301	28/28	0.94	0.13	11,20,32,39	0
2	P4I	F	301	28/28	0.94	0.13	16,23,30,53	0
2	P4I	C	301	28/28	0.95	0.10	13,22,30,44	0
2	P4I	G	301	28/28	0.95	0.12	13,19,30,39	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.

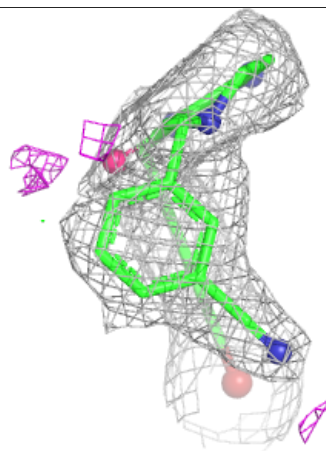
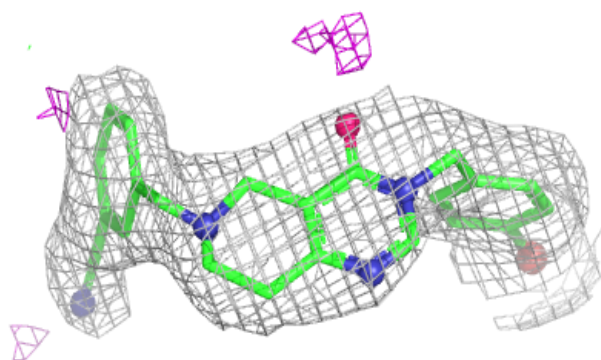
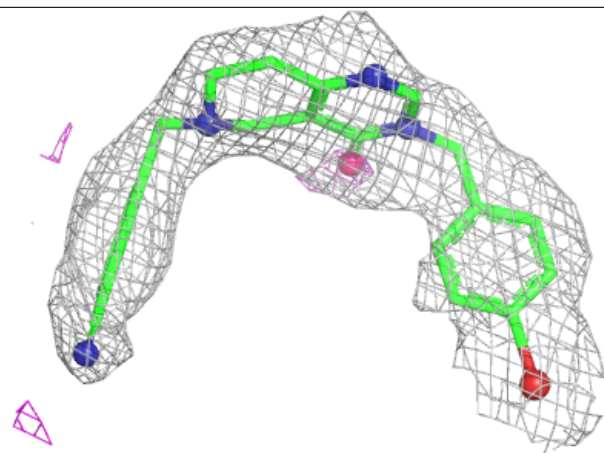
Electron density around P4I B 301:

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



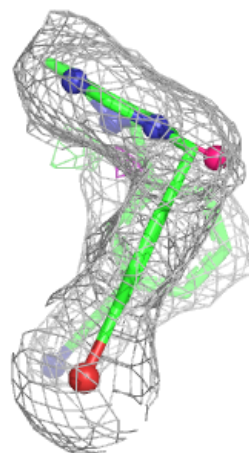
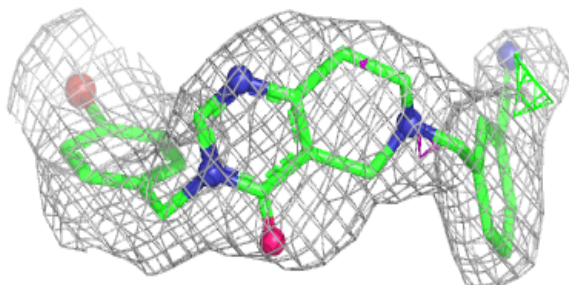
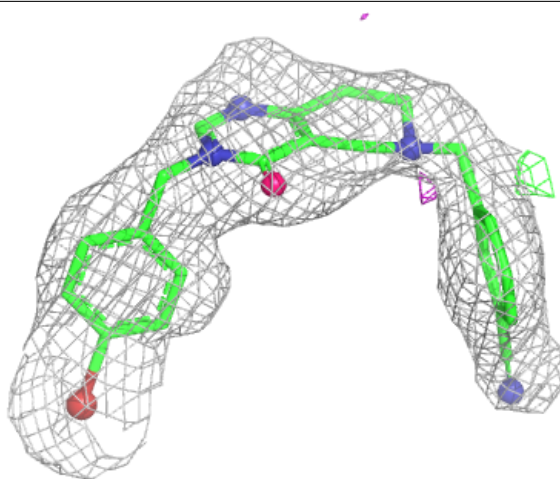
Electron density around P4I A 301:

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



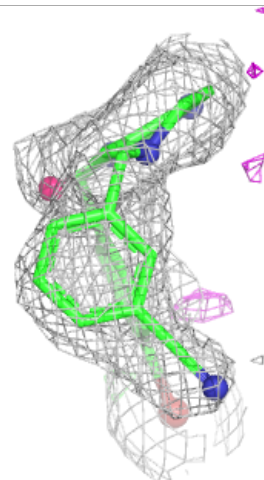
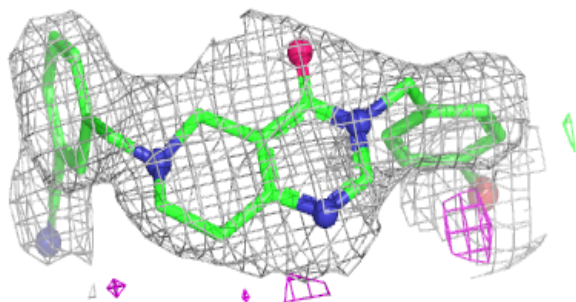
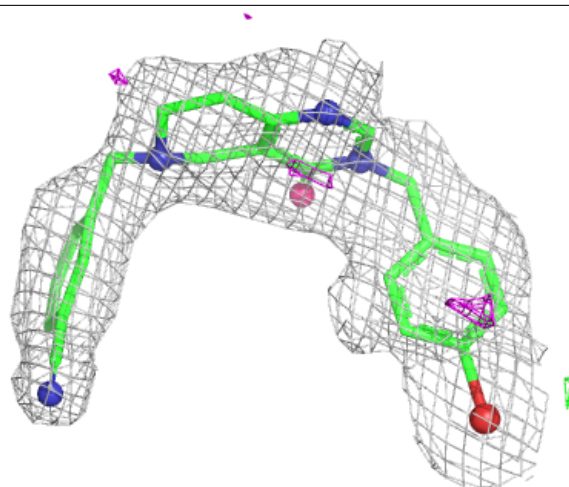
Electron density around P4I D 301:

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



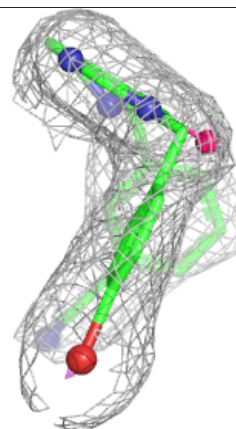
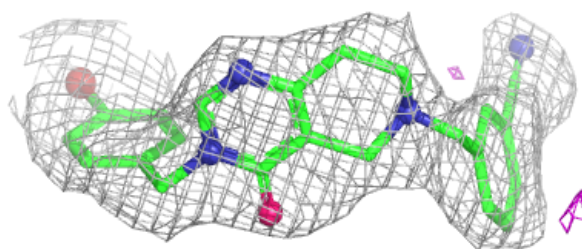
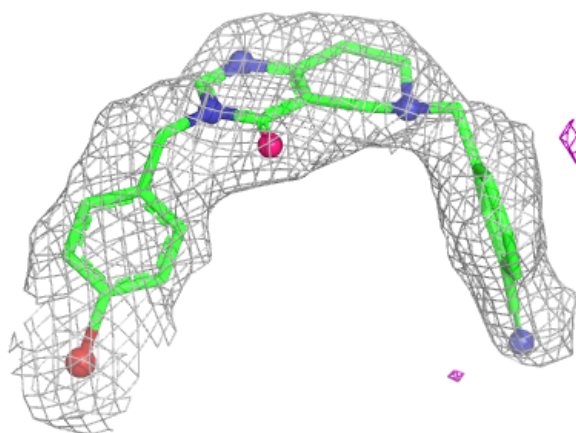
Electron density around P4I E 301:

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



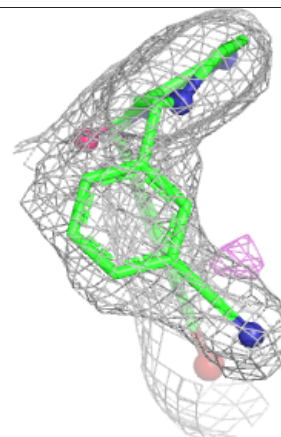
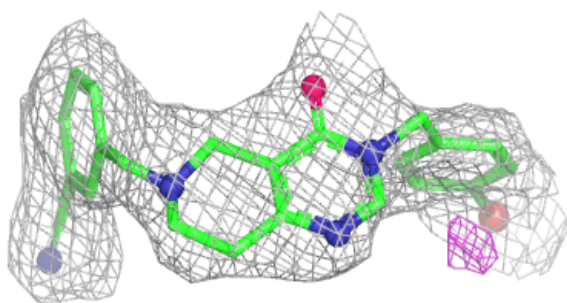
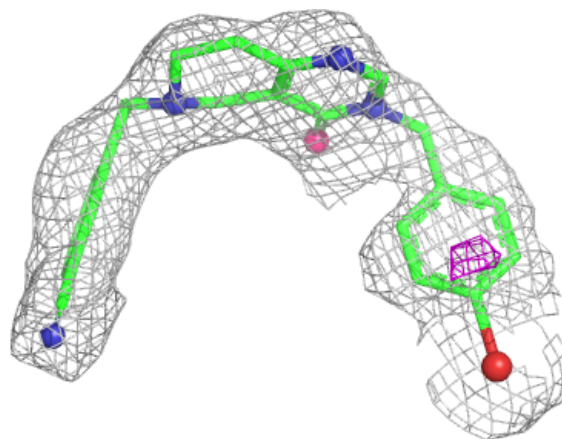
Electron density around P4I F 301:

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



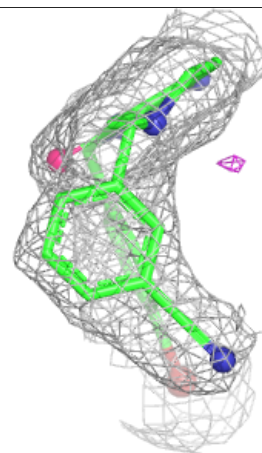
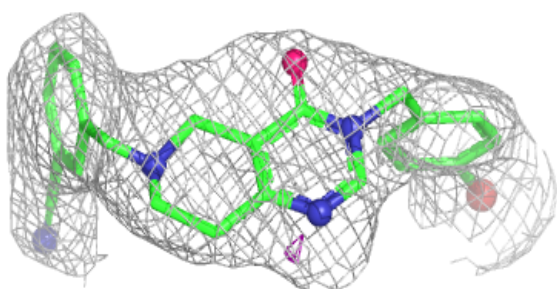
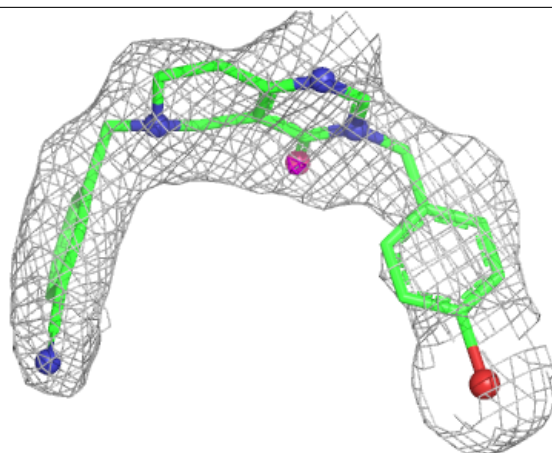
Electron density around P4I C 301:

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



Electron density around P4I G 301:

$2mF_o-DF_c$ (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.