



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 04:46 pm GMT

PDB ID : 4Z4Q  
Title : Quinazolinedione(PD 0305970)-DNA cleavage complex of topoisomerase IV from *S. pneumoniae*  
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Selvarajah, J.; Crevel, I.M.-T.; Fisher, L.M.; Sanderson, M.R.  
Deposited on : 2015-04-02  
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

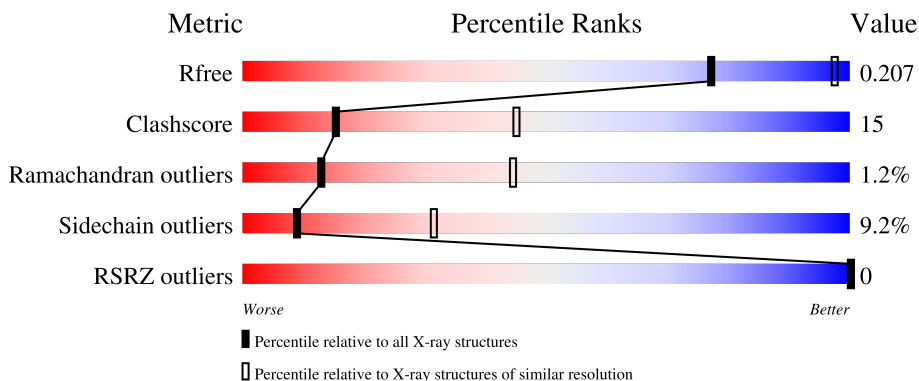
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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.



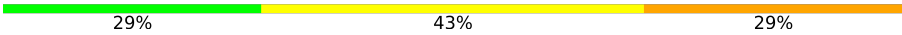
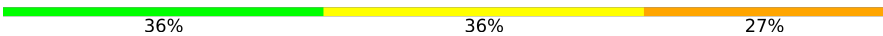
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	742	 67% 23% 7%
1	B	742	 68% 24% 5%
2	E	7	 29% 43% 29%
3	F	11	 45% 36% 18%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	G	7	
5	H	11	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	B	1502	-	-	-	X
7	PDQ	H	101	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11338 atoms, of which 48 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 DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	690	5215	3308	905	983	19	0	0	0
1	B	708	5292	3362	909	1002	19	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	expression tag	UNP Q59961
A	460	ILE	VAL	conflict	UNP Q59961
A	996	ALA	-	linker	UNP Q59961
A	997	THR	-	linker	UNP Q59961
A	998	VAL	-	linker	UNP Q59961
A	999	PHE	-	linker	UNP Q59961
A	1000	HIS	-	linker	UNP Q59961
A	1001	MET	-	linker	UNP Q59961
A	1002	SER	-	linker	UNP Q59961
A	1257	THR	ILE	conflict	UNP P72525
A	1485	THR	-	expression tag	UNP P72525
A	1486	ALA	-	expression tag	UNP P72525
A	1487	LYS	-	expression tag	UNP P72525
A	1488	ALA	-	expression tag	UNP P72525
A	1489	LEU	-	expression tag	UNP P72525
A	1490	GLU	-	expression tag	UNP P72525
A	1491	HIS	-	expression tag	UNP P72525
A	1492	HIS	-	expression tag	UNP P72525
A	1493	HIS	-	expression tag	UNP P72525
A	1494	HIS	-	expression tag	UNP P72525
A	1495	HIS	-	expression tag	UNP P72525
A	1496	HIS	-	expression tag	UNP P72525
B	403	MET	-	expression tag	UNP Q59961
B	460	ILE	VAL	conflict	UNP Q59961

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	996	ALA	-	linker	UNP Q59961
B	997	THR	-	linker	UNP Q59961
B	998	VAL	-	linker	UNP Q59961
B	999	PHE	-	linker	UNP Q59961
B	1000	HIS	-	linker	UNP Q59961
B	1001	MET	-	linker	UNP Q59961
B	1002	SER	-	linker	UNP Q59961
B	1257	THR	ILE	conflict	UNP P72525
B	1485	THR	-	expression tag	UNP P72525
B	1486	ALA	-	expression tag	UNP P72525
B	1487	LYS	-	expression tag	UNP P72525
B	1488	ALA	-	expression tag	UNP P72525
B	1489	LEU	-	expression tag	UNP P72525
B	1490	GLU	-	expression tag	UNP P72525
B	1491	HIS	-	expression tag	UNP P72525
B	1492	HIS	-	expression tag	UNP P72525
B	1493	HIS	-	expression tag	UNP P72525
B	1494	HIS	-	expression tag	UNP P72525
B	1495	HIS	-	expression tag	UNP P72525
B	1496	HIS	-	expression tag	UNP P72525

- Molecule 2 is a DNA chain called V-site DNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				P
2	E	7	138	67	27	38	6	0	0	0

- Molecule 3 is a DNA chain called V-site DNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				P
3	F	11	220	104	40	65	11	0	0	0

- Molecule 4 is a DNA chain called V-site DNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				P
4	G	7	140	67	26	41	6	0	0	0

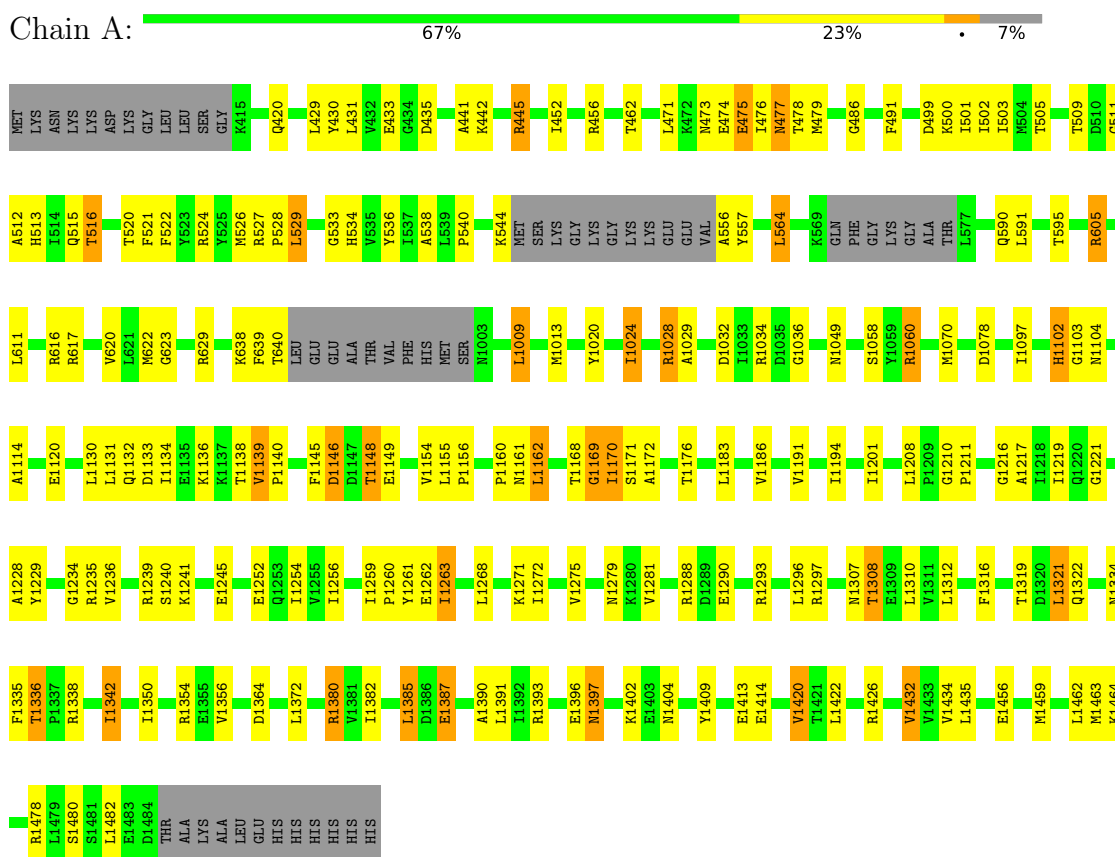
- Molecule 5 is a DNA chain called V-site DNA.



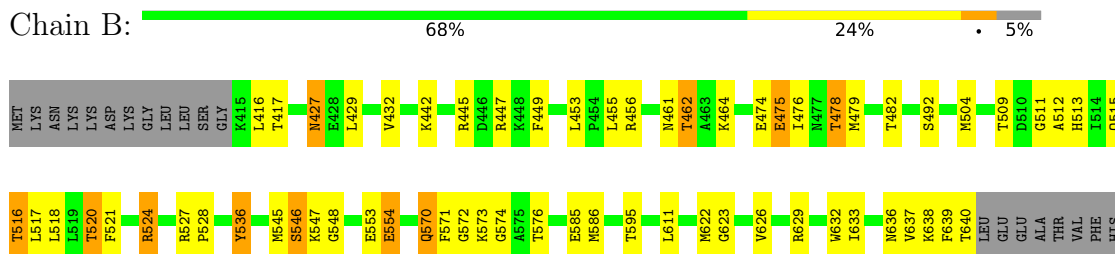
### 3 Residue-property plots

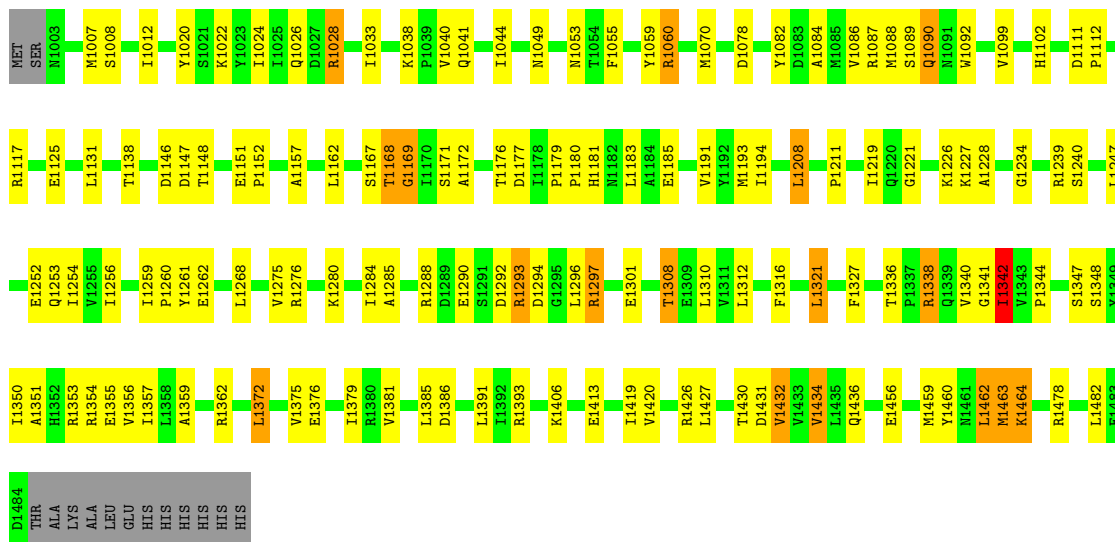
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A

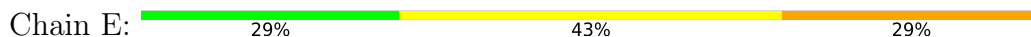


- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A





- Molecule 2: V-site DNA



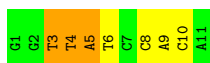
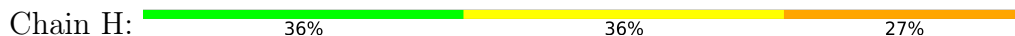
- Molecule 3: V-site DNA



- Molecule 4: V-site DNA



- Molecule 5: V-site DNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.02Å 158.02Å 211.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.59 – 3.04 44.59 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.59-3.04) 95.7 (44.59-2.88)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.162 , 0.205 0.164 , 0.207	Depositor DCC
$R_{free}$ test set	3369 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtrriage
Anisotropy	0.435	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11338	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.51	0/5302	0.68	2/7196 (0.0%)
1	B	0.48	0/5382	0.66	1/7313 (0.0%)
2	E	1.13	1/155 (0.6%)	2.10	4/237 (1.7%)
3	F	1.10	0/246	2.03	10/375 (2.7%)
4	G	0.90	0/157	1.90	8/241 (3.3%)
5	H	0.99	1/247 (0.4%)	1.87	8/377 (2.1%)
All	All	0.55	2/11489 (0.0%)	0.85	33/15739 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	13	DT	N1-C2	5.77	1.42	1.38
5	H	4	DT	C3'-O3'	-5.00	1.37	1.44

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	13	DT	N3-C2-O2	-12.99	114.51	122.30
3	F	3	DC	O4'-C4'-C3'	-9.96	100.02	106.00
3	F	6	DT	O4'-C4'-C3'	-9.75	100.15	106.00
5	H	10	DC	O4'-C4'-C3'	-9.22	100.47	106.00
2	E	13	DT	N1-C2-O2	8.59	129.97	123.10
3	F	7	DA	N1-C6-N6	8.55	123.73	118.60
3	F	6	DT	O4'-C1'-N1	8.06	113.65	108.00
5	H	3	DT	O4'-C4'-C3'	-7.94	101.24	106.00
1	A	1183	LEU	CA-CB-CG	7.52	132.60	115.30
4	G	14	DA	O4'-C4'-C3'	-7.29	101.58	104.50
3	F	7	DA	C5-C6-N6	-7.28	117.87	123.70
5	H	10	DC	C1'-O4'-C4'	-7.20	102.90	110.10
3	F	8	DT	C5-C4-O4	-7.04	119.97	124.90

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	DA	O4'-C1'-N9	6.79	112.75	108.00
2	E	12	DA	O4'-C1'-C2'	-6.74	100.51	105.90
4	G	11	DT	O4'-C1'-N1	6.67	112.67	108.00
3	F	6	DT	C4'-C3'-C2'	-6.54	97.22	103.10
2	E	14	DA	O4'-C4'-C3'	-6.53	101.89	104.50
3	F	8	DT	N3-C4-O4	6.37	123.72	119.90
5	H	6	DT	O4'-C4'-C3'	-6.32	101.97	104.50
5	H	4	DT	O4'-C1'-N1	6.14	112.30	108.00
4	G	15	DT	C5-C4-O4	-5.90	120.77	124.90
5	H	3	DT	O4'-C1'-N1	5.89	112.12	108.00
4	G	15	DT	N3-C4-O4	5.86	123.42	119.90
5	H	5	DA	O4'-C1'-N9	5.76	112.03	108.00
5	H	8	DC	O4'-C1'-N1	5.75	112.03	108.00
1	B	1463	MET	CG-SD-CE	-5.56	91.31	100.20
4	G	9	DT	N3-C4-O4	5.39	123.14	119.90
4	G	15	DT	P-O5'-C5'	-5.36	112.33	120.90
4	G	13	DG	C5-N7-C8	-5.11	101.75	104.30
1	A	1170	ILE	CB-CA-C	-5.08	101.44	111.60
4	G	15	DT	O4'-C1'-N1	5.06	111.54	108.00
3	F	5	DG	O4'-C4'-C3'	5.02	109.01	106.00

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	5215	0	4973	142	0
1	B	5292	0	5005	162	0
2	E	138	0	72	2	0
3	F	220	0	116	3	0
4	G	140	0	70	1	0
5	H	221	0	116	4	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	F	26	24	24	6	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	26	24	24	10	0
8	A	5	0	0	0	0
8	B	3	0	0	1	0
All	All	11290	48	10400	320	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (320) 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:A:1028:ARG:HG3	1:A:1028:ARG:HH11	1.07	1.11
1:B:1028:ARG:HG3	1:B:1028:ARG:HH11	1.14	1.06
1:B:1070:MET:HE1	1:B:1078:ASP:HB3	1.40	1.04
1:A:1070:MET:HE1	1:A:1078:ASP:HB3	1.42	1.00
1:A:1235:ARG:NH2	3:F:11:DC:O3'	1.95	0.99
1:B:546:SER:CB	1:B:547:LYS:HA	1.93	0.99
1:A:520:THR:HG21	1:A:622:MET:HG3	1.50	0.94
1:B:478:THR:O	1:B:482:THR:HG23	1.70	0.92
1:B:524:ARG:HH11	1:B:524:ARG:HB3	1.37	0.90
1:B:1146:ASP:HB3	1:B:1148:THR:HG23	1.55	0.88
1:B:1194:ILE:HD13	1:B:1463:MET:HE2	1.55	0.88
1:A:1396:GLU:O	1:A:1397:ASN:HB3	1.75	0.87
7:F:101:PDQ:H29	7:F:101:PDQ:C18	2.04	0.87
1:A:1288:ARG:NH1	1:A:1290:GLU:OE2	2.08	0.87
1:B:524:ARG:HH11	1:B:524:ARG:CB	1.86	0.87
1:B:474:GLU:O	1:B:478:THR:HG23	1.75	0.86
1:B:1254:ILE:HD13	1:B:1312:LEU:HD13	1.56	0.86
1:A:1060:ARG:HH11	1:A:1060:ARG:CG	1.88	0.86
1:B:1169:GLY:HA2	1:B:1176:THR:HG22	1.57	0.85
1:B:1288:ARG:NH1	1:B:1290:GLU:OE2	2.10	0.84
1:B:546:SER:CB	1:B:547:LYS:CA	2.55	0.84
1:A:1060:ARG:HH11	1:A:1060:ARG:HG3	1.43	0.83
1:A:1169:GLY:HA2	1:A:1176:THR:HG22	1.59	0.83
7:H:101:PDQ:H29	7:H:101:PDQ:C18	2.09	0.82
1:B:1194:ILE:CD1	1:B:1463:MET:HE2	2.10	0.81
1:A:1028:ARG:HH11	1:A:1028:ARG:CG	1.93	0.80
1:B:1256:ILE:HD13	1:B:1321:LEU:HD21	1.62	0.80
1:A:1028:ARG:HG3	1:A:1028:ARG:NH1	1.89	0.80
1:A:1271:LYS:HE3	1:A:1319:THR:HB	1.65	0.78
1:B:1169:GLY:CA	1:B:1176:THR:HG22	2.14	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1194:ILE:HD11	1:B:1463:MET:HE1	1.64	0.77
1:A:471:LEU:O	1:A:477:ASN:ND2	2.19	0.76
1:B:611:LEU:HD13	1:B:611:LEU:O	1.83	0.76
1:B:1194:ILE:HD11	1:B:1463:MET:CE	2.16	0.76
1:A:623:GLY:O	1:A:629:ARG:NH2	2.17	0.75
1:B:456:ARG:HB2	7:H:101:PDQ:N51	2.01	0.75
1:A:1296:LEU:HD23	1:A:1297:ARG:N	2.00	0.75
1:A:1350:ILE:HA	1:A:1463:MET:HE1	1.70	0.74
1:B:1194:ILE:HG13	1:B:1350:ILE:HD13	1.68	0.73
1:B:516:THR:O	1:B:520:THR:HG23	1.89	0.72
1:A:529:LEU:HD22	1:A:534:HIS:HB2	1.72	0.72
1:A:1296:LEU:HD23	1:A:1296:LEU:C	2.10	0.72
1:B:1194:ILE:CD1	1:B:1463:MET:CE	2.68	0.72
1:A:1191:VAL:HG13	1:A:1464:LYS:HG2	1.70	0.71
1:A:1171:SER:OG	1:A:1172:ALA:N	2.22	0.71
1:B:1146:ASP:HB3	1:B:1148:THR:CG2	2.22	0.69
1:B:456:ARG:HB2	7:H:101:PDQ:HN51	1.57	0.68
1:A:1391:LEU:HD21	1:A:1404:ASN:HB3	1.75	0.68
1:A:1146:ASP:HB3	1:A:1148:THR:OG1	1.93	0.68
1:B:1044:ILE:HG21	1:B:1088:MET:HE1	1.74	0.68
1:A:1396:GLU:O	1:A:1397:ASN:CB	2.42	0.68
1:B:623:GLY:O	1:B:629:ARG:NH2	2.26	0.68
1:B:570:GLN:O	1:B:572:GLY:N	2.27	0.68
1:A:1239:ARG:HB2	1:A:1322:GLN:HG3	1.74	0.67
1:B:1431:ASP:CG	1:B:1434:VAL:HG12	2.15	0.67
1:A:1132:GLN:O	1:A:1133:ASP:HB2	1.96	0.66
1:B:513:HIS:HB2	1:B:1020:TYR:CD1	2.31	0.66
1:A:475:GLU:OE1	7:F:101:PDQ:N51	2.27	0.65
1:B:1028:ARG:NH1	8:B:1601:HOH:O	2.29	0.65
1:B:524:ARG:HH11	1:B:524:ARG:CG	2.07	0.65
1:B:1239:ARG:NH1	1:B:1316:PHE:CE2	2.64	0.65
1:A:500:LYS:HG2	1:A:536:TYR:CE1	2.31	0.65
1:A:486:GLY:O	1:A:491:PHE:HD1	1.79	0.65
7:F:101:PDQ:H29	7:F:101:PDQ:C20	2.27	0.65
1:A:1139:VAL:HG22	1:A:1154:VAL:HG13	1.79	0.64
1:B:1007:MET:HB3	1:B:1012:ILE:CG1	2.27	0.64
1:A:1169:GLY:CA	1:A:1176:THR:HG22	2.27	0.64
1:B:520:THR:HG21	1:B:622:MET:HG3	1.80	0.64
7:H:101:PDQ:H29	7:H:101:PDQ:C20	2.26	0.64
1:A:1256:ILE:HD13	1:A:1321:LEU:HD21	1.79	0.64
1:A:1252:GLU:OE1	1:A:1308:THR:HG21	1.98	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ARG:NH1	1:A:605:ARG:HG3	2.14	0.63
1:B:1028:ARG:HG3	1:B:1028:ARG:NH1	1.95	0.63
1:A:557:TYR:OH	1:A:590:GLN:HG2	1.98	0.63
1:A:1316:PHE:CE1	1:A:1321:LEU:HD13	2.34	0.63
1:A:605:ARG:HG3	1:A:605:ARG:HH11	1.64	0.62
1:B:611:LEU:HD13	1:B:611:LEU:C	2.20	0.62
1:B:1341:GLY:O	1:B:1344:PRO:HD2	2.00	0.62
1:B:524:ARG:HB3	1:B:524:ARG:NH1	2.10	0.62
1:A:1024:ILE:HD11	1:A:1028:ARG:NE	2.15	0.61
1:B:516:THR:CG2	1:B:622:MET:CE	2.79	0.61
5:H:4:DT:H2''	5:H:5:DA:H5''	1.80	0.61
1:A:516:THR:O	1:A:520:THR:HG23	2.01	0.61
1:B:1028:ARG:HH11	1:B:1028:ARG:CG	2.00	0.60
1:B:545:MET:O	1:B:546:SER:O	2.19	0.60
1:B:1185:GLU:OE1	1:B:1478:ARG:NH1	2.33	0.60
1:B:1391:LEU:C	1:B:1391:LEU:HD23	2.21	0.60
7:F:101:PDQ:H29	7:F:101:PDQ:H18	1.83	0.60
1:B:1252:GLU:OE1	1:B:1308:THR:HG21	2.01	0.60
1:B:1070:MET:CE	1:B:1078:ASP:HB3	2.24	0.60
1:B:1359:ALA:HA	1:B:1362:ARG:NH1	2.16	0.60
1:B:1296:LEU:HD23	1:B:1297:ARG:N	2.17	0.59
1:A:1350:ILE:HG23	1:A:1463:MET:CE	2.32	0.59
1:B:1167:SER:C	1:B:1168:THR:HG22	2.22	0.59
1:B:1211:PRO:O	1:B:1478:ARG:NH2	2.36	0.59
5:H:3:DT:H4'	5:H:4:DT:OP1	2.02	0.59
1:A:1060:ARG:CG	1:A:1060:ARG:NH1	2.59	0.59
1:B:513:HIS:O	1:B:516:THR:HB	2.03	0.59
1:B:633:ILE:HG23	1:B:637:VAL:HG21	1.84	0.58
1:A:638:LYS:C	1:A:640:THR:H	2.06	0.58
1:A:1434:VAL:HG13	1:A:1435:LEU:N	2.17	0.58
4:G:13:DG:H2''	4:G:14:DA:O5'	2.03	0.58
1:B:1375:VAL:O	1:B:1379:ILE:HG13	2.04	0.58
1:B:1191:VAL:HG13	1:B:1464:LYS:HG2	1.84	0.58
1:A:431:LEU:HD12	1:A:503:ILE:HG12	1.86	0.58
1:A:1254:ILE:HD13	1:A:1312:LEU:HD13	1.85	0.58
1:A:1382:ILE:HD12	1:A:1432:VAL:HG23	1.86	0.58
1:B:1357:ILE:HD12	1:B:1463:MET:HG3	1.86	0.58
1:A:1060:ARG:HG3	1:A:1060:ARG:NH1	2.17	0.57
1:A:1259:ILE:HD12	1:A:1263:ILE:HG22	1.86	0.57
1:A:509:THR:O	1:A:512:ALA:HB3	2.04	0.57
1:A:527:ARG:N	1:A:528:PRO:CD	2.68	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1390:ALA:O	1:A:1393:ARG:HB3	2.03	0.57
1:B:1381:VAL:CG2	1:B:1419:ILE:HD13	2.34	0.57
1:B:1022:LYS:HE2	1:B:1026:GLN:HE22	1.70	0.57
1:B:1194:ILE:HG13	1:B:1350:ILE:CD1	2.32	0.57
2:E:13:DT:H2''	2:E:14:DA:O5'	2.04	0.56
1:A:1169:GLY:HA3	1:A:1176:THR:O	2.05	0.56
1:A:1211:PRO:O	1:A:1478:ARG:NH2	2.39	0.56
1:B:1169:GLY:HA3	1:B:1176:THR:O	2.05	0.56
1:B:1022:LYS:HE2	1:B:1026:GLN:NE2	2.21	0.56
1:A:1380:ARG:NH2	1:A:1409:TYR:O	2.26	0.56
1:B:1261:TYR:CD2	1:B:1262:GLU:HG3	2.41	0.55
1:A:511:GLY:O	1:A:515:GLN:HG3	2.06	0.55
1:A:1245:GLU:OE2	1:A:1297:ARG:NH2	2.40	0.55
1:A:1160:PRO:HG2	1:A:1186:VAL:HG11	1.88	0.54
7:H:101:PDQ:H29B	7:H:101:PDQ:C34	2.37	0.54
1:A:442:LYS:O	1:A:445:ARG:HD3	2.07	0.54
1:B:509:THR:O	1:B:512:ALA:HB3	2.07	0.54
1:A:1402:LYS:HE3	1:A:1413:GLU:OE1	2.07	0.54
1:A:1049:ASN:HB2	1:A:1131:LEU:HD13	1.89	0.54
1:B:1171:SER:OG	1:B:1172:ALA:N	2.40	0.54
1:A:513:HIS:HB2	1:A:1020:TYR:CD1	2.42	0.53
1:A:1261:TYR:CD2	1:A:1262:GLU:HG3	2.43	0.53
1:A:433:GLU:HB2	1:A:505:THR:HG22	1.90	0.53
1:A:1160:PRO:HG2	1:A:1186:VAL:CG1	2.38	0.53
1:A:513:HIS:O	1:A:516:THR:HB	2.08	0.53
1:B:475:GLU:O	1:B:479:MET:HG3	2.08	0.53
1:B:516:THR:O	1:B:520:THR:CG2	2.56	0.53
1:A:1350:ILE:HG23	1:A:1463:MET:HE2	1.89	0.53
1:B:632:TRP:CE2	1:B:636:ASN:ND2	2.77	0.53
1:B:638:LYS:C	1:B:640:THR:H	2.13	0.53
1:B:476:ILE:HD12	1:B:521:PHE:CE1	2.43	0.53
1:B:1020:TYR:CE2	1:B:1024:ILE:HD13	2.44	0.53
7:H:101:PDQ:H29	7:H:101:PDQ:H18	1.91	0.52
1:B:1008:SER:O	1:B:1012:ILE:HG13	2.09	0.52
1:B:1193:MET:HE1	1:B:1347:SER:HB3	1.90	0.52
1:A:1024:ILE:HD11	1:A:1028:ARG:CZ	2.39	0.52
1:A:476:ILE:HD12	1:A:521:PHE:CE1	2.45	0.52
1:B:516:THR:HG22	1:B:517:LEU:N	2.24	0.52
1:A:430:TYR:CE1	1:A:502:ILE:HD12	2.45	0.52
1:A:1354:ARG:NE	1:A:1456:GLU:OE1	2.33	0.52
1:B:1146:ASP:O	1:B:1147:ASP:HB2	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1247:LEU:HD11	1:B:1253:GLN:HB2	1.92	0.51
1:A:564:LEU:HD22	1:A:564:LEU:O	2.09	0.51
1:A:1219:ILE:HB	1:A:1482:LEU:HD23	1.93	0.51
1:A:1350:ILE:HG12	1:A:1463:MET:HE2	1.93	0.51
1:A:1434:VAL:CG1	1:A:1435:LEU:N	2.73	0.51
1:A:1216:GLY:O	1:A:1217:ALA:HB3	2.10	0.51
1:B:511:GLY:O	1:B:515:GLN:HG3	2.11	0.51
1:B:1259:ILE:HB	1:B:1260:PRO:CD	2.40	0.51
1:B:1432:VAL:O	1:B:1436:GLN:HG3	2.11	0.51
1:B:1355:GLU:OE2	1:B:1355:GLU:HA	2.10	0.50
1:A:1296:LEU:C	1:A:1296:LEU:CD2	2.78	0.50
1:B:516:THR:CG2	1:B:622:MET:HE2	2.42	0.50
1:B:1082:TYR:O	1:B:1086:VAL:HG23	2.11	0.50
1:B:1219:ILE:HB	1:B:1482:LEU:HD23	1.93	0.50
1:A:1391:LEU:HD21	1:A:1404:ASN:CB	2.42	0.50
1:A:605:ARG:HH11	1:A:605:ARG:CG	2.23	0.50
1:B:1193:MET:CE	1:B:1347:SER:HB3	2.42	0.50
1:A:1070:MET:HE1	1:A:1078:ASP:CB	2.28	0.50
1:B:1296:LEU:HD23	1:B:1296:LEU:C	2.32	0.50
1:B:1285:ALA:HB3	1:B:1301:GLU:O	2.12	0.49
1:A:564:LEU:O	1:A:564:LEU:CD2	2.60	0.49
1:B:476:ILE:HD12	1:B:521:PHE:CD1	2.48	0.49
2:E:9:DG:H1'	2:E:10:DT:H5''	1.93	0.49
1:B:1040:VAL:HG13	1:B:1041:GLN:N	2.27	0.49
1:A:1393:ARG:NH1	1:B:1386:ASP:OD1	2.39	0.49
1:A:441:ALA:HB1	1:A:452:ILE:HD12	1.94	0.49
1:A:1104:ASN:HB3	1:A:1114:ALA:HB2	1.94	0.49
7:F:101:PDQ:H29B	7:F:101:PDQ:C34	2.43	0.49
1:B:1084:ALA:O	1:B:1088:MET:HG3	2.13	0.48
1:B:1275:VAL:HG13	1:B:1280:LYS:HB2	1.94	0.48
1:A:1170:ILE:O	1:A:1170:ILE:HG22	2.12	0.48
1:B:1240:SER:OG	1:B:1321:LEU:HD22	2.13	0.48
1:A:1240:SER:OG	1:A:1260:PRO:HD3	2.14	0.48
1:B:524:ARG:CG	1:B:524:ARG:NH1	2.72	0.48
1:A:533:GLY:HA3	1:A:605:ARG:HE	1.78	0.48
1:B:1342:ILE:HD12	1:B:1342:ILE:HA	1.60	0.48
1:A:1259:ILE:HB	1:A:1260:PRO:CD	2.43	0.48
1:A:1350:ILE:HG12	1:A:1463:MET:CE	2.43	0.48
1:B:1406:LYS:HE2	1:B:1413:GLU:HA	1.96	0.48
1:A:1259:ILE:HB	1:A:1260:PRO:HD2	1.96	0.47
1:A:433:GLU:OE2	1:A:505:THR:HB	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1055:PHE:CD2	1:B:1125:GLU:HB2	2.49	0.47
1:B:1038:LYS:NZ	1:B:1168:THR:O	2.46	0.47
1:A:1138:THR:HB	1:A:1356:VAL:HG13	1.96	0.47
1:B:1169:GLY:HA3	1:B:1176:THR:HG22	1.93	0.47
1:B:548:GLY:HA3	1:B:553:GLU:HA	1.97	0.47
1:B:1276:ARG:HB2	1:B:1284:ILE:HG21	1.96	0.47
1:A:526:MET:HE1	1:A:529:LEU:HD12	1.97	0.47
1:B:432:VAL:HG22	1:B:504:MET:CE	2.45	0.47
1:B:462:THR:HG21	1:B:521:PHE:HD1	1.78	0.47
1:A:1049:ASN:CB	1:A:1131:LEU:HD13	2.44	0.47
1:B:1020:TYR:CZ	1:B:1024:ILE:HD13	2.50	0.47
1:A:1272:ILE:O	1:A:1275:VAL:HB	2.15	0.46
1:A:1097:ILE:O	1:A:1097:ILE:HG13	2.14	0.46
1:B:1044:ILE:CG2	1:B:1088:MET:HE1	2.41	0.46
1:A:1316:PHE:HE1	1:A:1321:LEU:HD13	1.80	0.46
1:B:516:THR:HG22	1:B:622:MET:CE	2.45	0.46
1:B:1179:PRO:HG3	1:B:1327:PHE:CE2	2.50	0.46
1:A:474:GLU:O	1:A:478:THR:HG23	2.15	0.46
1:B:527:ARG:N	1:B:528:PRO:CD	2.78	0.46
1:B:1033:ILE:HG12	1:B:1033:ILE:O	2.14	0.46
1:B:1053:ASN:ND2	1:B:1060:ARG:HD2	2.31	0.46
1:A:616:ARG:O	1:A:620:VAL:HG23	2.16	0.46
1:B:1292:ASP:O	1:B:1294:ASP:N	2.48	0.46
1:A:520:THR:CG2	1:A:622:MET:HG3	2.35	0.46
1:B:1040:VAL:CG1	1:B:1041:GLN:N	2.79	0.46
1:A:1029:ALA:HB3	1:A:1171:SER:HB2	1.97	0.46
1:A:1201:ILE:HD12	1:A:1201:ILE:H	1.81	0.46
1:B:1456:GLU:HG3	1:B:1460:TYR:CE2	2.50	0.46
7:H:101:PDQ:C34	7:H:101:PDQ:C29	2.94	0.46
1:B:516:THR:HG22	1:B:622:MET:HE2	1.97	0.46
1:B:1007:MET:HB3	1:B:1012:ILE:HG13	1.97	0.46
1:A:1136:LYS:HE2	1:A:1364:ASP:OD1	2.16	0.45
1:B:1430:THR:HG23	1:B:1430:THR:O	2.16	0.45
7:F:101:PDQ:C20	7:F:101:PDQ:C29	2.94	0.45
1:B:626:VAL:HG11	5:H:9:DA:H3'	1.99	0.45
1:B:1426:ARG:HA	1:B:1426:ARG:HD3	1.79	0.45
1:B:475:GLU:OE2	7:H:101:PDQ:H47	2.17	0.45
1:B:520:THR:O	1:B:524:ARG:HG2	2.17	0.45
7:H:101:PDQ:C20	7:H:101:PDQ:C29	2.94	0.45
1:B:476:ILE:HG23	1:B:521:PHE:CE1	2.51	0.45
1:B:1462:LEU:HA	1:B:1462:LEU:HD23	1.66	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:TYR:CD1	1:B:536:TYR:N	2.84	0.45
1:B:1181:HIS:HD2	1:B:1208:LEU:HD21	1.81	0.45
1:B:1087:ARG:HA	1:B:1090:GLN:HG3	1.99	0.44
1:A:1426:ARG:HA	1:A:1426:ARG:HD3	1.60	0.44
1:A:544:LYS:HA	1:A:556:ALA:O	2.17	0.44
1:A:1350:ILE:CA	1:A:1463:MET:HE1	2.43	0.44
1:B:1431:ASP:CG	1:B:1434:VAL:CG1	2.85	0.44
1:A:538:ALA:O	1:A:540:PRO:HD3	2.18	0.44
1:A:1334:ASN:O	1:A:1336:THR:HG23	2.18	0.44
1:B:1239:ARG:NH1	1:B:1316:PHE:CD2	2.86	0.44
1:B:1431:ASP:OD1	1:B:1434:VAL:HG12	2.17	0.44
1:A:1354:ARG:HG3	1:A:1459:MET:CE	2.48	0.44
1:B:1049:ASN:CB	1:B:1131:LEU:HD13	2.48	0.43
1:B:1157:ALA:O	1:B:1353:ARG:HD3	2.17	0.43
1:A:526:MET:C	1:A:528:PRO:HD2	2.38	0.43
1:B:1168:THR:HA	1:B:1176:THR:O	2.19	0.43
7:H:101:PDQ:H29B	7:H:101:PDQ:H34	1.99	0.43
1:A:1387:GLU:OE2	1:A:1387:GLU:N	2.51	0.43
1:A:475:GLU:H	1:A:475:GLU:HG2	1.48	0.43
1:A:1103:GLY:HA2	1:B:586:MET:O	2.19	0.43
1:A:1139:VAL:HG22	1:A:1140:PRO:HD2	2.01	0.43
1:A:1194:ILE:HG13	1:A:1350:ILE:CD1	2.49	0.43
1:A:1145:PHE:CD1	1:A:1146:ASP:N	2.87	0.43
1:A:1009:LEU:HD22	1:A:1013:MET:HG3	2.01	0.43
1:A:1217:ALA:O	1:A:1480:SER:HA	2.19	0.43
1:B:455:LEU:HD13	1:B:518:LEU:HD11	2.00	0.43
1:A:1342:ILE:HA	1:A:1342:ILE:HD12	1.50	0.42
1:B:1090:GLN:HB3	1:B:1092:TRP:CH2	2.54	0.42
1:A:1210:GLY:HA2	1:A:1229:TYR:OH	2.19	0.42
1:A:1334:ASN:O	1:A:1335:PHE:HB2	2.18	0.42
1:B:432:VAL:HG22	1:B:504:MET:HE1	2.01	0.42
1:B:546:SER:O	1:B:554:GLU:O	2.37	0.42
1:B:1463:MET:HE2	1:B:1463:MET:HB3	1.86	0.42
1:A:1032:ASP:OD1	1:A:1034:ARG:HB2	2.20	0.42
1:A:1060:ARG:HH11	1:A:1060:ARG:HG2	1.76	0.42
1:B:546:SER:CB	1:B:547:LYS:CB	2.98	0.42
1:B:1351:ALA:O	1:B:1354:ARG:HB3	2.19	0.42
1:A:473:ASN:ND2	3:F:6:DT:OP1	2.53	0.42
1:A:1201:ILE:HD12	1:A:1201:ILE:N	2.35	0.42
1:A:479:MET:CE	1:A:522:PHE:CZ	3.03	0.42
1:B:1372:LEU:HD22	1:B:1372:LEU:O	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:LEU:HD21	1:A:1161:ASN:HB2	2.01	0.42
1:B:1354:ARG:HG3	1:B:1459:MET:CE	2.49	0.42
1:B:1226:LYS:O	1:B:1227:LYS:C	2.58	0.41
1:A:1288:ARG:HD2	1:A:1290:GLU:OE2	2.20	0.41
1:B:461:ASN:ND2	1:B:464:LYS:HD2	2.35	0.41
1:A:1420:VAL:O	1:A:1420:VAL:HG13	2.20	0.41
1:B:1321:LEU:HD23	1:B:1321:LEU:HA	1.78	0.41
1:B:1381:VAL:HG21	1:B:1419:ILE:HD13	2.03	0.41
3:F:6:DT:H2'	3:F:7:DA:C8	2.55	0.41
1:A:611:LEU:HD12	1:A:611:LEU:O	2.20	0.41
1:A:638:LYS:C	1:A:640:THR:N	2.74	0.41
1:B:476:ILE:HG23	1:B:521:PHE:CZ	2.56	0.41
1:B:546:SER:CB	1:B:576:THR:H	2.34	0.41
1:B:611:LEU:C	1:B:611:LEU:CD1	2.89	0.41
1:B:442:LYS:O	1:B:445:ARG:HD3	2.20	0.41
1:B:1179:PRO:HA	1:B:1180:PRO:HD3	1.92	0.41
1:A:479:MET:CE	1:A:522:PHE:HZ	2.33	0.41
1:A:1155:LEU:HB3	1:A:1156:PRO:HD2	2.02	0.41
1:B:633:ILE:HG23	1:B:637:VAL:CG2	2.49	0.41
1:B:1138:THR:HB	1:B:1356:VAL:HG13	2.01	0.41
1:B:1239:ARG:HG3	1:B:1316:PHE:CE1	2.56	0.41
1:B:1290:GLU:OE1	1:B:1297:ARG:HD3	2.21	0.41
1:A:462:THR:HG21	1:A:521:PHE:HD1	1.86	0.41
1:A:1385:LEU:HD12	1:B:1393:ARG:CZ	2.50	0.41
1:B:1111:ASP:HB2	1:B:1112:PRO:CD	2.51	0.41
1:B:1372:LEU:HD22	1:B:1376:GLU:HG3	2.03	0.41
1:B:416:LEU:HG	1:B:417:THR:N	2.35	0.41
1:B:1089:SER:HA	1:B:1099:VAL:O	2.21	0.41
1:A:1385:LEU:HD23	1:A:1385:LEU:HA	1.80	0.40
1:B:1228:ALA:HB2	1:B:1234:GLY:HA3	2.04	0.40
1:B:1338:ARG:HB3	1:B:1340:VAL:HG13	2.03	0.40
1:A:1036:GLY:HA2	1:A:1162:LEU:HD23	2.03	0.40
1:A:1102:HIS:HB2	1:A:1120:GLU:HG3	2.03	0.40
1:A:1422:LEU:HD22	1:A:1426:ARG:HG3	2.02	0.40
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.85	0.40
1:A:1024:ILE:HA	1:A:1024:ILE:HD13	1.45	0.40
1:A:1171:SER:HG	1:A:1172:ALA:H	1.62	0.40
1:B:427:ASN:HA	1:B:449:PHE:O	2.20	0.40
1:B:573:LYS:HA	1:B:574:GLY:HA2	1.67	0.40
1:B:1354:ARG:HG3	1:B:1459:MET:HE1	2.02	0.40
1:A:1393:ARG:HA	1:A:1393:ARG:HD2	1.96	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1151:GLU:HB2	1:B:1152:PRO:HD2	2.04	0.40
1:A:1228:ALA:HB2	1:A:1234:GLY:HA3	2.02	0.40
5:H:4:DT:H2''	5:H:5:DA:C5'	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	682/742 (92%)	639 (94%)	38 (6%)	5 (1%)	22 57
1	B	704/742 (95%)	652 (93%)	40 (6%)	12 (2%)	9 35
All	All	1386/1484 (93%)	1291 (93%)	78 (6%)	17 (1%)	13 44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1397	ASN
1	B	546	SER
1	A	639	PHE
1	A	1169	GLY
1	B	571	PHE
1	B	1169	GLY
1	B	1427	LEU
1	B	427	ASN
1	B	570	GLN
1	B	639	PHE
1	B	1059	TYR
1	B	1293	ARG
1	A	1307	ASN
1	B	462	THR
1	B	1221	GLY

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1342	ILE
1	A	1221	GLY

### 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	501/635 (79%)	449 (90%)	52 (10%)	7 25
1	B	500/635 (79%)	460 (92%)	40 (8%)	12 38
All	All	1001/1270 (79%)	909 (91%)	92 (9%)	9 31

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	429	LEU
1	A	435	ASP
1	A	445	ARG
1	A	456	ARG
1	A	475	GLU
1	A	477	ASN
1	A	499	ASP
1	A	501	ILE
1	A	516	THR
1	A	524	ARG
1	A	529	LEU
1	A	564	LEU
1	A	591	LEU
1	A	595	THR
1	A	605	ARG
1	A	617	ARG
1	A	1009	LEU
1	A	1024	ILE
1	A	1028	ARG
1	A	1058	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1060	ARG
1	A	1102	HIS
1	A	1134	ILE
1	A	1139	VAL
1	A	1146	ASP
1	A	1148	THR
1	A	1149	GLU
1	A	1162	LEU
1	A	1168	THR
1	A	1208	LEU
1	A	1236	VAL
1	A	1241	LYS
1	A	1263	ILE
1	A	1268	LEU
1	A	1279	ASN
1	A	1281	VAL
1	A	1293	ARG
1	A	1308	THR
1	A	1310	LEU
1	A	1321	LEU
1	A	1336	THR
1	A	1338	ARG
1	A	1342	ILE
1	A	1372	LEU
1	A	1380	ARG
1	A	1385	LEU
1	A	1387	GLU
1	A	1414	GLU
1	A	1420	VAL
1	A	1432	VAL
1	A	1462	LEU
1	B	429	LEU
1	B	447	ARG
1	B	453	LEU
1	B	475	GLU
1	B	478	THR
1	B	492	SER
1	B	516	THR
1	B	520	THR
1	B	524	ARG
1	B	536	TYR
1	B	554	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	585	GLU
1	B	595	THR
1	B	1028	ARG
1	B	1060	ARG
1	B	1090	GLN
1	B	1102	HIS
1	B	1117	ARG
1	B	1162	LEU
1	B	1168	THR
1	B	1177	ASP
1	B	1183	LEU
1	B	1208	LEU
1	B	1268	LEU
1	B	1293	ARG
1	B	1297	ARG
1	B	1308	THR
1	B	1310	LEU
1	B	1321	LEU
1	B	1336	THR
1	B	1338	ARG
1	B	1342	ILE
1	B	1348	SER
1	B	1372	LEU
1	B	1385	LEU
1	B	1420	VAL
1	B	1432	VAL
1	B	1434	VAL
1	B	1462	LEU
1	B	1464	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1026	GLN
1	B	1094	ASN

### 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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
7	PDQ	F	101	-	26,29,29	5.28	14 (53%)	30,45,45	1.69	5 (16%)
7	PDQ	H	101	-	26,29,29	5.53	16 (61%)	30,45,45	1.72	6 (20%)

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
7	PDQ	F	101	-	-	4/11/23/23	0/4/4/4
7	PDQ	H	101	-	-	4/11/23/23	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	101	PDQ	C12-C10	15.33	1.65	1.40
7	F	101	PDQ	C12-C10	14.20	1.63	1.40
7	H	101	PDQ	C4-C3	13.65	1.61	1.39
7	F	101	PDQ	C4-C3	13.11	1.60	1.39
7	H	101	PDQ	C12-N13	11.71	1.62	1.42
7	F	101	PDQ	C12-N13	11.47	1.61	1.42

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	101	PDQ	C3-C1	6.92	1.61	1.47
7	H	101	PDQ	C8-C6	6.81	1.54	1.39
7	F	101	PDQ	C34-C37	-6.69	1.43	1.52
7	F	101	PDQ	C8-C6	6.57	1.53	1.39
7	H	101	PDQ	C34-C37	-6.46	1.43	1.52
7	F	101	PDQ	C3-C1	6.17	1.60	1.47
7	H	101	PDQ	C39-C37	-5.04	1.40	1.53
7	F	101	PDQ	C39-C37	-4.76	1.41	1.53
7	F	101	PDQ	C3-C12	-3.26	1.36	1.40
7	F	101	PDQ	C37-C45	-3.12	1.43	1.52
7	H	101	PDQ	C8-N33	3.12	1.49	1.40
7	H	101	PDQ	C34-N33	3.04	1.50	1.46
7	F	101	PDQ	C20-C18	2.90	1.55	1.48
7	H	101	PDQ	C37-C45	-2.82	1.44	1.52
7	F	101	PDQ	C8-N33	2.81	1.48	1.40
7	H	101	PDQ	C3-C12	-2.78	1.37	1.40
7	F	101	PDQ	C34-N33	2.77	1.50	1.46
7	H	101	PDQ	C23-C18	2.65	1.54	1.48
7	H	101	PDQ	C20-C18	2.63	1.54	1.48
7	F	101	PDQ	C23-C18	2.61	1.54	1.48
7	H	101	PDQ	C8-C10	2.24	1.44	1.40
7	H	101	PDQ	O2-C1	-2.14	1.18	1.22
7	F	101	PDQ	O2-C1	-2.09	1.18	1.22
7	H	101	PDQ	C4-C6	2.09	1.41	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	101	PDQ	C23-C18-N13	-5.09	113.15	118.29
7	F	101	PDQ	C18-N13-C15	3.86	123.05	117.33
7	F	101	PDQ	C23-C18-N13	-3.69	114.57	118.29
7	F	101	PDQ	C20-C18-N13	-3.47	114.79	118.29
7	H	101	PDQ	C18-N13-C15	3.26	122.17	117.33
7	H	101	PDQ	C1-N17-C15	-2.85	121.58	126.61
7	H	101	PDQ	C20-C18-N13	-2.71	115.55	118.29
7	F	101	PDQ	C39-C37-C34	2.71	108.49	102.19
7	H	101	PDQ	C3-C12-N13	-2.55	116.39	119.73
7	F	101	PDQ	C1-N17-C15	-2.41	122.35	126.61
7	H	101	PDQ	C42-N33-C34	-2.28	105.67	111.55

There are no chirality outliers.

All (8) torsion outliers are listed below:

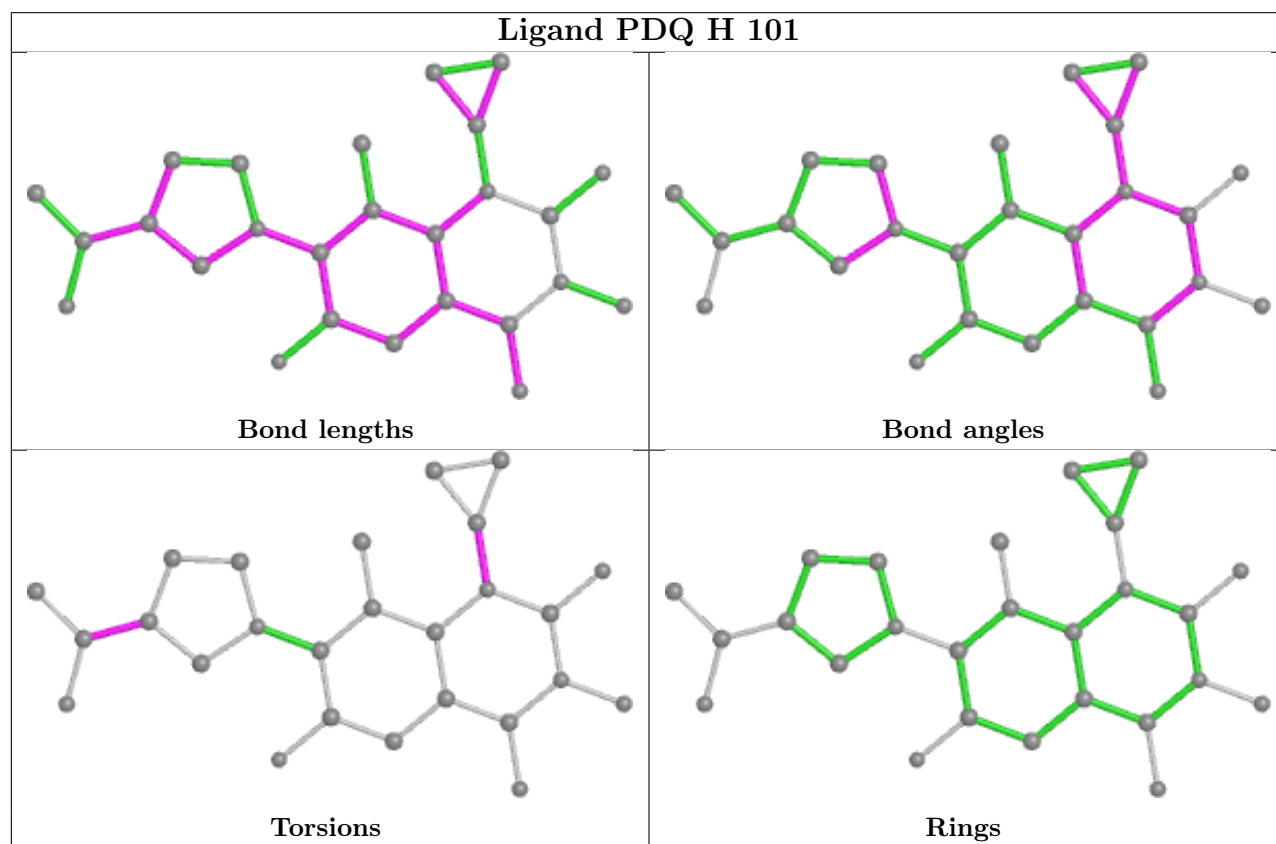
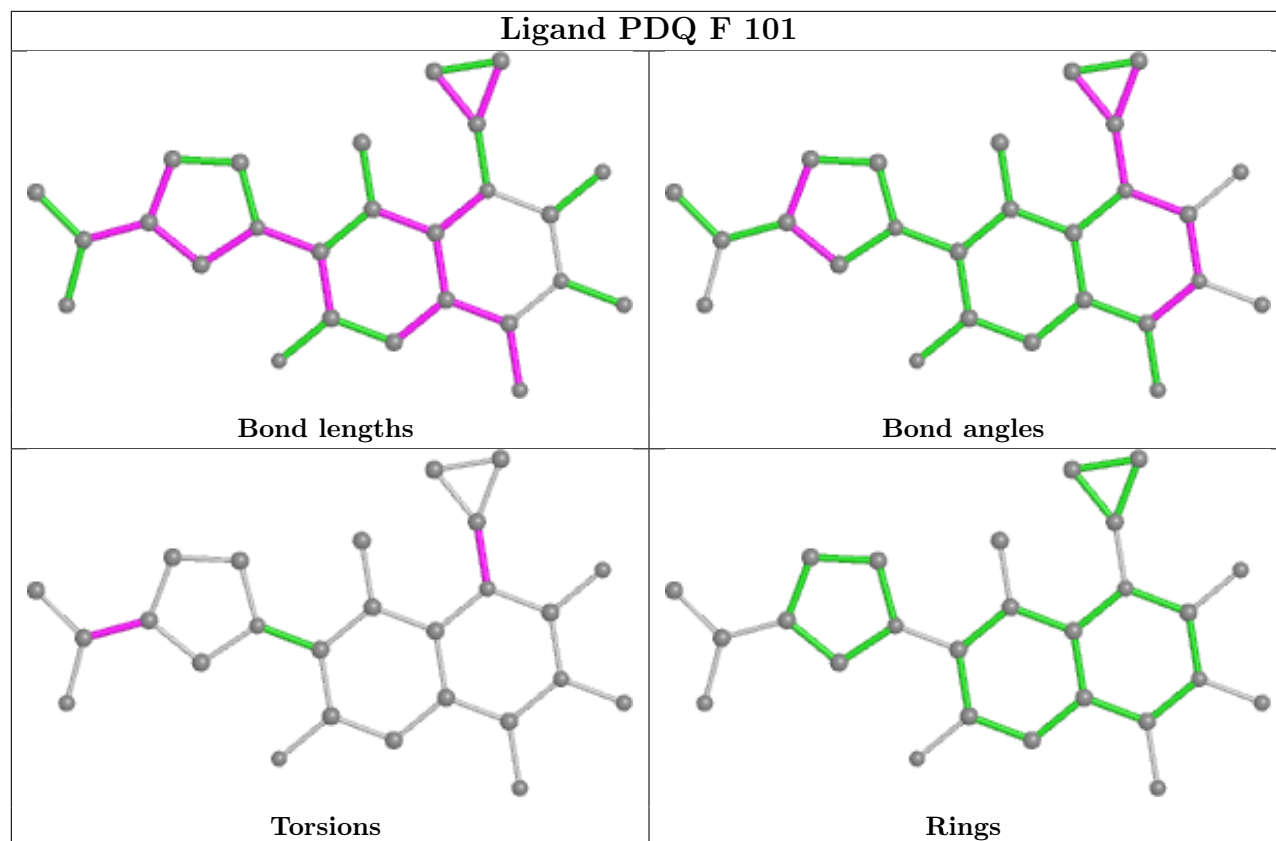
Mol	Chain	Res	Type	Atoms
7	F	101	PDQ	C39-C37-C45-C47
7	H	101	PDQ	C39-C37-C45-N51
7	F	101	PDQ	C20-C18-N13-C15
7	F	101	PDQ	C34-C37-C45-C47
7	H	101	PDQ	C34-C37-C45-C47
7	H	101	PDQ	C39-C37-C45-C47
7	F	101	PDQ	C23-C18-N13-C15
7	H	101	PDQ	C20-C18-N13-C15

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	101	PDQ	6	0
7	H	101	PDQ	10	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	690/742 (92%)	-0.81	0 100 100	35, 66, 111, 150	0
1	B	708/742 (95%)	-0.76	0 100 100	40, 69, 114, 138	0
2	E	7/7 (100%)	-0.46	0 100 100	56, 65, 102, 143	0
3	F	11/11 (100%)	-0.70	0 100 100	65, 79, 89, 126	0
4	G	7/7 (100%)	-0.04	0 100 100	56, 63, 111, 136	0
5	H	11/11 (100%)	-0.62	0 100 100	66, 79, 87, 126	0
All	All	1434/1520 (94%)	-0.77	0 100 100	35, 68, 113, 150	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 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.

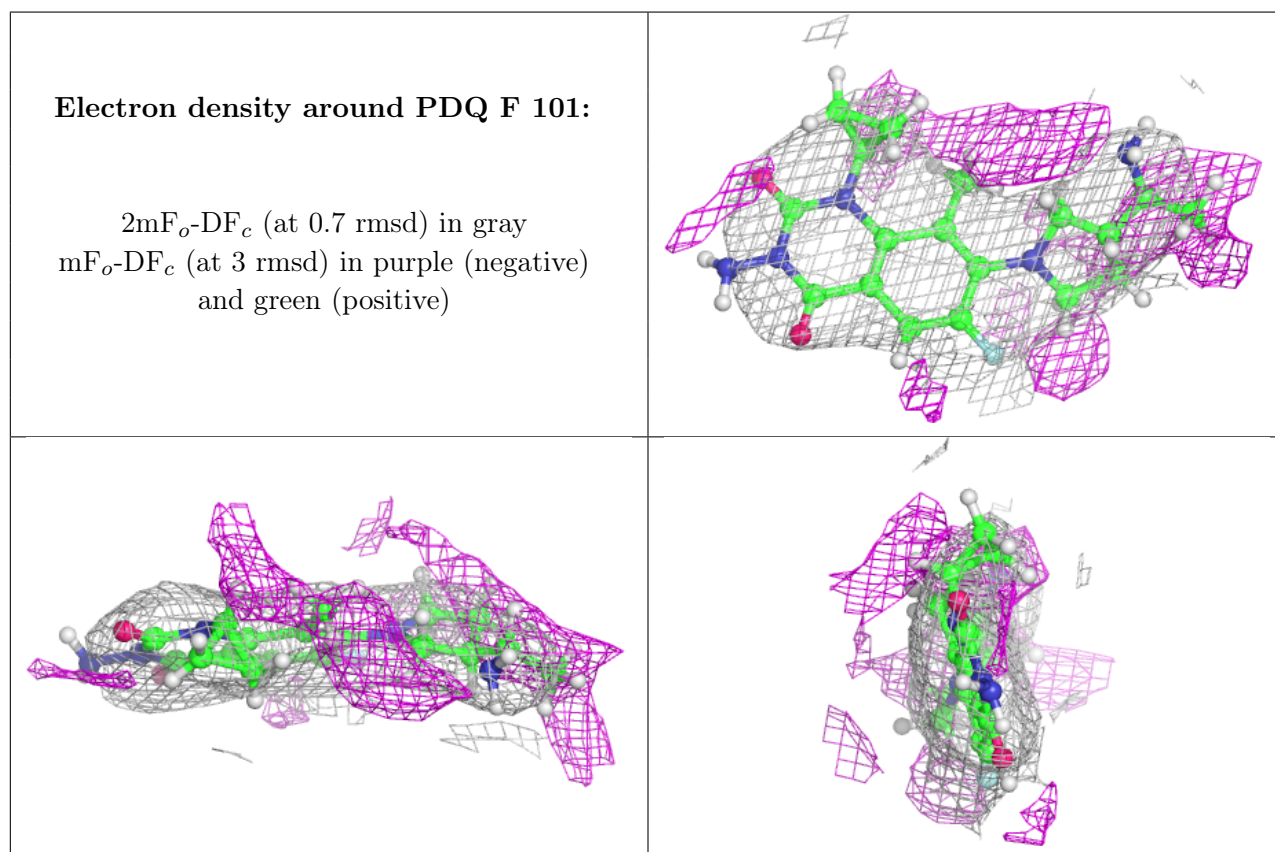
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	B	1502	1/1	0.50	0.58	79,79,79,79	0

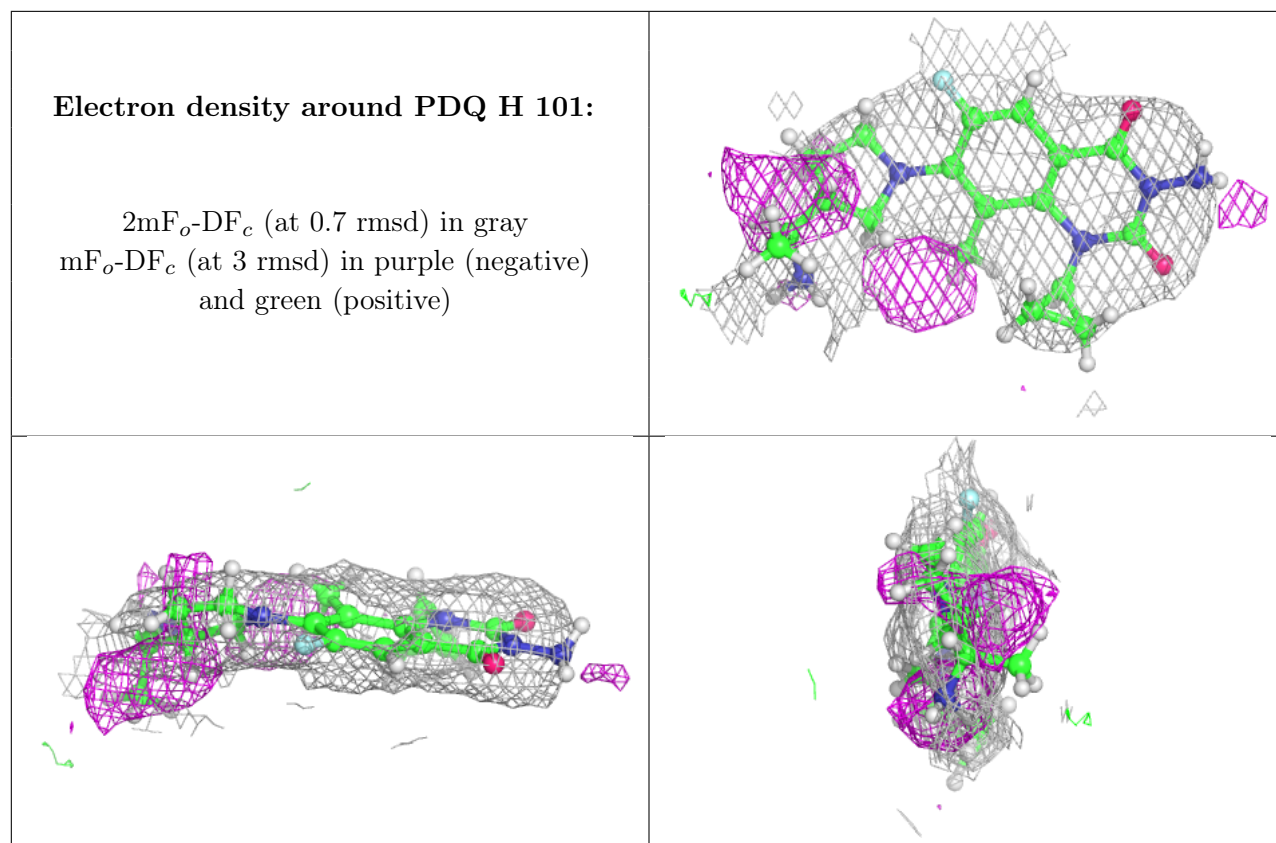
*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	1501	1/1	0.72	0.12	102,102,102,102	0
6	MG	A	1502	1/1	0.81	0.59	94,94,94,94	0
6	MG	A	1501	1/1	0.86	0.09	96,96,96,96	0
7	PDQ	F	101	26/26	0.90	0.23	64,81,105,126	0
7	PDQ	H	101	26/26	0.90	0.25	70,84,101,118	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.