



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:03 AM BST

PDB ID : 4MSK  
Title : Co-crystal structure of tankyrase 1 with compound 34  
Authors : Huang, X.  
Deposited on : 2013-09-18  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

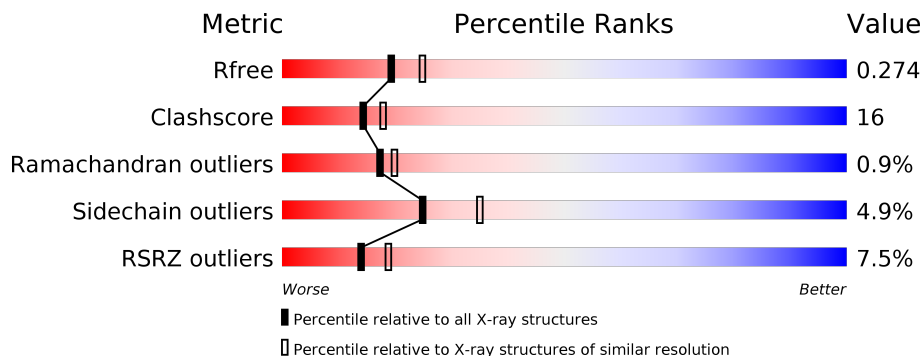
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	217	 5% 70% 25%
1	B	217	 5% 62% 32%
1	C	217	 10% 65% 25%
1	D	217	 9% 61% 28%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	D	1401	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7031 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 Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	Total 1695	C 1066	N 310	O 307	S 12	0	0	0
1	B	211	Total 1692	C 1065	N 308	O 307	S 12	0	0	0
1	C	200	Total 1634	C 1032	N 298	O 293	S 11	0	0	0
1	D	201	Total 1641	C 1037	N 300	O 292	S 12	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1315	HIS	-	EXPRESSION TAG	UNP O95271
A	1316	HIS	-	EXPRESSION TAG	UNP O95271
A	1317	HIS	-	EXPRESSION TAG	UNP O95271
A	1318	HIS	-	EXPRESSION TAG	UNP O95271
A	1319	HIS	-	EXPRESSION TAG	UNP O95271
A	1320	HIS	-	EXPRESSION TAG	UNP O95271
B	1315	HIS	-	EXPRESSION TAG	UNP O95271
B	1316	HIS	-	EXPRESSION TAG	UNP O95271
B	1317	HIS	-	EXPRESSION TAG	UNP O95271
B	1318	HIS	-	EXPRESSION TAG	UNP O95271
B	1319	HIS	-	EXPRESSION TAG	UNP O95271
B	1320	HIS	-	EXPRESSION TAG	UNP O95271
C	1315	HIS	-	EXPRESSION TAG	UNP O95271
C	1316	HIS	-	EXPRESSION TAG	UNP O95271
C	1317	HIS	-	EXPRESSION TAG	UNP O95271
C	1318	HIS	-	EXPRESSION TAG	UNP O95271
C	1319	HIS	-	EXPRESSION TAG	UNP O95271
C	1320	HIS	-	EXPRESSION TAG	UNP O95271
D	1315	HIS	-	EXPRESSION TAG	UNP O95271
D	1316	HIS	-	EXPRESSION TAG	UNP O95271
D	1317	HIS	-	EXPRESSION TAG	UNP O95271

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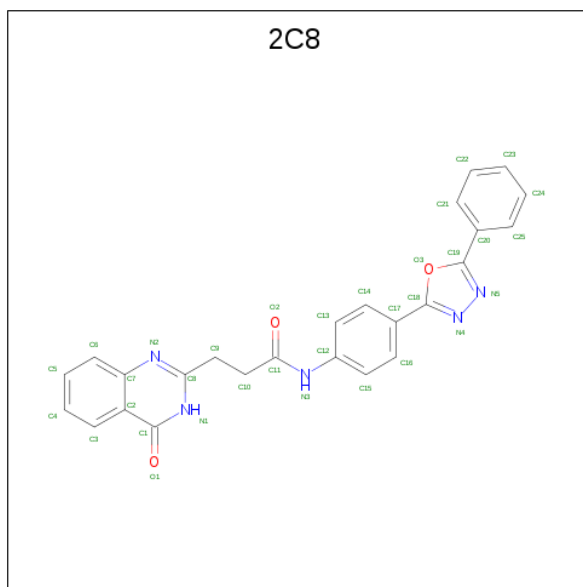
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1318	HIS	-	EXPRESSION TAG	UNP O95271
D	1319	HIS	-	EXPRESSION TAG	UNP O95271
D	1320	HIS	-	EXPRESSION TAG	UNP O95271

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 3-(4-oxo-3,4-dihydroquinazolin-2-yl)-N-[4-(5-phenyl-1,3,4-oxadiazol-2-yl)phenyl]propanamide (three-letter code: 2C8) (formula: C<sub>25</sub>H<sub>19</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 33 25 5 3	0	0
3	B	1	Total C N O 33 25 5 3	0	0
3	C	1	Total C N O 33 25 5 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	D	1	33	25	5	3	0	0

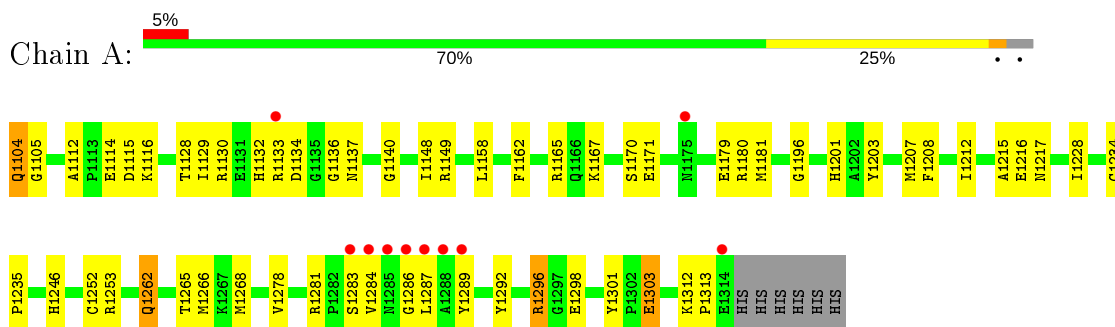
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	62	Total	O	0	0
			62	62		
4	C	62	Total	O	0	0
			62	62		
4	D	46	Total	O	0	0
			46	46		

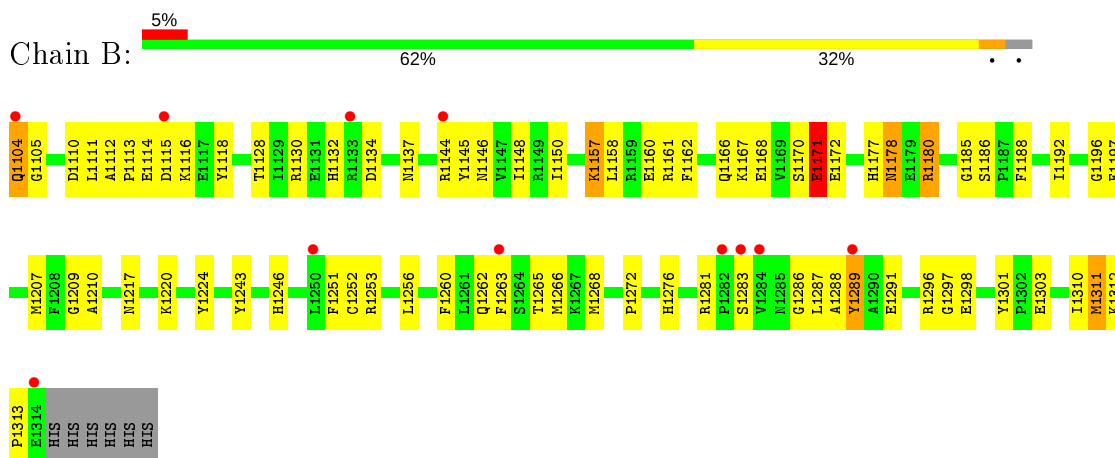
### 3 Residue-property plots [i](#)

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.

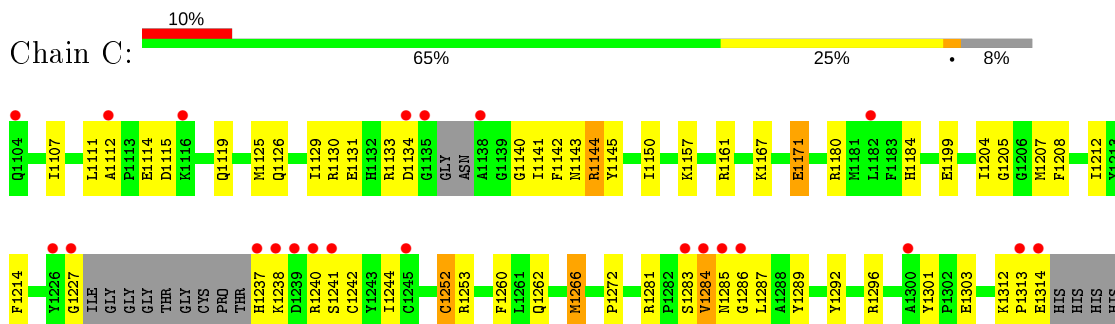
- Molecule 1: Tankyrase-1



- Molecule 1: Tankyrase-1



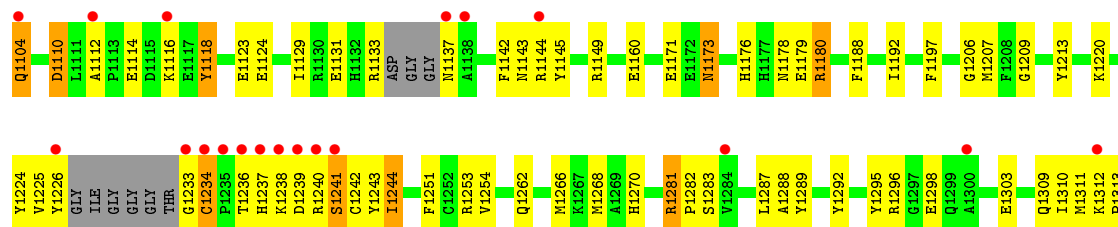
- Molecule 1: Tankyrase-1



HIS  
HIS

• Molecule 1: Tankyrase-1

Chain D: 



GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.23Å 79.78Å 85.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 25.53 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.30) 95.3 (25.53-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 1.99Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.239 , 0.285 0.243 , 0.274	Depositor DCC
$R_{free}$ test set	3544 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtrriage
Anisotropy	0.370	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7523e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2C8

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	0.50	1/1738 (0.1%)	0.68	0/2336
1	B	0.50	1/1734 (0.1%)	0.71	3/2331 (0.1%)
1	C	0.49	1/1674 (0.1%)	0.67	0/2246
1	D	0.48	1/1682 (0.1%)	0.65	0/2259
All	All	0.49	4/6828 (0.1%)	0.68	3/9172 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1171	GLU	CG-CD	8.20	1.64	1.51
1	D	1160	GLU	CG-CD	7.42	1.63	1.51
1	B	1171	GLU	CG-CD	6.32	1.61	1.51
1	A	1216	GLU	CG-CD	5.22	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1281	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	B	1281	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	1251	PHE	N-CA-C	-5.11	97.21	111.00

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	1695	0	1623	43	1
1	B	1692	0	1625	64	0
1	C	1634	0	1571	46	1
1	D	1641	0	1582	56	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	33	0	19	2	0
3	B	33	0	19	1	0
3	C	33	0	19	1	0
3	D	33	0	19	1	0
4	A	63	0	0	3	0
4	B	62	0	0	3	0
4	C	62	0	0	4	0
4	D	46	0	0	1	0
All	All	7031	0	6477	206	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 16.

All (206) 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:B:1178:ASN:HD21	1:B:1180:ARG:HH12	1.10	0.99
1:B:1134:ASP:OD1	1:B:1137:ASN:HB3	1.66	0.93
1:C:1167:LYS:O	1:C:1171:GLU:HG3	1.74	0.88
1:B:1112:ALA:HB1	1:B:1114:GLU:OE2	1.74	0.88
1:A:1167:LYS:O	1:A:1171:GLU:HG3	1.78	0.84
1:B:1157:LYS:H	1:B:1157:LYS:HZ2	1.26	0.84
1:C:1283:SER:HB3	4:C:1506:HOH:O	1.77	0.83
1:B:1207:MET:SD	1:B:1287:LEU:HD21	2.20	0.81
1:A:1207:MET:SD	1:A:1287:LEU:HD21	2.25	0.77
1:A:1203:TYR:CE1	1:A:1228:ILE:HD11	2.20	0.76
1:A:1104:GLN:HG3	1:A:1105:GLY:H	1.49	0.76
1:C:1180:ARG:HG3	4:C:1552:HOH:O	1.85	0.75
1:C:1284:VAL:HG23	1:C:1285:ASN:H	1.51	0.75
1:B:1178:ASN:ND2	1:B:1180:ARG:HH12	1.84	0.73
1:C:1253:ARG:HG3	1:C:1303:GLU:HG3	1.71	0.72
1:B:1220:LYS:HB2	1:B:1289:TYR:CE2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1244:ILE:HG13	1:D:1237:HIS:HE1	1.56	0.70
1:D:1244:ILE:N	1:D:1244:ILE:HD13	2.06	0.70
1:D:1268:MET:HG2	1:D:1270:HIS:O	1.94	0.68
1:B:1220:LYS:HB2	1:B:1289:TYR:CD2	2.28	0.68
1:B:1178:ASN:HD21	1:B:1180:ARG:NH1	1.89	0.68
1:B:1167:LYS:O	1:B:1171:GLU:HG2	1.96	0.66
1:D:1240:ARG:O	1:D:1241:SER:OG	2.13	0.66
1:D:1112:ALA:HB1	1:D:1114:GLU:OE2	1.97	0.65
1:D:1234:CYS:SG	1:D:1237:HIS:HB2	2.37	0.64
1:D:1253:ARG:CG	1:D:1303:GLU:HG3	2.29	0.63
1:D:1253:ARG:HG3	1:D:1303:GLU:HG3	1.80	0.62
1:B:1298:GLU:H	1:B:1298:GLU:CD	2.03	0.61
1:A:1203:TYR:HE1	1:A:1228:ILE:HD11	1.65	0.61
1:B:1180:ARG:HG3	1:B:1256:LEU:CD1	2.31	0.60
1:D:1243:TYR:CD2	1:D:1312:LYS:HD3	2.36	0.60
1:C:1252:CYS:HB3	1:C:1301:TYR:O	2.01	0.60
1:C:1240:ARG:HH11	1:C:1240:ARG:HG2	1.66	0.60
1:B:1144:ARG:HG2	1:B:1145:TYR:N	2.16	0.60
1:C:1212:ILE:HG23	3:C:1402:2C8:H14	1.83	0.59
1:A:1148:ILE:HD13	1:A:1246:HIS:CE1	2.37	0.59
1:A:1253:ARG:HG3	1:A:1303:GLU:HG2	1.84	0.59
1:D:1242:CYS:SG	1:D:1244:ILE:HG12	2.42	0.59
1:D:1207:MET:SD	1:D:1287:LEU:HD21	2.43	0.59
1:B:1180:ARG:HG3	1:B:1256:LEU:HD12	1.83	0.59
1:C:1296:ARG:NH2	4:C:1514:HOH:O	2.37	0.58
1:D:1144:ARG:HG2	1:D:1145:TYR:N	2.18	0.58
1:D:1295:TYR:O	1:D:1296:ARG:HG3	2.04	0.58
1:D:1244:ILE:H	1:D:1244:ILE:HD13	1.68	0.58
1:D:1234:CYS:SG	1:D:1239:ASP:N	2.72	0.57
1:B:1178:ASN:ND2	1:B:1180:ARG:NH1	2.51	0.57
1:A:1104:GLN:CG	1:A:1105:GLY:H	2.16	0.56
1:B:1289:TYR:N	1:B:1289:TYR:CD1	2.74	0.56
1:C:1237:HIS:O	1:C:1238:LYS:C	2.44	0.56
1:C:1141:ILE:HG22	1:C:1313:PRO:HG2	1.88	0.56
1:B:1157:LYS:HD3	1:B:1157:LYS:N	2.19	0.56
1:C:1115:ASP:O	1:C:1119:GLN:HG3	2.06	0.56
1:C:1244:ILE:HD11	1:D:1236:THR:HG21	1.86	0.56
1:B:1180:ARG:HG2	1:B:1180:ARG:HH11	1.71	0.55
1:A:1115:ASP:OD1	1:A:1116:LYS:N	2.39	0.55
1:A:1129:ILE:O	1:A:1130:ARG:HG2	2.07	0.55
1:B:1289:TYR:HD1	1:B:1289:TYR:N	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1111:LEU:HD12	1:C:1150:ILE:HG22	1.86	0.55
1:C:1129:ILE:O	1:C:1130:ARG:HD2	2.07	0.55
1:A:1112:ALA:HB1	1:A:1114:GLU:OE2	2.07	0.55
1:D:1129:ILE:HD11	1:D:1145:TYR:CE2	2.42	0.55
1:A:1104:GLN:HG3	1:A:1105:GLY:N	2.21	0.54
1:C:1112:ALA:HB1	1:C:1114:GLU:OE2	2.07	0.54
1:D:1253:ARG:HG3	1:D:1303:GLU:CG	2.38	0.54
1:A:1132:HIS:C	1:A:1134:ASP:H	2.11	0.53
1:B:1188:PHE:O	1:B:1192:ILE:HG13	2.09	0.53
1:B:1312:LYS:HD3	1:B:1313:PRO:HD2	1.89	0.53
1:B:1312:LYS:HD3	1:B:1313:PRO:CD	2.39	0.53
1:A:1148:ILE:O	1:A:1149:ARG:HB3	2.09	0.53
1:B:1312:LYS:HD3	1:B:1313:PRO:N	2.24	0.53
1:C:1207:MET:SD	1:C:1287:LEU:HD21	2.49	0.53
1:D:1310:ILE:HG13	1:D:1310:ILE:O	2.09	0.52
1:A:1104:GLN:CG	1:A:1105:GLY:N	2.72	0.52
1:D:1225:VAL:O	1:D:1225:VAL:HG12	2.09	0.52
1:B:1288:ALA:C	1:B:1289:TYR:HD1	2.12	0.52
1:C:1260:PHE:CD2	1:C:1272:PRO:HG2	2.44	0.52
1:B:1148:ILE:HD13	1:B:1246:HIS:CE1	2.44	0.52
1:B:1128:THR:HB	1:B:1217:ASN:HA	1.93	0.51
1:C:1114:GLU:H	1:C:1114:GLU:CD	2.14	0.51
1:D:1309:GLN:HA	4:D:1518:HOH:O	2.10	0.51
1:A:1268:MET:CE	1:A:1278:VAL:HG21	2.40	0.51
1:C:1140:GLY:HA2	1:C:1241:SER:HB2	1.93	0.51
1:D:1281:ARG:HH21	1:D:1282:PRO:HD2	1.74	0.51
1:C:1244:ILE:HG13	1:D:1237:HIS:CE1	2.41	0.51
1:A:1283:SER:O	1:A:1286:GLY:N	2.36	0.51
1:B:1146:ASN:HB2	1:B:1311:MET:SD	2.51	0.50
1:D:1209:GLY:HA3	1:D:1268:MET:H	1.77	0.50
1:C:1292:TYR:CD2	1:C:1292:TYR:N	2.79	0.50
1:C:1129:ILE:HD11	1:C:1145:TYR:CE2	2.47	0.49
1:D:1118:TYR:CD2	1:D:1118:TYR:C	2.85	0.49
1:C:1284:VAL:HG23	1:C:1285:ASN:N	2.22	0.49
1:D:1206:GLY:HA3	1:D:1213:TYR:OH	2.12	0.49
1:D:1292:TYR:N	1:D:1292:TYR:CD2	2.80	0.49
1:B:1114:GLU:H	1:B:1114:GLU:CD	2.15	0.49
1:C:1283:SER:HB3	1:C:1286:GLY:HA3	1.94	0.49
1:D:1129:ILE:HD11	1:D:1145:TYR:CD2	2.48	0.49
1:C:1142:PHE:HA	1:C:1313:PRO:HG3	1.95	0.49
1:A:1128:THR:HB	1:A:1217:ASN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1204:ILE:HG13	1:C:1205:GLY:N	2.27	0.49
1:D:1179:GLU:OE2	1:D:1253:ARG:HD2	2.12	0.48
1:B:1157:LYS:O	1:B:1160:GLU:HB2	2.13	0.48
1:D:1124:GLU:HG2	1:D:1251:PHE:CZ	2.49	0.48
1:A:1253:ARG:HG3	1:A:1303:GLU:CG	2.43	0.48
1:A:1289:TYR:CD1	1:A:1289:TYR:N	2.81	0.48
1:B:1180:ARG:CG	1:B:1180:ARG:HH11	2.26	0.48
1:B:1207:MET:HE1	1:B:1287:LEU:HD11	1.95	0.48
1:D:1239:ASP:OD1	1:D:1241:SER:HB2	2.14	0.48
1:D:1137:ASN:OD1	1:D:1240:ARG:NH2	2.46	0.48
1:C:1242:CYS:SG	1:C:1244:ILE:N	2.86	0.48
1:C:1131:GLU:CD	1:C:1143:ASN:HB3	2.35	0.48
1:A:1181:MET:HA	1:A:1252:CYS:O	2.15	0.47
1:D:1237:HIS:O	1:D:1238:LYS:C	2.52	0.47
1:B:1185:GLY:O	1:B:1186:SER:HB3	2.14	0.47
1:D:1236:THR:HB	1:D:1237:HIS:CE1	2.49	0.47
1:B:1207:MET:O	1:B:1265:THR:HG23	2.14	0.47
1:A:1165:ARG:HD3	1:A:1296:ARG:NH1	2.30	0.47
1:B:1197:PHE:O	1:B:1297:GLY:HA3	2.15	0.47
1:B:1260:PHE:HE2	1:B:1262:GLN:NE2	2.11	0.47
1:C:1240:ARG:CG	1:C:1240:ARG:HH11	2.28	0.47
1:B:1144:ARG:HE	1:B:1311:MET:HE1	1.78	0.47
1:D:1236:THR:C	1:D:1237:HIS:ND1	2.69	0.47
1:D:1243:TYR:HD1	1:D:1310:ILE:O	1.98	0.47
1:A:1132:HIS:C	1:A:1134:ASP:N	2.68	0.46
1:D:1295:TYR:C	1:D:1296:ARG:HG3	2.36	0.46
1:B:1253:ARG:HG3	1:B:1303:GLU:HG3	1.98	0.46
1:D:1233:GLY:O	1:D:1234:CYS:C	2.53	0.46
1:A:1201:HIS:CE1	4:A:1528:HOH:O	2.68	0.46
1:B:1262:GLN:NE2	1:B:1266:MET:SD	2.88	0.46
1:C:1157:LYS:O	1:C:1161:ARG:HG3	2.15	0.46
1:D:1224:TYR:C	1:D:1226:TYR:H	2.17	0.46
1:B:1134:ASP:O	1:B:1134:ASP:OD1	2.34	0.46
1:D:1192:ILE:HD13	1:D:1197:PHE:CE1	2.51	0.46
1:B:1113:PRO:HA	1:B:1118:TYR:CD2	2.51	0.46
1:A:1179:GLU:CG	1:A:1180:ARG:N	2.79	0.46
1:B:1263:PHE:CD2	1:B:1263:PHE:N	2.83	0.45
1:B:1209:GLY:HA3	1:B:1268:MET:H	1.81	0.45
1:D:1180:ARG:HH11	1:D:1180:ARG:CG	2.30	0.45
1:D:1133:ARG:HD3	1:D:1288:ALA:O	2.16	0.45
1:B:1260:PHE:CD2	1:B:1272:PRO:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:TYR:N	1:A:1292:TYR:CD2	2.85	0.45
1:D:1124:GLU:HG2	1:D:1251:PHE:HZ	1.82	0.45
1:A:1158:LEU:HD22	1:A:1196:GLY:HA3	1.99	0.45
1:D:1262:GLN:NE2	1:D:1266:MET:SD	2.90	0.45
1:B:1132:HIS:C	1:B:1134:ASP:H	2.19	0.45
1:C:1111:LEU:HD12	1:C:1150:ILE:CG2	2.46	0.45
1:A:1132:HIS:O	1:A:1134:ASP:N	2.49	0.45
1:B:1158:LEU:HD22	1:B:1196:GLY:HA3	1.99	0.45
1:A:1298:GLU:CD	1:A:1298:GLU:H	2.20	0.44
1:B:1111:LEU:HD12	1:B:1150:ILE:HG22	1.99	0.44
1:A:1201:HIS:HE1	4:A:1528:HOH:O	1.99	0.44
1:A:1208:PHE:CE1	1:A:1262:GLN:HG2	2.52	0.44
1:B:1104:GLN:HG3	1:B:1105:GLY:H	1.83	0.44
1:C:1126:GLN:OE1	1:C:1144:ARG:HD3	2.17	0.44
1:B:1162:PHE:HA	1:B:1298:GLU:O	2.16	0.44
1:C:1208:PHE:HA	1:C:1266:MET:O	2.17	0.44
1:A:1136:GLY:O	1:A:1140:GLY:N	2.42	0.44
1:A:1252:CYS:HB3	1:A:1301:TYR:O	2.18	0.44
1:B:1130:ARG:HG2	1:B:1217:ASN:HD22	1.82	0.44
1:C:1129:ILE:HD11	1:C:1145:TYR:CD2	2.53	0.44
1:B:1243:TYR:HD1	1:B:1310:ILE:O	2.00	0.43
1:D:1173:ASN:HB3	1:D:1176:HIS:O	2.18	0.43
1:A:1265:THR:O	1:A:1266:MET:HG3	2.19	0.43
1:B:1252:CYS:HB3	1:B:1301:TYR:O	2.18	0.43
1:B:1180:ARG:NH1	1:B:1180:ARG:CG	2.81	0.43
1:C:1312:LYS:HA	1:C:1313:PRO:HD3	1.89	0.43
1:D:1224:TYR:C	1:D:1226:TYR:N	2.72	0.43
1:B:1207:MET:HB2	4:B:1522:HOH:O	2.18	0.43
1:D:1179:GLU:HA	1:D:1254:VAL:O	2.19	0.43
1:A:1130:ARG:HH11	1:A:1130:ARG:HG2	1.84	0.43
1:C:1199:GLU:N	1:C:1199:GLU:OE1	2.34	0.43
1:C:1262:GLN:HE22	1:C:1266:MET:CE	2.31	0.42
1:A:1136:GLY:O	1:A:1137:ASN:C	2.58	0.42
1:D:1236:THR:O	1:D:1236:THR:HG22	2.19	0.42
1:A:1162:PHE:HA	1:A:1298:GLU:O	2.19	0.42
1:C:1184:HIS:HB2	1:C:1214:PHE:CD1	2.55	0.42
1:D:1188:PHE:O	1:D:1192:ILE:HG13	2.19	0.42
1:D:1188:PHE:CD2	3:D:1402:2C8:H12	2.55	0.42
1:B:1166:GLN:HG2	1:B:1177:HIS:CD2	2.55	0.42
1:B:1186:SER:HA	1:B:1224:TYR:O	2.19	0.42
1:C:1227:GLY:HA2	4:C:1530:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1130:ARG:HG2	1:C:1133:ARG:HD2	2.01	0.41
1:B:1168:GLU:O	1:B:1171:GLU:HG3	2.20	0.41
1:B:1283:SER:OG	1:B:1286:GLY:N	2.53	0.41
1:C:1253:ARG:HG3	1:C:1303:GLU:CG	2.46	0.41
1:D:1110:ASP:OD2	1:D:1149:ARG:NH2	2.44	0.41
1:B:1144:ARG:HD3	4:B:1531:HOH:O	2.19	0.41
1:D:1244:ILE:O	1:D:1309:GLN:NE2	2.38	0.41
1:D:1144:ARG:NE	1:D:1311:MET:SD	2.92	0.41
1:B:1172:GLU:OE1	1:B:1276:HIS:NE2	2.52	0.41
1:D:1220:LYS:HD3	1:D:1289:TYR:CD1	2.55	0.41
1:B:1180:ARG:HG3	1:B:1256:LEU:HD11	2.01	0.41
1:D:1131:GLU:OE2	1:D:1143:ASN:HB2	2.20	0.41
1:A:1180:ARG:NH1	4:A:1527:HOH:O	2.53	0.41
1:B:1161:ARG:HD3	4:B:1530:HOH:O	2.19	0.41
1:D:1142:PHE:HA	1:D:1313:PRO:HG3	2.03	0.41
1:A:1215:ALA:HB2	3:A:1402:2C8:H2	2.03	0.41
1:A:1234:CYS:HA	1:A:1235:PRO:HD3	1.93	0.41
1:B:1115:ASP:OD1	1:B:1116:LYS:N	2.54	0.41
1:B:1291:GLU:HG2	3:B:1402:2C8:H4	2.03	0.41
1:C:1131:GLU:OE1	1:C:1143:ASN:HB3	2.20	0.41
1:C:1125:MET:HG2	1:C:1145:TYR:CD2	2.56	0.40
1:A:1212:ILE:HG23	3:A:1402:2C8:H14	2.04	0.40
1:A:1312:LYS:HE3	1:A:1312:LYS:HB2	1.94	0.40
1:C:1134:ASP:HB2	1:C:1289:TYR:HE1	1.86	0.40
1:A:1130:ARG:NH1	1:A:1130:ARG:HG2	2.35	0.40
1:B:1144:ARG:HD3	1:B:1311:MET:HE2	2.04	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:A:1104:GLN:OE1	1:D:1104:GLN:N[3_546]	2.10	0.10
1:C:1107:ILE:CD1	1:C:1107:ILE:CD1[2_665]	2.16	0.04

## 5.3 Torsion angles [i](#)

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

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



of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/217 (96%)	195 (93%)	11 (5%)	3 (1%)	11	11
1	B	209/217 (96%)	201 (96%)	7 (3%)	1 (0%)	29	35
1	C	194/217 (89%)	182 (94%)	11 (6%)	1 (0%)	29	35
1	D	195/217 (90%)	183 (94%)	10 (5%)	2 (1%)	15	17
All	All	807/868 (93%)	761 (94%)	39 (5%)	7 (1%)	17	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1313	PRO
1	D	1241	SER
1	A	1133	ARG
1	B	1210	ALA
1	C	1284	VAL
1	D	1234	CYS
1	A	1284	VAL

### 5.3.2 Protein sidechains [i](#)

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	177/185 (96%)	171 (97%)	6 (3%)	37	51
1	B	177/185 (96%)	167 (94%)	10 (6%)	21	29
1	C	172/185 (93%)	167 (97%)	5 (3%)	42	58
1	D	174/185 (94%)	161 (92%)	13 (8%)	13	17
All	All	700/740 (95%)	666 (95%)	34 (5%)	25	35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1104	GLN
1	A	1170	SER
1	A	1262	GLN
1	A	1281	ARG
1	A	1296	ARG
1	A	1303	GLU
1	B	1104	GLN
1	B	1110	ASP
1	B	1157	LYS
1	B	1170	SER
1	B	1171	GLU
1	B	1178	ASN
1	B	1180	ARG
1	B	1289	TYR
1	B	1296	ARG
1	B	1311	MET
1	C	1144	ARG
1	C	1252	CYS
1	C	1266	MET
1	C	1281	ARG
1	C	1314	GLU
1	D	1104	GLN
1	D	1110	ASP
1	D	1116	LYS
1	D	1118	TYR
1	D	1123	GLU
1	D	1171	GLU
1	D	1173	ASN
1	D	1178	ASN
1	D	1180	ARG
1	D	1244	ILE
1	D	1281	ARG
1	D	1283	SER
1	D	1298	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1104	GLN
1	A	1166	GLN
1	A	1173	ASN
1	A	1176	HIS
1	A	1177	HIS

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Mol	Chain	Res	Type
1	A	1223	GLN
1	A	1248	GLN
1	B	1104	GLN
1	B	1166	GLN
1	B	1177	HIS
1	B	1178	ASN
1	B	1217	ASN
1	C	1104	GLN
1	C	1119	GLN
1	C	1151	GLN
1	C	1166	GLN
1	C	1173	ASN
1	C	1223	GLN
1	C	1248	GLN
1	C	1262	GLN
1	D	1119	GLN
1	D	1166	GLN
1	D	1173	ASN
1	D	1176	HIS
1	D	1178	ASN
1	D	1223	GLN
1	D	1237	HIS
1	D	1248	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	2C8	D	1402	-	30,37,37	3.25	21 (70%)	42,51,51	3.09	11 (26%)
3	2C8	B	1402	-	30,37,37	3.14	21 (70%)	42,51,51	3.10	11 (26%)
3	2C8	C	1402	-	30,37,37	3.11	21 (70%)	42,51,51	3.27	12 (28%)
3	2C8	A	1402	-	30,37,37	2.97	22 (73%)	42,51,51	3.17	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2C8	D	1402	-	-	3/13/17/17	0/5/5/5
3	2C8	B	1402	-	-	2/13/17/17	0/5/5/5
3	2C8	C	1402	-	-	2/13/17/17	0/5/5/5
3	2C8	A	1402	-	-	1/13/17/17	0/5/5/5

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	2C8	C2-C7	5.16	1.51	1.41
3	D	1402	2C8	C4-C3	5.14	1.48	1.36
3	D	1402	2C8	C2-C7	5.13	1.51	1.41
3	C	1402	2C8	C2-C7	4.95	1.50	1.41
3	A	1402	2C8	C4-C3	4.81	1.47	1.36
3	D	1402	2C8	C15-C12	4.78	1.47	1.39
3	B	1402	2C8	C4-C3	4.67	1.47	1.36
3	C	1402	2C8	C5-C6	4.63	1.47	1.36
3	C	1402	2C8	C4-C3	4.56	1.47	1.36
3	C	1402	2C8	C25-C20	4.55	1.49	1.39
3	B	1402	2C8	C25-C20	4.54	1.49	1.39
3	B	1402	2C8	C14-C17	4.38	1.48	1.39
3	A	1402	2C8	C25-C20	4.38	1.48	1.39
3	D	1402	2C8	C5-C6	4.35	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1402	2C8	C8-N1	4.32	1.39	1.33
3	D	1402	2C8	C5-C4	4.31	1.49	1.38
3	D	1402	2C8	C14-C17	4.30	1.48	1.39
3	B	1402	2C8	C5-C6	4.28	1.46	1.36
3	D	1402	2C8	C25-C20	4.14	1.48	1.39
3	D	1402	2C8	C13-C12	4.10	1.46	1.39
3	A	1402	2C8	C5-C6	4.08	1.46	1.36
3	B	1402	2C8	C13-C12	4.08	1.46	1.39
3	D	1402	2C8	C8-N1	4.03	1.39	1.33
3	B	1402	2C8	C15-C12	3.99	1.46	1.39
3	A	1402	2C8	C13-C12	3.98	1.46	1.39
3	A	1402	2C8	C2-C7	3.97	1.49	1.41
3	D	1402	2C8	C21-C20	3.87	1.47	1.39
3	D	1402	2C8	C14-C13	3.86	1.45	1.38
3	C	1402	2C8	C5-C4	3.86	1.48	1.38
3	C	1402	2C8	C6-C7	3.84	1.48	1.41
3	D	1402	2C8	C22-C21	3.83	1.47	1.38
3	B	1402	2C8	C21-C20	3.80	1.47	1.39
3	A	1402	2C8	C21-C20	3.76	1.47	1.39
3	C	1402	2C8	C21-C20	3.75	1.47	1.39
3	A	1402	2C8	C3-C2	3.70	1.48	1.41
3	A	1402	2C8	C15-C12	3.69	1.45	1.39
3	A	1402	2C8	C22-C21	3.67	1.46	1.38
3	B	1402	2C8	C24-C23	3.67	1.47	1.38
3	D	1402	2C8	C6-C7	3.65	1.48	1.41
3	A	1402	2C8	C24-C25	3.65	1.46	1.38
3	C	1402	2C8	C16-C17	3.63	1.47	1.39
3	B	1402	2C8	C22-C21	3.62	1.46	1.38
3	B	1402	2C8	C23-C22	3.60	1.47	1.38
3	B	1402	2C8	C16-C17	3.58	1.47	1.39
3	B	1402	2C8	C5-C4	3.56	1.47	1.38
3	C	1402	2C8	C14-C17	3.53	1.46	1.39
3	A	1402	2C8	C14-C13	3.52	1.45	1.38
3	C	1402	2C8	C15-C12	3.51	1.45	1.39
3	D	1402	2C8	C23-C22	3.50	1.47	1.38
3	B	1402	2C8	C1-N1	3.48	1.39	1.33
3	B	1402	2C8	C14-C13	3.46	1.45	1.38
3	C	1402	2C8	C13-C12	3.46	1.45	1.39
3	D	1402	2C8	C16-C17	3.43	1.46	1.39
3	A	1402	2C8	C14-C17	3.41	1.46	1.39
3	A	1402	2C8	C23-C22	3.39	1.47	1.38
3	A	1402	2C8	C5-C4	3.38	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1402	2C8	C24-C23	3.33	1.46	1.38
3	C	1402	2C8	C24-C23	3.27	1.46	1.38
3	A	1402	2C8	C10-C11	-3.25	1.45	1.51
3	B	1402	2C8	C16-C15	3.21	1.44	1.38
3	C	1402	2C8	C23-C22	3.20	1.46	1.38
3	C	1402	2C8	C16-C15	3.20	1.44	1.38
3	C	1402	2C8	C22-C21	3.15	1.45	1.38
3	C	1402	2C8	C3-C2	3.10	1.47	1.41
3	C	1402	2C8	C14-C13	3.08	1.44	1.38
3	B	1402	2C8	C24-C25	3.06	1.45	1.38
3	A	1402	2C8	C1-N1	3.02	1.38	1.33
3	B	1402	2C8	C8-N1	2.98	1.37	1.33
3	D	1402	2C8	C16-C15	2.92	1.44	1.38
3	D	1402	2C8	C3-C2	2.86	1.46	1.41
3	D	1402	2C8	C24-C25	2.86	1.44	1.38
3	A	1402	2C8	C16-C17	2.84	1.45	1.39
3	C	1402	2C8	C24-C25	2.79	1.44	1.38
3	D	1402	2C8	C1-N1	2.76	1.37	1.33
3	C	1402	2C8	C12-N3	-2.76	1.36	1.41
3	A	1402	2C8	C24-C23	2.71	1.45	1.38
3	C	1402	2C8	C1-N1	2.60	1.37	1.33
3	B	1402	2C8	C6-C7	2.54	1.46	1.41
3	A	1402	2C8	C16-C15	2.43	1.43	1.38
3	A	1402	2C8	C12-N3	-2.40	1.36	1.41
3	D	1402	2C8	C12-N3	-2.37	1.36	1.41
3	B	1402	2C8	C12-N3	-2.32	1.37	1.41
3	A	1402	2C8	C8-N1	2.27	1.36	1.33
3	A	1402	2C8	C6-C7	2.10	1.45	1.41
3	B	1402	2C8	C10-C11	-2.10	1.47	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1402	2C8	C8-N2-C7	13.07	125.40	116.54
3	A	1402	2C8	C8-N2-C7	13.00	125.35	116.54
3	D	1402	2C8	C8-N2-C7	12.61	125.09	116.54
3	B	1402	2C8	C8-N2-C7	11.50	124.34	116.54
3	C	1402	2C8	C2-C7-N2	-10.38	117.97	123.60
3	A	1402	2C8	C2-C7-N2	-9.04	118.69	123.60
3	D	1402	2C8	C2-C7-N2	-8.72	118.86	123.60
3	B	1402	2C8	C2-C1-N1	-8.04	118.80	124.40
3	B	1402	2C8	C2-C7-N2	-7.70	119.42	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1402	2C8	N2-C8-N1	-6.62	117.32	126.06
3	A	1402	2C8	N2-C8-N1	-6.15	117.95	126.06
3	C	1402	2C8	N2-C8-N1	-6.09	118.01	126.06
3	D	1402	2C8	N2-C8-N1	-6.07	118.04	126.06
3	D	1402	2C8	C1-C2-C7	-5.62	113.70	118.59
3	A	1402	2C8	C1-C2-C7	-5.59	113.72	118.59
3	C	1402	2C8	C9-C8-N1	5.18	124.60	116.67
3	C	1402	2C8	C2-C1-N1	-4.97	120.94	124.40
3	A	1402	2C8	C9-C8-N1	4.83	124.06	116.67
3	D	1402	2C8	C2-C1-N1	-4.35	121.37	124.40
3	A	1402	2C8	C3-C2-C1	4.32	127.96	121.61
3	C	1402	2C8	C1-C2-C7	-4.21	114.93	118.59
3	B	1402	2C8	C9-C8-N1	4.20	123.10	116.67
3	B	1402	2C8	C1-C2-C7	-4.20	114.94	118.59
3	B	1402	2C8	C20-C19-N5	4.13	131.11	124.12
3	D	1402	2C8	C3-C2-C1	4.10	127.62	121.61
3	B	1402	2C8	C17-C18-N4	3.68	130.36	124.12
3	C	1402	2C8	C17-C18-N4	3.55	130.13	124.12
3	C	1402	2C8	C20-C19-N5	3.48	130.02	124.12
3	A	1402	2C8	C17-C18-N4	3.46	129.99	124.12
3	D	1402	2C8	C9-C8-N1	3.42	121.91	116.67
3	D	1402	2C8	C17-C18-N4	3.24	129.60	124.12
3	C	1402	2C8	C3-C2-C1	3.16	126.24	121.61
3	D	1402	2C8	C20-C19-N5	3.08	129.33	124.12
3	A	1402	2C8	C2-C1-N1	-2.96	122.34	124.40
3	B	1402	2C8	C3-C2-C1	2.80	125.72	121.61
3	A	1402	2C8	C20-C19-N5	2.74	128.76	124.12
3	B	1402	2C8	O2-C11-N3	2.70	128.55	123.63
3	A	1402	2C8	O2-C11-N3	2.53	128.25	123.63
3	C	1402	2C8	O2-C11-N3	2.31	127.84	123.63
3	D	1402	2C8	O2-C11-N3	2.17	127.59	123.63
3	D	1402	2C8	C9-C8-N2	2.14	120.03	116.72
3	C	1402	2C8	C6-C7-N2	2.08	121.86	118.69
3	C	1402	2C8	C10-C11-N3	-2.05	110.98	114.59
3	B	1402	2C8	C10-C11-N3	-2.03	111.01	114.59

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1402	2C8	N1-C8-C9-C10
3	D	1402	2C8	N1-C8-C9-C10

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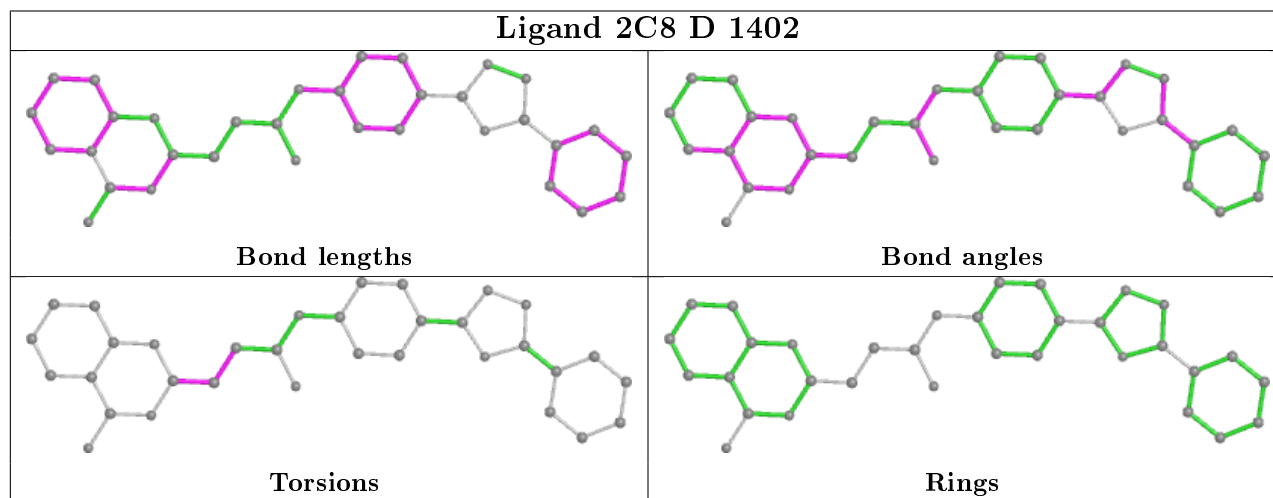
Mol	Chain	Res	Type	Atoms
3	D	1402	2C8	N2-C8-C9-C10
3	B	1402	2C8	N1-C8-C9-C10
3	A	1402	2C8	N1-C8-C9-C10
3	C	1402	2C8	N2-C8-C9-C10
3	D	1402	2C8	C11-C10-C9-C8
3	B	1402	2C8	C11-C10-C9-C8

There are no ring outliers.

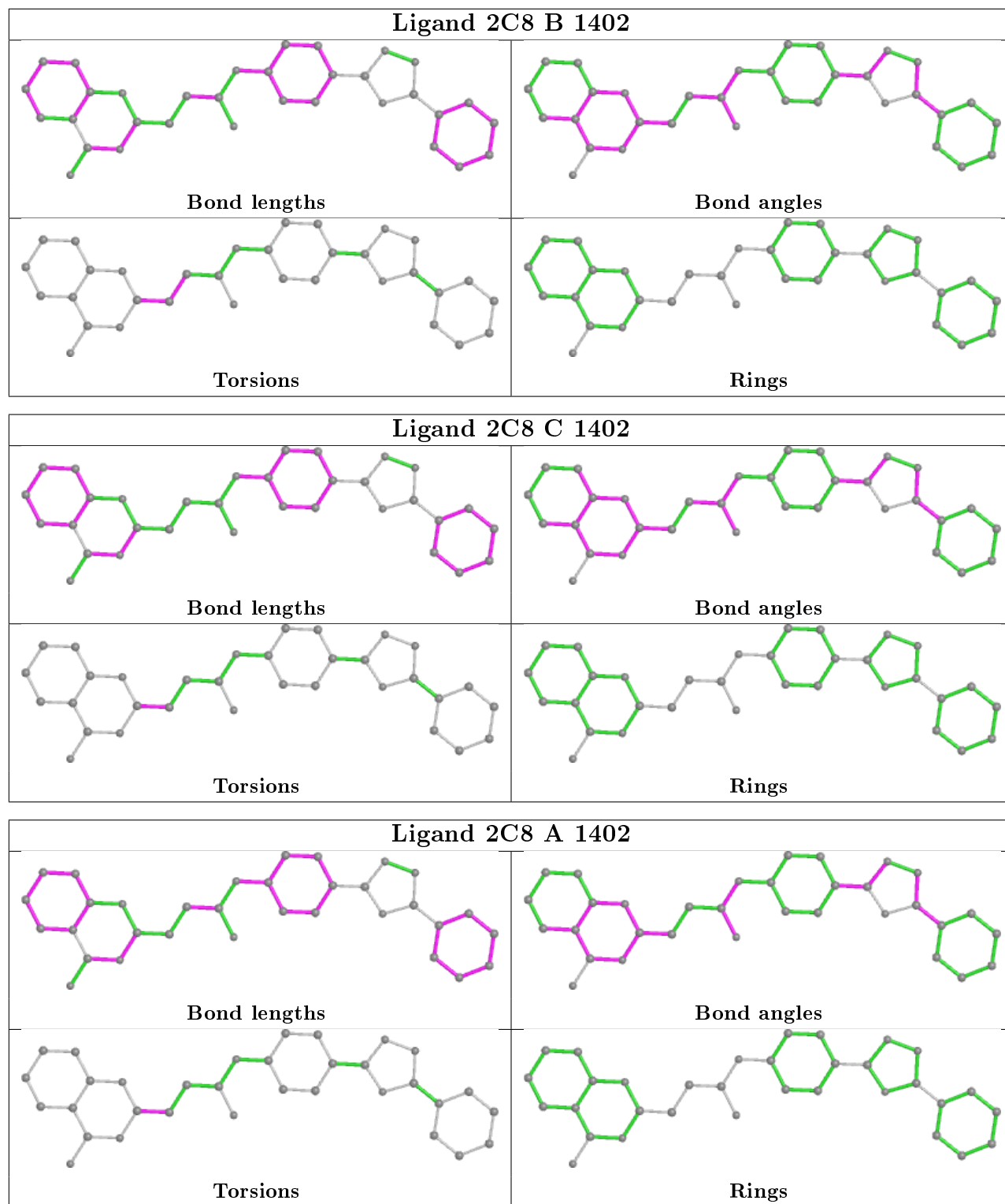
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1402	2C8	1	0
3	B	1402	2C8	1	0
3	C	1402	2C8	1	0
3	A	1402	2C8	2	0

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







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	211/217 (97%)	0.30	10 (4%) 31 38	19, 31, 52, 69	0
1	B	211/217 (97%)	0.22	11 (5%) 27 34	17, 30, 54, 71	0
1	C	200/217 (92%)	0.46	22 (11%) 5 7	19, 32, 57, 85	0
1	D	201/217 (92%)	0.64	19 (9%) 8 11	18, 31, 62, 88	0
All	All	823/868 (94%)	0.40	62 (7%) 14 19	17, 31, 56, 88	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1234	CYS	18.6
1	D	1236	THR	14.7
1	D	1237	HIS	11.2
1	C	1238	LYS	9.2
1	D	1238	LYS	8.9
1	D	1235	PRO	8.9
1	D	1138	ALA	8.3
1	D	1233	GLY	7.8
1	C	1237	HIS	7.7
1	A	1284	VAL	7.3
1	C	1135	GLY	6.9
1	C	1239	ASP	6.6
1	C	1240	ARG	6.4
1	A	1285	ASN	6.3
1	D	1239	ASP	6.1
1	D	1137	ASN	5.5
1	A	1283	SER	5.4
1	D	1104	GLN	5.2
1	C	1104	GLN	4.9
1	C	1241	SER	4.8
1	C	1227	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	1314	GLU	4.5
1	D	1226	TYR	4.5
1	B	1283	SER	4.4
1	D	1240	ARG	4.3
1	A	1314	GLU	4.2
1	B	1133	ARG	4.2
1	B	1314	GLU	4.2
1	B	1284	VAL	4.0
1	A	1133	ARG	4.0
1	C	1134	ASP	3.9
1	C	1226	TYR	3.8
1	D	1241	SER	3.8
1	D	1112	ALA	3.4
1	C	1116	LYS	3.3
1	C	1285	ASN	3.2
1	B	1104	GLN	3.2
1	B	1289	TYR	3.1
1	C	1313	PRO	3.1
1	A	1286	GLY	3.1
1	A	1289	TYR	2.9
1	B	1115	ASP	2.9
1	C	1138	ALA	2.7
1	C	1245	CYS	2.7
1	A	1287	LEU	2.7
1	D	1284	VAL	2.6
1	B	1250	LEU	2.5
1	B	1144	ARG	2.4
1	B	1282	PRO	2.4
1	D	1116	LYS	2.3
1	C	1300	ALA	2.3
1	C	1182	LEU	2.3
1	C	1284	VAL	2.3
1	A	1288	ALA	2.3
1	C	1283	SER	2.2
1	B	1263	PHE	2.2
1	D	1144	ARG	2.1
1	C	1112	ALA	2.1
1	A	1175	ASN	2.1
1	C	1286	GLY	2.1
1	D	1300	ALA	2.0
1	D	1312	LYS	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

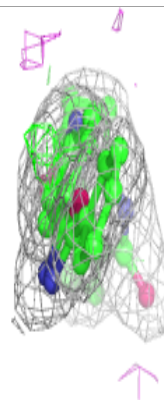
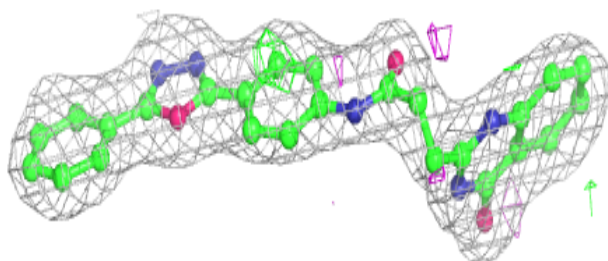
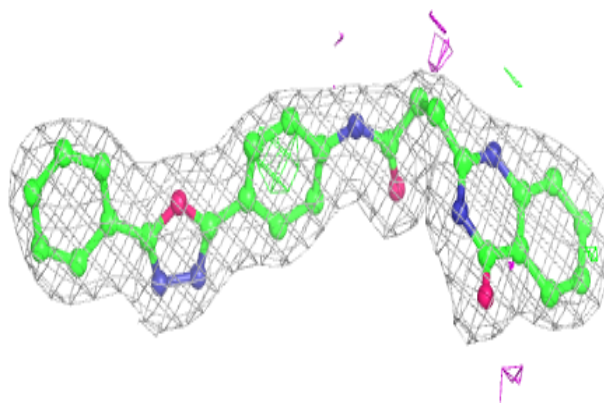
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	D	1401	1/1	0.47	0.44	175,175,175,175	0
2	ZN	C	1401	1/1	0.88	0.14	80,80,80,80	0
3	2C8	A	1402	33/33	0.92	0.15	21,23,25,26	0
3	2C8	C	1402	33/33	0.93	0.12	19,22,25,26	0
3	2C8	D	1402	33/33	0.94	0.12	22,24,26,26	0
2	ZN	A	1401	1/1	0.95	0.08	42,42,42,42	0
3	2C8	B	1402	33/33	0.95	0.13	21,23,27,28	0
2	ZN	B	1401	1/1	0.96	0.06	40,40,40,40	0

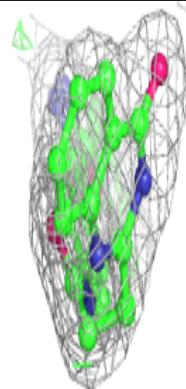
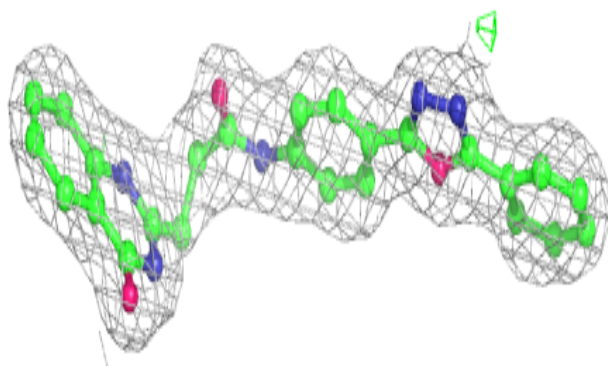
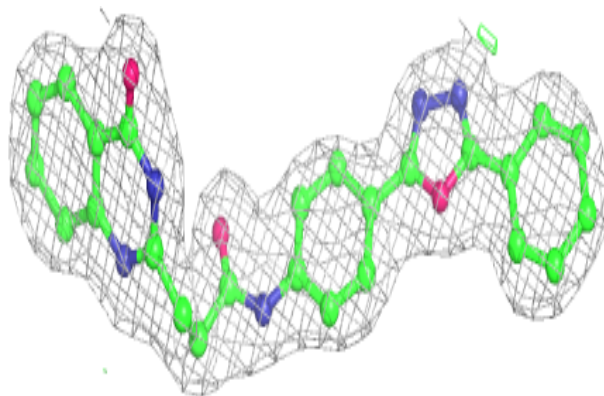
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

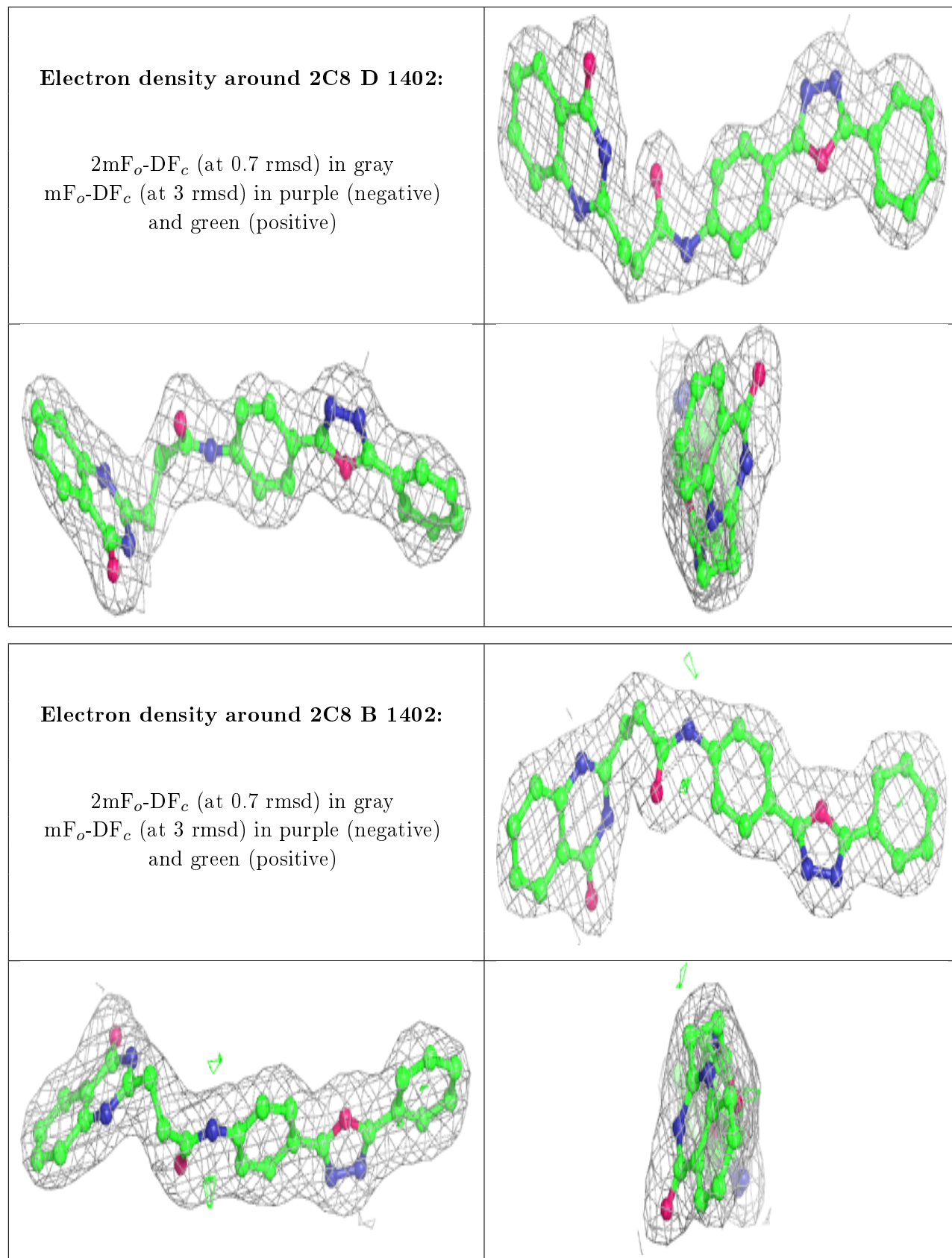
**Electron density around 2C8 A 1402:**

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

**Electron density around 2C8 C 1402:**

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





## 6.5 Other polymers

There are no such residues in this entry.