Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:00 pm BST

PDB ID	:	4Z2E
Title	:	Quinolone(Trovafloxacin)-DNA cleavage complex of gyrase 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	:	2015-03-29
Resolution	:	3.46 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 following versions of software and data (see references ⓘ) were used in the production of this report:

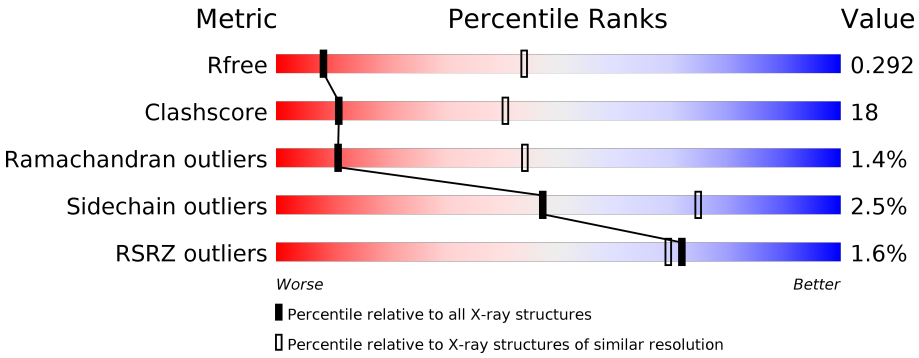
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.46 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 >=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 <=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	499	69% 27%
1	B	499	2% 66% 28% 5%
2	C	269	3% 54% 19% 27%
2	D	269	% 52% 19% 29%
3	E	15	20% 33% 47%
3	G	15	20% 27% 53%

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Mol	Chain	Length	Quality of chain
4	F	19	37% 26% 37%
4	H	19	21% 37% 42%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9755 atoms, of which 28 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 gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3340	2082	617	625	16			
1	B	472	Total	C	N	O	S	0	0	0
			3129	1966	564	587	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	HIS	-	expression tag	UNP Q9R867
A	495	HIS	-	expression tag	UNP Q9R867
A	496	HIS	-	expression tag	UNP Q9R867
A	497	HIS	-	expression tag	UNP Q9R867
A	498	HIS	-	expression tag	UNP Q9R867
A	499	HIS	-	expression tag	UNP Q9R867
B	494	HIS	-	expression tag	UNP Q9R867
B	495	HIS	-	expression tag	UNP Q9R867
B	496	HIS	-	expression tag	UNP Q9R867
B	497	HIS	-	expression tag	UNP Q9R867
B	498	HIS	-	expression tag	UNP Q9R867
B	499	HIS	-	expression tag	UNP Q9R867

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	197	Total	C	N	O	S	0	0	0
			1224	765	223	230	6			
2	D	191	Total	C	N	O	S	0	0	0
			1205	758	218	223	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	initiating methionine	UNP Q59957
C	381	GLY	-	expression tag	UNP Q59957
C	382	HIS	-	expression tag	UNP Q59957
C	383	HIS	-	expression tag	UNP Q59957
C	384	HIS	-	expression tag	UNP Q59957
C	385	HIS	-	expression tag	UNP Q59957
C	386	HIS	-	expression tag	UNP Q59957
C	387	HIS	-	expression tag	UNP Q59957
C	388	HIS	-	expression tag	UNP Q59957
C	389	HIS	-	expression tag	UNP Q59957
C	390	HIS	-	expression tag	UNP Q59957
C	391	HIS	-	expression tag	UNP Q59957
C	392	SER	-	expression tag	UNP Q59957
C	393	SER	-	expression tag	UNP Q59957
C	394	GLY	-	expression tag	UNP Q59957
C	395	HIS	-	expression tag	UNP Q59957
C	396	ILE	-	expression tag	UNP Q59957
C	397	ASP	-	expression tag	UNP Q59957
C	398	ASP	-	expression tag	UNP Q59957
C	399	ASP	-	expression tag	UNP Q59957
C	400	ASP	-	expression tag	UNP Q59957
C	401	LYS	-	expression tag	UNP Q59957
C	402	HIS	-	expression tag	UNP Q59957
C	403	MET	-	expression tag	UNP Q59957
D	380	MET	-	initiating methionine	UNP Q59957
D	381	GLY	-	expression tag	UNP Q59957
D	382	HIS	-	expression tag	UNP Q59957
D	383	HIS	-	expression tag	UNP Q59957
D	384	HIS	-	expression tag	UNP Q59957
D	385	HIS	-	expression tag	UNP Q59957
D	386	HIS	-	expression tag	UNP Q59957
D	387	HIS	-	expression tag	UNP Q59957
D	388	HIS	-	expression tag	UNP Q59957
D	389	HIS	-	expression tag	UNP Q59957
D	390	HIS	-	expression tag	UNP Q59957
D	391	HIS	-	expression tag	UNP Q59957
D	392	SER	-	expression tag	UNP Q59957
D	393	SER	-	expression tag	UNP Q59957
D	394	GLY	-	expression tag	UNP Q59957
D	395	HIS	-	expression tag	UNP Q59957
D	396	ILE	-	expression tag	UNP Q59957
D	397	ASP	-	expression tag	UNP Q59957
D	398	ASP	-	expression tag	UNP Q59957

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Chain	Residue	Modelled	Actual	Comment	Reference
D	399	ASP	-	expression tag	UNP Q59957
D	400	ASP	-	expression tag	UNP Q59957
D	401	LYS	-	expression tag	UNP Q59957
D	402	HIS	-	expression tag	UNP Q59957
D	403	MET	-	expression tag	UNP Q59957

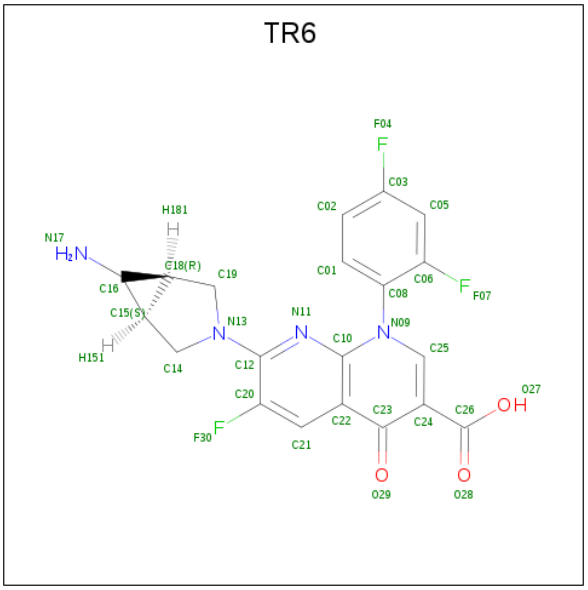
- Molecule 3 is a DNA chain called Symmetrized E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	P	0	0	0
			160	79	26	48	7			
3	G	7	Total	C	N	O	P	0	0	0
			141	70	23	42	6			

- Molecule 4 is a DNA chain called Symmetrized E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	12	Total	C	N	O	P	0	0	0
			243	117	48	67	11			
4	H	11	Total	C	N	O	P	0	0	0
			221	107	43	61	10			

- Molecule 5 is Trovafloxacin (three-letter code: TR6) (formula: $C_{20}H_{15}F_3N_4O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	F	1	Total	C	F	H	N	O	0	0
			44	20	3	14	4	3		
5	H	1	Total	C	F	H	N	O	0	0
			44	20	3	14	4	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is water.

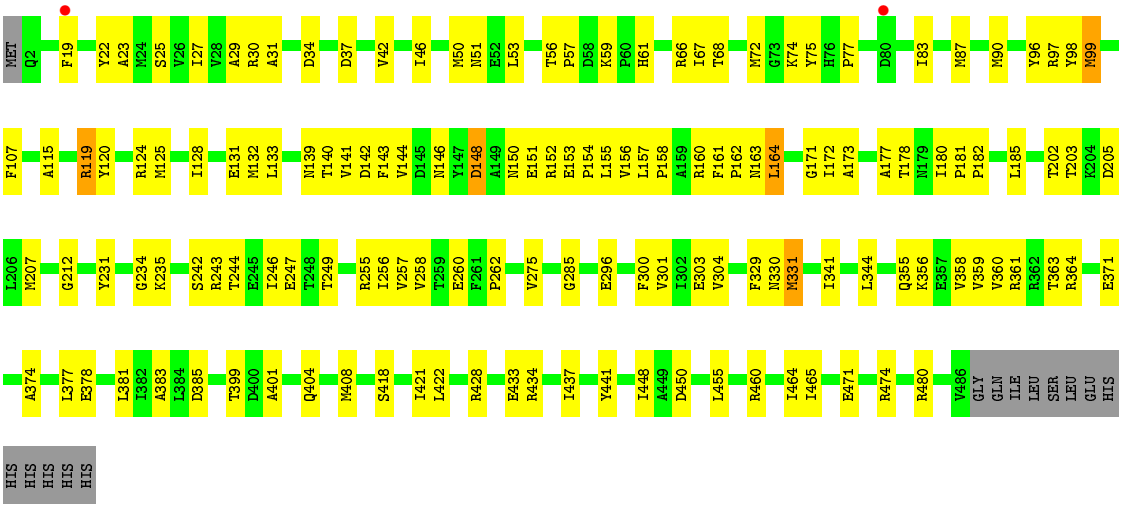
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

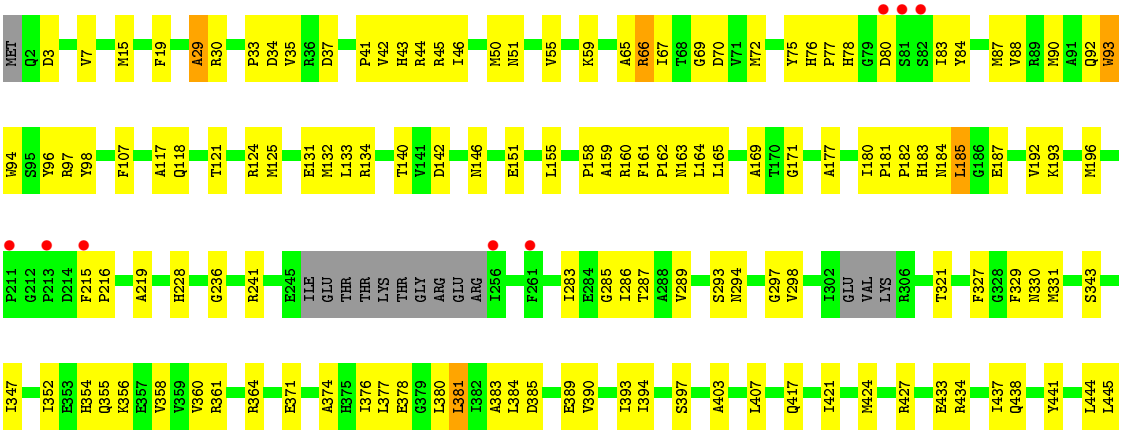
- Molecule 1: DNA gyrase subunit A

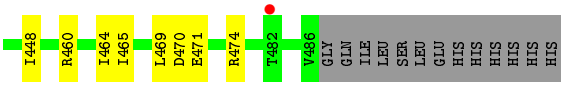
Chain A:



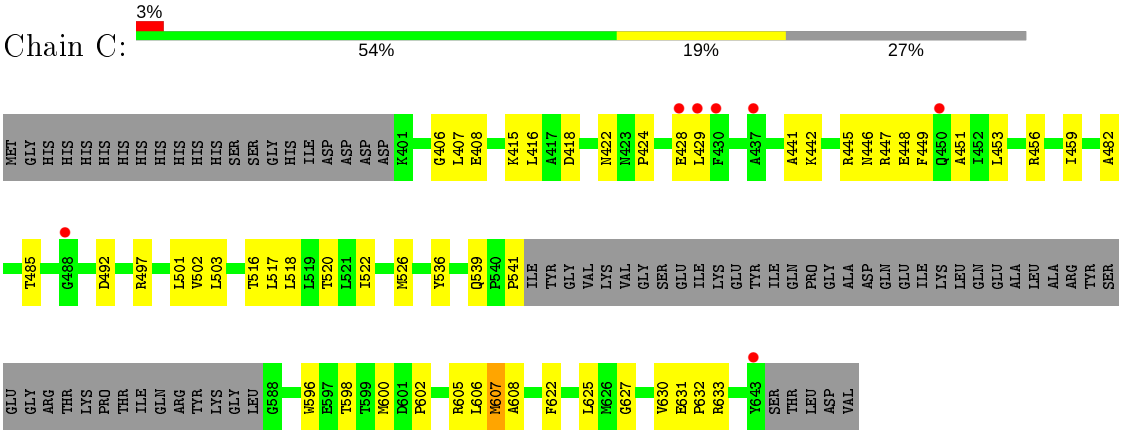
- Molecule 1: DNA gyrase subunit A

Chain B:

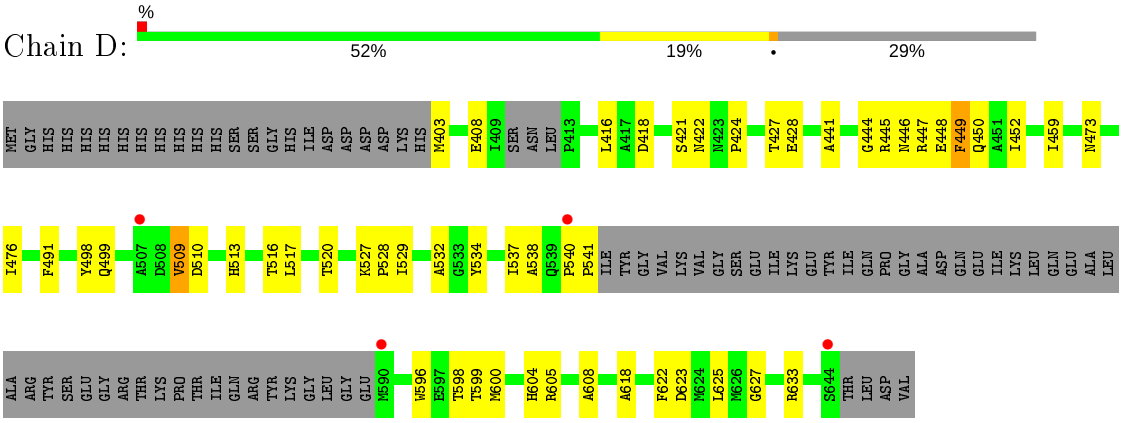




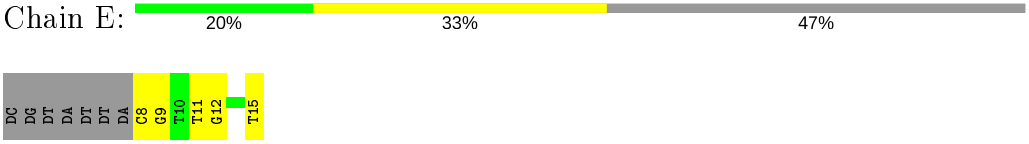
• Molecule 2: DNA gyrase subunit B



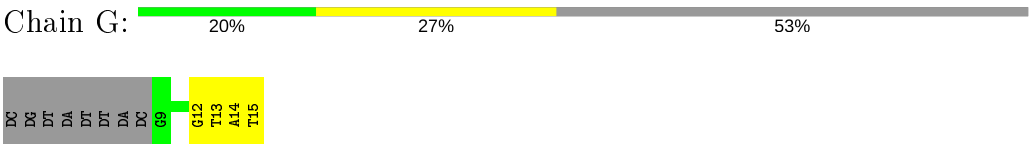
• Molecule 2: DNA gyrase subunit B



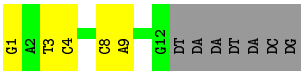
• Molecule 3: Symmetrized E-site DNA



• Molecule 3: Symmetrized E-site DNA

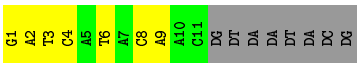


• Molecule 4: Symmetrized E-site DNA



- Molecule 4: Symmetrized E-site DNA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.19Å 96.62Å 275.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.05 – 3.46 56.04 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (56.05-3.46) 94.5 (56.04-3.37)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.247 , 0.292 0.249 , 0.292	Depositor DCC
R_{free} test set	1788 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	102.4	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 105.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9755	wwPDB-VP
Average B, all atoms (Å^2)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, TR6

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	0.19	0/3394	0.37	0/4637
1	B	0.19	0/3180	0.36	0/4355
2	C	0.19	0/1244	0.36	0/1708
2	D	0.19	0/1225	0.35	0/1676
3	E	0.43	0/178	1.09	0/274
3	G	0.44	0/157	1.10	0/242
4	F	0.45	0/273	0.97	0/419
4	H	0.44	0/248	0.97	1/380 (0.3%)
All	All	0.22	0/9899	0.47	1/13691 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	6	DT	O4'-C4'-C3'	-5.12	102.45	104.50

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	3340	0	2824	119	0
1	B	3129	0	2521	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1224	0	908	39	0
2	D	1205	0	906	40	0
3	E	160	0	91	4	0
3	G	141	0	80	5	0
4	F	243	0	136	8	0
4	H	221	0	125	8	0
5	F	30	14	14	3	0
5	H	30	14	14	1	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	A	2	0	0	0	0
All	All	9727	28	7619	307	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 18.

All (307) 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:234:GLY:HA2	1:A:331:MET:HE2	1.56	0.88
2:D:403:MET:HA	2:D:421:SER:HA	1.61	0.83
1:B:90:MET:HG2	1:B:96:TYR:HE2	1.45	0.80
1:A:74:LYS:HD3	1:B:66:ARG:HH21	1.50	0.77
2:D:520:THR:HG22	2:D:622:PHE:CD2	2.21	0.76
1:A:181:PRO:HG3	1:A:329:PHE:CZ	2.21	0.75
1:B:90:MET:HG2	1:B:96:TYR:CE2	2.23	0.72
2:C:520:THR:HG22	2:C:622:PHE:CD2	2.24	0.72
2:C:627:GLY:O	2:C:633:ARG:NH2	2.22	0.72
1:A:371:GLU:HG2	1:A:448:ILE:HD13	1.72	0.72
1:B:84:TYR:CD1	1:B:118:GLN:HG2	2.25	0.71
1:A:385:ASP:OD1	1:A:434:ARG:NH1	2.23	0.71
2:C:633:ARG:HD3	1:B:19:PHE:HZ	1.56	0.71
1:A:422:LEU:HB3	1:B:427:ARG:HB3	1.73	0.70
2:D:520:THR:HG22	2:D:622:PHE:HD2	1.54	0.70
1:A:156:VAL:HG22	1:A:157:LEU:H	1.57	0.69
1:B:67:ILE:HG21	1:B:87:MET:HE1	1.75	0.68
1:A:72:MET:HB2	1:A:83:ILE:HD12	1.76	0.68
2:C:596:TRP:HA	2:C:600:MET:HB2	1.75	0.68
1:A:471:GLU:OE1	1:A:474:ARG:NH2	2.27	0.68
2:C:520:THR:HG22	2:C:622:PHE:HD2	1.59	0.68
1:A:90:MET:HA	1:A:96:TYR:CD1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:416:LEU:HB2	2:C:453:LEU:HD23	1.76	0.67
4:H:8:DC:H2"	4:H:9:DA:H5"	1.75	0.66
2:C:503:LEU:HD22	2:C:518:LEU:HD13	1.77	0.66
1:A:25:SER:CB	2:D:509:VAL:HG11	2.26	0.66
1:A:255:ARG:HG3	1:A:303:GLU:HG2	1.78	0.66
1:A:74:LYS:HD3	1:B:66:ARG:NH2	2.11	0.65
1:B:125:MET:HE1	1:B:133:LEU:HD12	1.78	0.65
1:B:385:ASP:OD1	1:B:434:ARG:NH1	2.29	0.65
1:B:383:ALA:HB2	1:B:421:ILE:HD13	1.78	0.65
2:D:510:ASP:HB3	3:E:15:DT:H4'	1.78	0.65
2:C:441:ALA:O	2:C:445:ARG:HB3	1.98	0.64
2:D:627:GLY:O	2:D:633:ARG:NH2	2.31	0.64
1:A:177:ALA:O	1:A:330:ASN:ND2	2.31	0.63
1:A:404:GLN:HG3	1:A:418:SER:HB2	1.80	0.63
1:B:142:ASP:OD1	1:B:361:ARG:NH2	2.32	0.63
1:A:98:TYR:CZ	1:A:185:LEU:HB2	2.34	0.62
2:C:602:PRO:HA	2:C:605:ARG:HG2	1.82	0.62
2:C:442:LYS:O	2:C:445:ARG:NH1	2.31	0.62
2:C:446:ASN:O	2:C:448:GLU:N	2.32	0.62
1:B:44:ARG:NH1	1:B:155:LEU:O	2.33	0.62
1:B:177:ALA:O	1:B:330:ASN:ND2	2.32	0.61
1:A:74:LYS:HE3	1:A:75:TYR:CE1	2.36	0.61
2:D:445:ARG:HA	2:D:600:MET:HE2	1.80	0.61
1:A:51:ASN:HB2	1:A:133:LEU:HD13	1.82	0.60
1:B:97:ARG:HG3	1:B:98:TYR:CE1	2.36	0.60
1:A:22:TYR:CD1	2:D:513:HIS:HB2	2.36	0.60
1:A:255:ARG:NH1	1:A:303:GLU:OE2	2.35	0.60
1:A:66:ARG:NH1	1:B:70:ASP:OD1	2.35	0.60
4:H:9:DA:H5'	4:H:9:DA:H8	1.66	0.60
4:H:9:DA:H5'	4:H:9:DA:C8	2.37	0.60
1:B:355:GLN:HB3	1:B:465:ILE:HD13	1.84	0.59
2:C:625:LEU:HD22	1:B:19:PHE:CD1	2.37	0.59
4:F:3:DT:H2"	4:F:4:DC:O5'	2.02	0.59
1:A:142:ASP:OD1	1:A:361:ARG:NH2	2.33	0.59
1:A:242:SER:OG	1:A:262:PRO:HD3	2.02	0.59
2:D:604:HIS:O	2:D:605:ARG:HG2	2.02	0.59
1:A:383:ALA:HB2	1:A:421:ILE:HD13	1.85	0.59
2:D:633:ARG:NH1	4:F:9:DA:OP1	2.36	0.58
2:D:520:THR:HA	2:D:622:PHE:CE2	2.39	0.58
1:A:399:THR:HG22	1:A:401:ALA:H	1.69	0.58
2:D:499:GLN:HA	2:D:534:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:O	1:B:183:HIS:ND1	2.34	0.58
1:A:141:VAL:HG11	1:A:156:VAL:O	2.04	0.57
1:A:125:MET:HE1	1:A:133:LEU:HD12	1.85	0.57
1:A:97:ARG:HG3	1:A:98:TYR:CE1	2.39	0.57
1:B:59:LYS:O	1:B:124:ARG:NH1	2.38	0.56
1:B:192:VAL:O	1:B:196:MET:HG3	2.05	0.56
2:C:428:GLU:N	2:C:449:PHE:O	2.38	0.56
1:A:140:THR:HA	1:A:361:ARG:HD3	1.86	0.56
2:C:422:ASN:O	2:C:424:PRO:HD3	2.05	0.56
1:B:125:MET:CE	1:B:133:LEU:HD12	2.36	0.56
1:A:249:THR:HA	1:A:255:ARG:HH21	1.71	0.56
1:B:97:ARG:HG3	1:B:98:TYR:CD1	2.41	0.56
1:A:66:ARG:HD3	1:B:70:ASP:HA	1.89	0.55
1:B:131:GLU:OE1	1:B:134:ARG:HD2	2.06	0.55
1:B:140:THR:CB	1:B:358:VAL:HG13	2.36	0.55
1:A:66:ARG:HG2	1:B:69:GLY:O	2.06	0.55
4:H:8:DC:H2"	4:H:9:DA:C5'	2.37	0.55
1:B:164:LEU:HD21	1:B:180:ILE:HD12	1.88	0.55
2:D:516:THR:O	2:D:520:THR:HG23	2.07	0.54
1:A:249:THR:HA	1:A:255:ARG:NH2	2.21	0.54
2:D:418:ASP:OD1	2:D:498:TYR:OH	2.25	0.54
1:B:35:VAL:HA	1:B:164:LEU:HD12	1.89	0.54
1:B:377:LEU:HD23	1:B:441:TYR:HB2	1.89	0.54
3:G:14:DA:H2'	3:G:15:DT:C6	2.43	0.54
1:B:50:MET:HB3	1:B:55:VAL:CG2	2.38	0.54
1:A:244:THR:HG22	1:A:258:VAL:HA	1.90	0.54
1:A:99:MET:HE2	1:A:99:MET:H	1.71	0.54
1:A:243:ARG:HB3	1:A:260:GLU:HB2	1.88	0.53
1:A:97:ARG:HB2	1:A:182:PRO:HB3	1.89	0.53
4:F:9:DA:C8	4:F:9:DA:H5'	2.44	0.53
1:A:125:MET:CE	1:A:133:LEU:HD12	2.38	0.53
1:A:31:ALA:CB	1:A:173:ALA:HB2	2.39	0.53
2:C:541:PRO:HG3	2:C:598:THR:HB	1.91	0.53
1:B:377:LEU:HG	1:B:437:ILE:CG2	2.39	0.53
1:A:172:ILE:HB	3:E:12:DG:N2	2.24	0.53
1:A:56:THR:HB	1:A:57:PRO:HD2	1.90	0.53
1:B:98:TYR:CZ	1:B:185:LEU:HB2	2.44	0.53
1:A:119:ARG:HB2	1:A:119:ARG:NH1	2.24	0.53
2:C:605:ARG:NE	1:B:3:ASP:OD1	2.38	0.52
1:A:143:PHE:HB3	1:A:152:ARG:HG2	1.90	0.52
1:A:460:ARG:O	1:A:464:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLY:O	1:B:329:PHE:N	2.40	0.52
1:B:67:ILE:CG2	1:B:87:MET:HE1	2.38	0.52
4:F:3:DT:H4'	4:F:4:DC:OP1	2.10	0.52
1:A:203:THR:O	1:A:207:MET:HG3	2.10	0.52
1:A:235:LYS:HE2	1:A:341:ILE:HD13	1.91	0.52
2:D:541:PRO:HG3	2:D:598:THR:HG21	1.91	0.52
1:B:381:LEU:HD11	1:B:437:ILE:HB	1.91	0.52
1:A:275:VAL:HG13	2:C:407:LEU:HA	1.93	0.51
1:A:474:ARG:HD2	1:A:474:ARG:O	2.10	0.51
2:D:449:PHE:HD1	2:D:449:PHE:H	1.58	0.51
1:B:90:MET:HA	1:B:96:TYR:CD2	2.46	0.51
1:A:404:GLN:HG3	1:A:418:SER:CB	2.40	0.51
1:A:144:VAL:HG11	1:A:155:LEU:HD21	1.91	0.51
1:A:131:GLU:O	1:A:160:ARG:HG2	2.11	0.51
1:A:171:GLY:HA2	1:A:178:THR:HG22	1.93	0.51
1:A:99:MET:H	1:A:99:MET:CE	2.24	0.51
1:B:164:LEU:HD21	1:B:180:ILE:CD1	2.42	0.50
1:B:55:VAL:O	1:B:124:ARG:HB2	2.11	0.50
1:B:75:TYR:O	1:B:77:PRO:HD3	2.11	0.50
1:A:377:LEU:HD23	1:A:441:TYR:HB2	1.94	0.50
1:B:294:ASN:N	1:B:297:GLY:O	2.37	0.50
1:A:258:VAL:HB	1:A:300:PHE:HB3	1.93	0.50
1:B:84:TYR:O	1:B:88:VAL:HG23	2.12	0.50
1:B:374:ALA:O	1:B:378:GLU:HG3	2.11	0.50
1:B:193:LYS:NZ	1:B:470:ASP:OD1	2.28	0.50
1:A:97:ARG:HG3	1:A:98:TYR:CD1	2.47	0.49
2:C:428:GLU:OE2	2:C:605:ARG:NH2	2.35	0.49
1:B:343:SER:O	1:B:347:ILE:HG13	2.12	0.49
1:A:119:ARG:HD3	1:A:120:TYR:CE2	2.47	0.49
1:B:371:GLU:HG2	1:B:448:ILE:HD13	1.92	0.49
1:B:42:VAL:O	1:B:46:ILE:HG13	2.13	0.49
2:D:529:ILE:HG23	2:D:534:TYR:HB2	1.93	0.49
1:B:78:HIS:CD2	3:G:14:DA:H5'	2.48	0.49
1:A:156:VAL:HG22	1:A:157:LEU:N	2.26	0.49
1:A:374:ALA:O	1:A:378:GLU:HG3	2.13	0.49
1:A:363:THR:CG2	1:A:455:LEU:HG	2.43	0.49
1:A:72:MET:CE	1:B:65:ALA:HB1	2.43	0.49
1:B:41:PRO:O	1:B:45:ARG:HG3	2.13	0.49
1:A:363:THR:HB	1:A:455:LEU:HD21	1.94	0.48
1:B:471:GLU:OE1	1:B:474:ARG:NH2	2.40	0.48
1:B:474:ARG:HD2	1:B:474:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:630:VAL:HA	2:C:633:ARG:NH1	2.27	0.48
2:D:446:ASN:O	2:D:448:GLU:N	2.42	0.48
1:A:244:THR:CG2	1:A:258:VAL:HG22	2.43	0.48
1:B:131:GLU:OE2	1:B:134:ARG:NH1	2.47	0.48
1:B:380:LEU:HD22	1:B:424:MET:SD	2.53	0.48
1:B:196:MET:HG2	1:B:352:ILE:HD13	1.95	0.48
1:B:184:ASN:HB3	1:B:187:GLU:CG	2.44	0.48
1:A:181:PRO:HG3	1:A:329:PHE:CE1	2.48	0.48
1:A:383:ALA:HB2	1:A:421:ILE:CD1	2.44	0.48
1:A:75:TYR:O	1:A:77:PRO:HD3	2.13	0.48
1:B:97:ARG:HA	1:B:216:PRO:HB3	1.96	0.48
1:A:19:PHE:HZ	2:D:633:ARG:HD3	1.79	0.48
1:B:50:MET:O	1:B:55:VAL:HG22	2.14	0.48
1:A:171:GLY:HA2	1:A:178:THR:CG2	2.44	0.48
3:E:8:DC:H2"	3:E:9:DG:OP1	2.14	0.47
1:A:140:THR:HB	1:A:358:VAL:HG13	1.96	0.47
1:A:171:GLY:O	1:A:177:ALA:HA	2.14	0.47
1:B:51:ASN:HB2	1:B:133:LEU:HD13	1.95	0.47
1:A:61:HIS:CE1	1:A:124:ARG:HG2	2.50	0.47
1:A:31:ALA:HB3	1:A:173:ALA:HB2	1.96	0.47
1:A:356:LYS:HA	1:A:465:ILE:HD11	1.95	0.47
2:C:633:ARG:HD3	1:B:19:PHE:CZ	2.43	0.47
1:A:164:LEU:HD21	1:A:180:ILE:HD12	1.97	0.47
4:F:1:DG:H1'	5:F:101:TR6:C01	2.45	0.47
4:H:2:DA:C8	4:H:2:DA:H5'	2.49	0.47
1:B:51:ASN:HB2	1:B:133:LEU:CD1	2.45	0.47
2:D:422:ASN:O	2:D:424:PRO:HD3	2.15	0.47
2:D:520:THR:HA	2:D:622:PHE:HE2	1.79	0.47
1:A:244:THR:HG22	1:A:258:VAL:HG22	1.96	0.47
1:A:72:MET:HE3	1:B:65:ALA:HB1	1.97	0.47
2:D:599:THR:O	2:D:605:ARG:HD2	2.15	0.47
1:B:376:ILE:O	1:B:380:LEU:HG	2.14	0.46
1:B:360:VAL:O	1:B:364:ARG:HG3	2.15	0.46
1:B:417:GLN:O	1:B:421:ILE:HG13	2.15	0.46
2:D:459:ILE:O	2:D:517:LEU:HD13	2.16	0.46
3:G:13:DT:H2"	3:G:14:DA:O5'	2.15	0.46
1:A:363:THR:HG21	1:A:455:LEU:HG	1.98	0.46
2:D:623:ASP:O	2:D:627:GLY:HA3	2.16	0.46
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.44	0.46
2:C:536:TYR:CB	2:C:607:MET:HE3	2.46	0.46
2:C:608:ALA:HA	1:B:7:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:428:GLU:N	2:D:449:PHE:O	2.47	0.46
1:B:132:MET:O	1:B:158:PRO:HD2	2.16	0.46
1:B:42:VAL:HG13	1:B:43:HIS:N	2.31	0.46
2:C:406:GLY:C	2:C:408:GLU:H	2.20	0.46
2:C:459:ILE:O	2:C:517:LEU:HD13	2.15	0.46
1:A:23:ALA:O	1:A:27:ILE:HG13	2.16	0.46
1:A:231:TYR:CD2	1:A:344:LEU:HD22	2.51	0.46
1:B:77:PRO:O	1:B:78:HIS:ND1	2.49	0.46
2:D:541:PRO:HG3	2:D:598:THR:CG2	2.46	0.46
1:B:182:PRO:HD2	1:B:215:PHE:CD1	2.52	0.45
1:B:181:PRO:HG3	1:B:329:PHE:CZ	2.51	0.45
1:A:428:ARG:O	1:A:433:GLU:HG2	2.16	0.45
1:A:42:VAL:O	1:A:46:ILE:HG13	2.15	0.45
2:C:539:GLN:HB2	2:C:606:LEU:O	2.17	0.45
2:D:427:THR:HG22	2:D:498:TYR:CD2	2.51	0.45
5:F:101:TR6:H051	3:G:15:DT:H2"	1.98	0.45
1:B:33:PRO:HG3	1:B:169:ALA:HB1	1.99	0.45
1:B:285:GLY:O	1:B:287:THR:N	2.50	0.45
1:B:397:SER:CB	1:B:403:ALA:HB2	2.47	0.45
1:B:441:TYR:CZ	1:B:445:LEU:HD21	2.52	0.45
1:A:433:GLU:O	1:A:437:ILE:HG13	2.16	0.45
1:B:131:GLU:O	1:B:160:ARG:HG2	2.16	0.45
1:B:161:PHE:O	1:B:163:ASN:N	2.50	0.45
2:D:416:LEU:HA	2:D:452:ILE:O	2.16	0.45
1:A:107:PHE:HA	1:A:115:ALA:CB	2.47	0.45
1:A:404:GLN:O	1:A:408:MET:HG3	2.17	0.45
2:C:482:ALA:O	2:C:497:ARG:HD3	2.16	0.45
1:B:444:LEU:O	1:B:448:ILE:HG13	2.17	0.45
1:B:92:GLN:HB3	1:B:94:TRP:CE2	2.52	0.45
1:B:389:GLU:O	1:B:393:ILE:HG12	2.17	0.45
2:C:503:LEU:HD22	2:C:518:LEU:CD1	2.46	0.44
2:D:618:ALA:O	2:D:622:PHE:HD1	2.00	0.44
2:D:625:LEU:O	2:D:633:ARG:NE	2.33	0.44
1:A:146:ASN:ND2	1:A:151:GLU:HB2	2.32	0.44
1:B:352:ILE:O	1:B:356:LYS:HG3	2.17	0.44
2:D:449:PHE:CD1	2:D:450:GLN:HG3	2.53	0.44
1:A:119:ARG:HH11	1:A:119:ARG:HB2	1.82	0.44
1:A:246:ILE:CD1	1:A:256:ILE:HG12	2.47	0.44
1:B:107:PHE:CE1	1:B:121:THR:HB	2.52	0.44
1:B:181:PRO:HD3	1:B:327:PHE:CE2	2.52	0.44
1:B:460:ARG:O	1:B:464:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:633:ARG:HD2	4:H:9:DA:OP1	2.18	0.44
1:B:131:GLU:HA	1:B:134:ARG:HG3	1.99	0.44
1:B:421:ILE:HA	1:B:424:MET:HG3	2.00	0.44
2:D:473:ASN:OD1	2:D:476:ILE:HG13	2.17	0.44
4:F:1:DG:H1'	5:F:101:TR6:H011	1.99	0.44
1:B:50:MET:HB3	1:B:55:VAL:HG23	1.99	0.44
1:A:50:MET:HE2	1:A:67:ILE:HD13	1.99	0.44
1:B:403:ALA:O	1:B:407:LEU:HG	2.18	0.44
2:C:445:ARG:HA	2:C:600:MET:HE2	2.00	0.43
2:C:520:THR:HG22	2:C:622:PHE:CE2	2.53	0.43
2:D:532:ALA:HB3	2:D:534:TYR:CD1	2.53	0.43
1:B:383:ALA:HB2	1:B:421:ILE:CD1	2.48	0.43
2:D:537:ILE:HB	2:D:608:ALA:HB3	2.00	0.43
1:B:117:ALA:HB2	4:H:1:DG:H5'	1.99	0.43
4:H:3:DT:H2'	4:H:4:DC:C6	2.53	0.43
2:C:631:GLU:CB	2:C:632:PRO:HD3	2.49	0.43
2:C:522:ILE:HA	2:C:526:MET:HB2	2.00	0.43
1:A:377:LEU:HG	1:A:437:ILE:HG23	2.01	0.43
4:F:8:DC:H2"	4:F:9:DA:H5"	2.00	0.43
1:A:257:VAL:HG22	1:A:301:VAL:HG22	2.00	0.43
2:C:429:LEU:HD12	2:C:501:LEU:CD1	2.49	0.43
1:A:153:GLU:HB2	1:A:154:PRO:HD2	2.01	0.43
1:B:93:TRP:O	1:B:216:PRO:HB2	2.19	0.43
1:B:34:ASP:HB3	1:B:37:ASP:OD1	2.18	0.43
2:C:502:VAL:HG22	2:C:607:MET:CE	2.49	0.43
1:A:172:ILE:HD11	3:E:11:DT:C2	2.54	0.43
1:A:180:ILE:HG23	1:A:181:PRO:HD2	2.01	0.43
1:A:50:MET:HE3	1:A:67:ILE:HG21	2.01	0.43
1:B:29:ALA:C	1:B:41:PRO:HG2	2.39	0.43
1:B:433:GLU:O	1:B:437:ILE:HG13	2.19	0.43
1:B:88:VAL:O	1:B:92:GLN:HG3	2.17	0.43
1:A:132:MET:O	1:A:158:PRO:HD2	2.19	0.43
1:A:56:THR:HB	1:A:57:PRO:CD	2.49	0.43
2:C:418:ASP:HA	2:C:451:ALA:CB	2.49	0.43
1:A:234:GLY:HA2	1:A:331:MET:CE	2.38	0.42
2:C:516:THR:HG23	1:B:15:MET:CE	2.48	0.42
2:D:538:ALA:C	2:D:540:PRO:HD3	2.40	0.42
1:B:465:ILE:O	1:B:469:LEU:HG	2.19	0.42
1:A:34:ASP:HB3	1:A:37:ASP:OD1	2.19	0.42
1:B:380:LEU:O	1:B:384:LEU:HG	2.20	0.42
2:D:441:ALA:O	2:D:445:ARG:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:THR:O	1:A:72:MET:HB3	2.20	0.42
1:A:247:GLU:O	1:A:255:ARG:N	2.52	0.42
2:D:427:THR:HG22	2:D:498:TYR:HD2	1.84	0.42
1:A:67:ILE:HB	1:A:87:MET:HE1	2.02	0.42
1:A:212:GLY:C	1:A:480:ARG:HH22	2.23	0.42
2:D:596:TRP:HA	2:D:600:MET:HB2	2.02	0.42
1:A:154:PRO:HB2	1:A:156:VAL:O	2.20	0.42
1:A:139:ASN:O	1:A:361:ARG:HB3	2.20	0.42
1:B:132:MET:HA	1:B:159:ALA:HA	2.02	0.42
1:A:381:LEU:HA	1:A:381:LEU:HD12	1.88	0.41
1:A:59:LYS:O	1:A:124:ARG:NH1	2.50	0.41
1:B:219:ALA:HB1	1:B:241:ARG:O	2.20	0.41
2:C:442:LYS:HA	2:C:445:ARG:HD3	2.01	0.41
1:A:355:GLN:O	1:A:359:VAL:HG23	2.21	0.41
1:A:181:PRO:HA	1:A:182:PRO:HD3	1.94	0.41
1:B:354:HIS:O	1:B:358:VAL:HG23	2.21	0.41
1:A:160:ARG:NE	1:A:355:GLN:OE1	2.50	0.41
5:H:101:TR6:C01	5:H:101:TR6:N11	2.82	0.41
1:A:25:SER:O	1:A:29:ALA:HB3	2.21	0.41
1:B:146:ASN:ND2	1:B:151:GLU:HB2	2.35	0.41
1:A:202:THR:OG1	1:A:205:ASP:OD2	2.31	0.41
2:C:418:ASP:HA	2:C:451:ALA:HB1	2.02	0.41
2:C:485:THR:HG23	2:C:492:ASP:O	2.21	0.41
1:A:128:ILE:HG12	1:A:161:PHE:CE1	2.57	0.40
1:A:161:PHE:O	1:A:163:ASN:N	2.54	0.40
2:D:527:LYS:N	2:D:528:PRO:CD	2.84	0.40
1:B:76:HIS:HB3	1:B:83:ILE:HD11	2.02	0.40
1:A:285:GLY:O	1:A:304:VAL:HG13	2.22	0.40
1:A:360:VAL:O	1:A:364:ARG:HG3	2.22	0.40
1:B:293:SER:HB3	1:B:298:VAL:HA	2.03	0.40
1:B:390:VAL:O	1:B:394:ILE:HG13	2.21	0.40
1:B:441:TYR:CE2	1:B:445:LEU:HD21	2.56	0.40
1:A:107:PHE:HA	1:A:115:ALA:HB1	2.03	0.40
1:A:148:ASP:HB3	1:A:150:ASN:OD1	2.22	0.40
1:A:156:VAL:O	1:A:157:LEU:HD23	2.22	0.40
1:B:72:MET:HE1	1:B:80:ASP:N	2.37	0.40
1:B:72:MET:HA	1:B:76:HIS:O	2.21	0.40
2:D:633:ARG:HD2	4:F:9:DA:OP1	2.22	0.40
3:G:12:DG:C2'	3:G:13:DT:H72	2.52	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	483/499 (97%)	449 (93%)	30 (6%)	4 (1%)	19	57
1	B	466/499 (93%)	431 (92%)	26 (6%)	9 (2%)	8	38
2	C	193/269 (72%)	166 (86%)	25 (13%)	2 (1%)	15	52
2	D	185/269 (69%)	165 (89%)	16 (9%)	4 (2%)	6	35
All	All	1327/1536 (86%)	1211 (91%)	97 (7%)	19 (1%)	11	44

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	447	ARG
1	B	29	ALA
1	B	286	ILE
1	B	289	VAL
1	A	30	ARG
1	A	331	MET
2	C	415	LYS
1	B	30	ARG
1	B	331	MET
2	D	447	ARG
1	A	296	GLU
1	B	283	ILE
1	B	321	THR
1	B	162	PRO
2	D	491	PHE
1	A	162	PRO
1	B	171	GLY
2	D	408	GLU
2	D	444	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	257/433 (59%)	252 (98%)	5 (2%)	57 80
1	B	215/433 (50%)	209 (97%)	6 (3%)	43 72
2	C	66/226 (29%)	64 (97%)	2 (3%)	41 70
2	D	66/226 (29%)	64 (97%)	2 (3%)	41 70
All	All	604/1318 (46%)	589 (98%)	15 (2%)	47 75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	99	MET
1	A	119	ARG
1	A	148	ASP
1	A	164	LEU
2	C	456	ARG
2	C	607	MET
1	B	66	ARG
1	B	93	TRP
1	B	185	LEU
1	B	228	HIS
1	B	381	LEU
1	B	438	GLN
2	D	449	PHE
2	D	509	VAL

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

Mol	Chain	Res	Type
1	B	118	GLN
1	B	404	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
5	TR6	F	101	6	26,34,34	1.85	8 (30%)	31,53,53	1.96	9 (29%)
5	TR6	H	101	6	26,34,34	1.87	9 (34%)	31,53,53	2.11	10 (32%)

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
5	TR6	F	101	6	-	0/8/29/29	0/5/5/5
5	TR6	H	101	6	-	1/8/29/29	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	101	TR6	C24-C26	4.34	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	TR6	C24-C26	4.26	1.51	1.47
5	H	101	TR6	C12-N13	3.78	1.47	1.37
5	F	101	TR6	C12-N13	3.65	1.46	1.37
5	H	101	TR6	C21-C20	3.31	1.40	1.35
5	F	101	TR6	C12-N11	3.31	1.35	1.31
5	F	101	TR6	C21-C20	3.23	1.40	1.35
5	H	101	TR6	C12-N11	3.23	1.35	1.31
5	F	101	TR6	C12-C20	-2.61	1.39	1.42
5	H	101	TR6	C12-C20	-2.49	1.39	1.42
5	F	101	TR6	F04-C03	-2.36	1.30	1.36
5	H	101	TR6	C14-C15	-2.34	1.50	1.52
5	H	101	TR6	F04-C03	-2.32	1.30	1.36
5	H	101	TR6	C22-C10	-2.27	1.38	1.41
5	F	101	TR6	C14-C15	-2.25	1.50	1.52
5	H	101	TR6	C19-C18	-2.03	1.50	1.52
5	F	101	TR6	C19-C18	-2.02	1.50	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	101	TR6	N11-C12-N13	-4.67	114.30	117.62
5	H	101	TR6	C25-N09-C10	4.44	122.29	118.14
5	F	101	TR6	C25-N09-C10	4.23	122.09	118.14
5	H	101	TR6	C21-C20-C12	-4.00	119.16	121.73
5	F	101	TR6	C21-C20-C12	-3.92	119.21	121.73
5	H	101	TR6	C12-N11-C10	3.81	124.21	118.69
5	F	101	TR6	C12-N11-C10	3.43	123.67	118.69
5	H	101	TR6	F30-C20-C12	3.28	123.06	119.92
5	F	101	TR6	C06-C05-C03	3.14	119.92	116.62
5	H	101	TR6	C06-C05-C03	3.06	119.83	116.62
5	F	101	TR6	N11-C12-N13	-2.96	115.52	117.62
5	F	101	TR6	C02-C03-C05	-2.70	119.78	123.29
5	H	101	TR6	C02-C03-C05	-2.65	119.84	123.29
5	H	101	TR6	C20-C12-N13	2.63	127.46	123.82
5	F	101	TR6	F30-C20-C12	2.55	122.36	119.92
5	F	101	TR6	C25-C24-C23	-2.53	118.69	119.97
5	F	101	TR6	C19-N13-C14	2.52	114.98	111.67
5	H	101	TR6	C25-C24-C23	-2.30	118.81	119.97
5	H	101	TR6	F30-C20-C21	-2.04	117.78	120.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	101	TR6	N11-C12-N13-C14

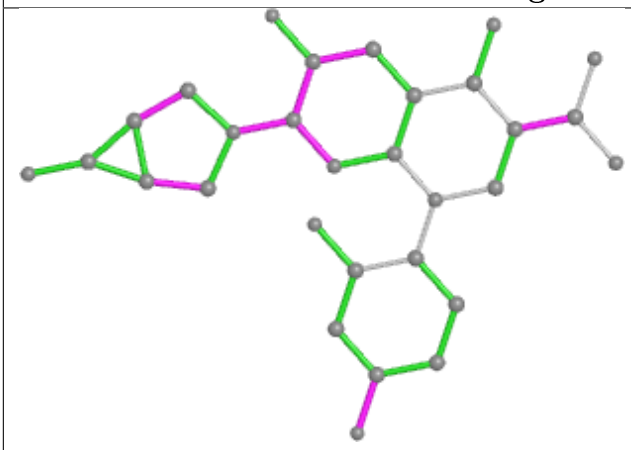
There are no ring outliers.

2 monomers are involved in 4 short contacts:

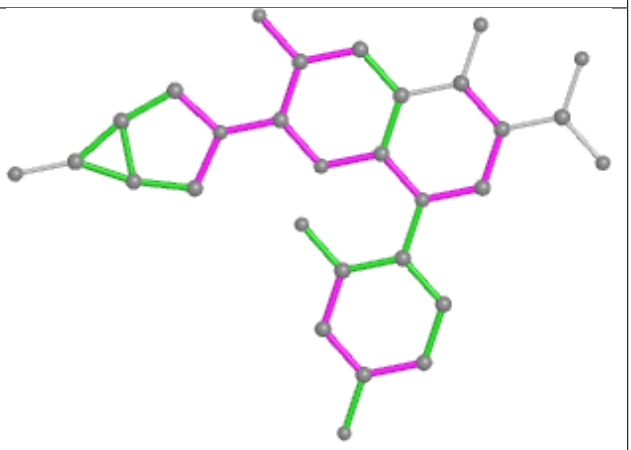
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	101	TR6	3	0
5	H	101	TR6	1	0

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

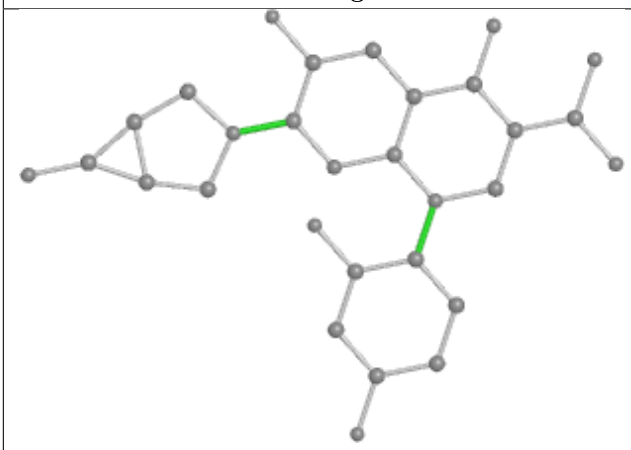
Ligand TR6 F 101



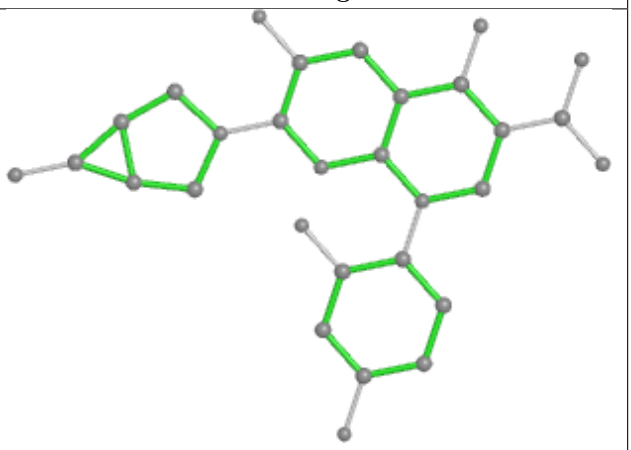
Bond lengths



Bond angles

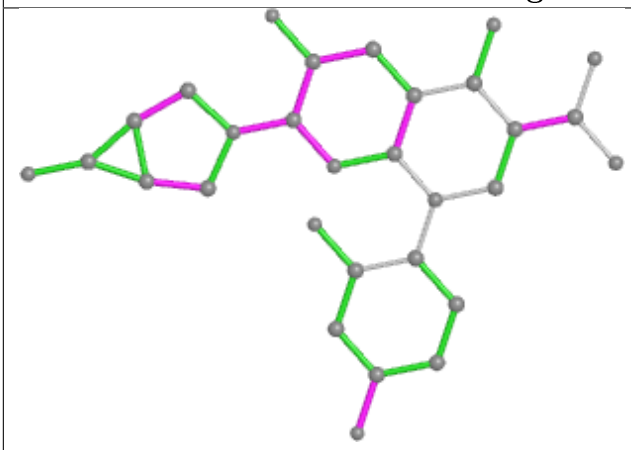


Torsions

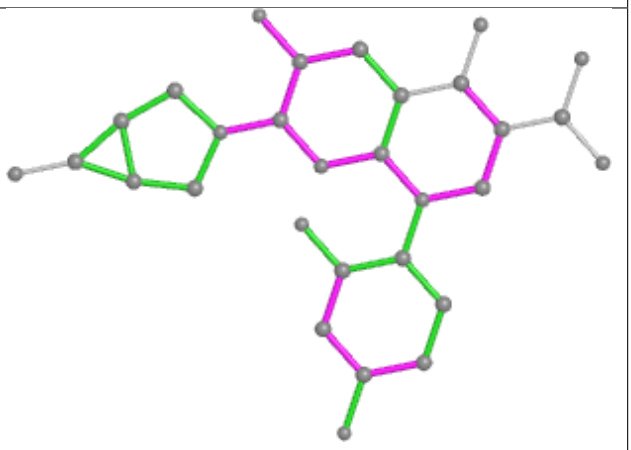


Rings

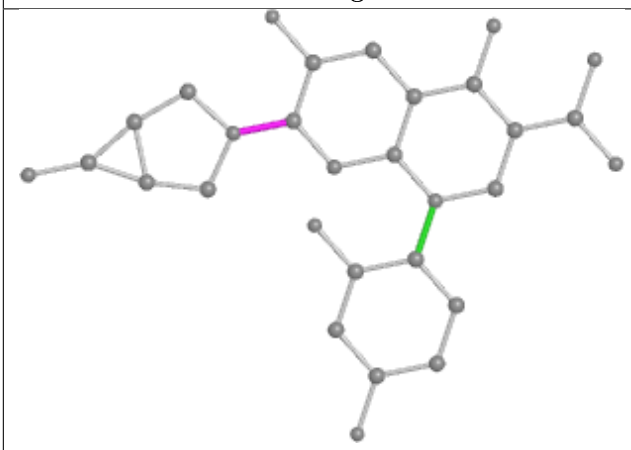
Ligand TR6 H 101



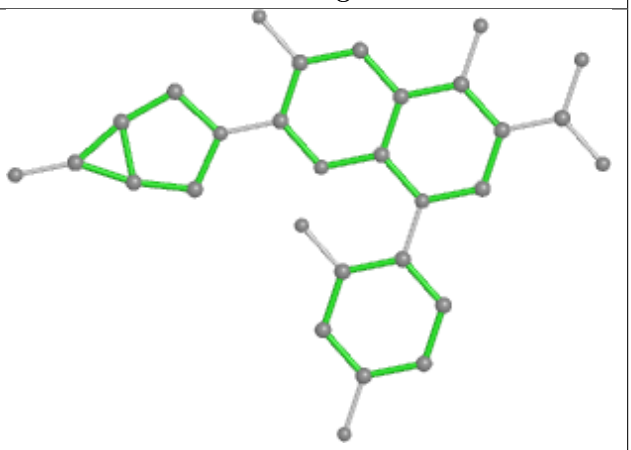
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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^{th} 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	485/499 (97%)	-0.24	2 (0%) 92 90	76, 117, 151, 190	0
1	B	472/499 (94%)	-0.21	9 (1%) 66 64	80, 125, 175, 206	0
2	C	197/269 (73%)	-0.05	7 (3%) 42 41	99, 144, 183, 197	0
2	D	191/269 (71%)	-0.14	4 (2%) 63 61	103, 142, 185, 199	0
3	E	8/15 (53%)	0.01	0 100 100	116, 123, 188, 205	0
3	G	7/15 (46%)	-0.05	0 100 100	115, 118, 164, 181	0
4	F	12/19 (63%)	-0.04	0 100 100	124, 144, 171, 197	0
4	H	11/19 (57%)	-0.26	0 100 100	112, 136, 166, 194	0
All	All	1383/1604 (86%)	-0.18	22 (1%) 72 69	76, 127, 177, 206	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	643	TYR	3.4
1	B	82	SER	3.3
1	B	256	ILE	2.9
1	B	81	SER	2.8
2	C	437	ALA	2.8
2	D	644	SER	2.8
2	D	507	ALA	2.7
2	C	428	GLU	2.5
1	B	482	THR	2.5
2	D	590	MET	2.5
2	C	429	LEU	2.4
1	B	261	PHE	2.4
1	B	213	PRO	2.3
1	B	80	ASP	2.3
1	A	80	ASP	2.2
1	B	211	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	450	GLN	2.2
2	C	430	PHE	2.1
2	C	488	GLY	2.1
1	B	215	PHE	2.1
1	A	19	PHE	2.0
2	D	540	PRO	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 carbohydrates in this entry.

6.4 Ligands (i)

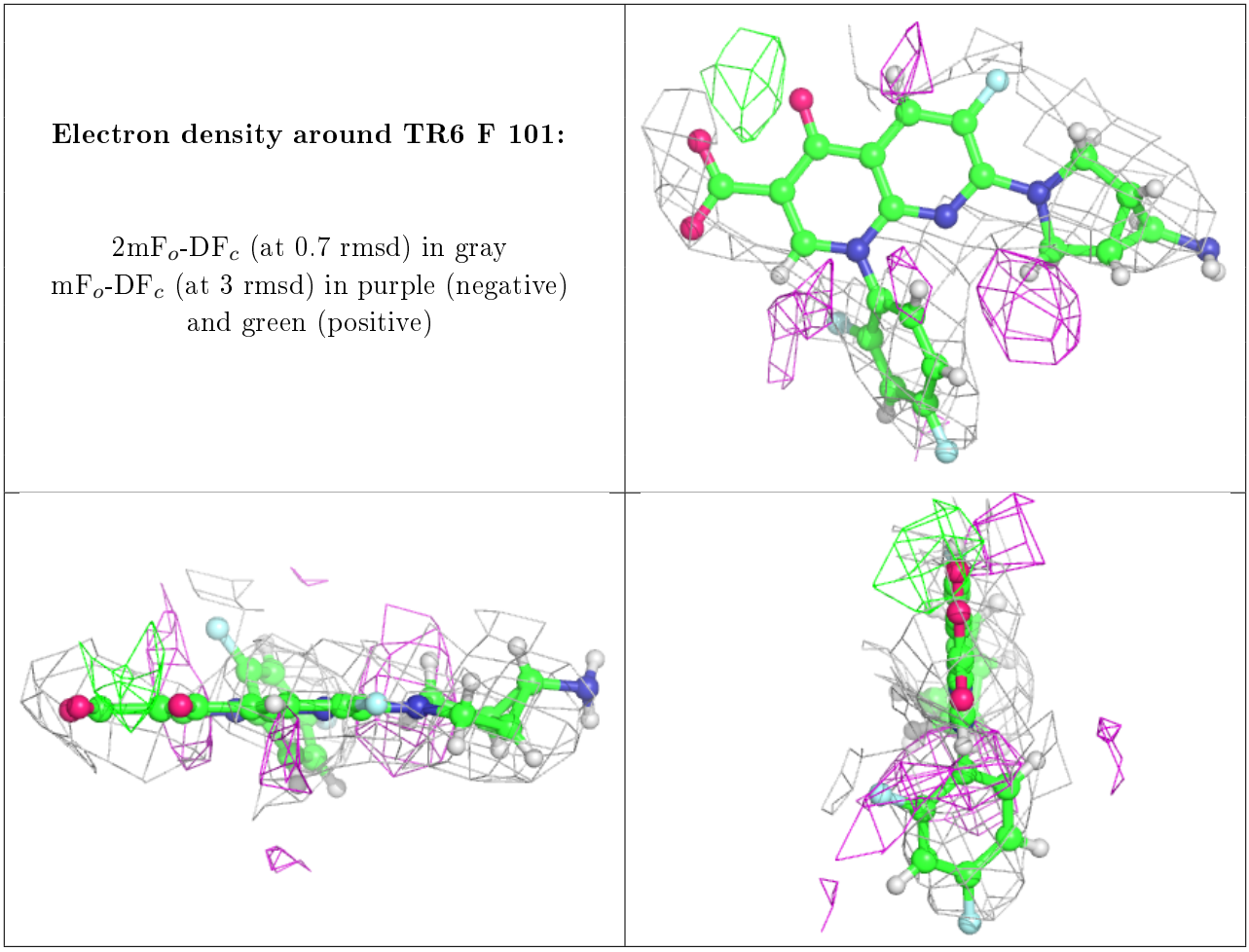
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	H	102	1/1	0.58	0.38	148,148,148,148	0
5	TR6	F	101	30/30	0.75	0.31	213,253,296,309	0
6	MG	F	102	1/1	0.83	0.77	201,201,201,201	0
5	TR6	H	101	30/30	0.83	0.30	136,191,236,244	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.

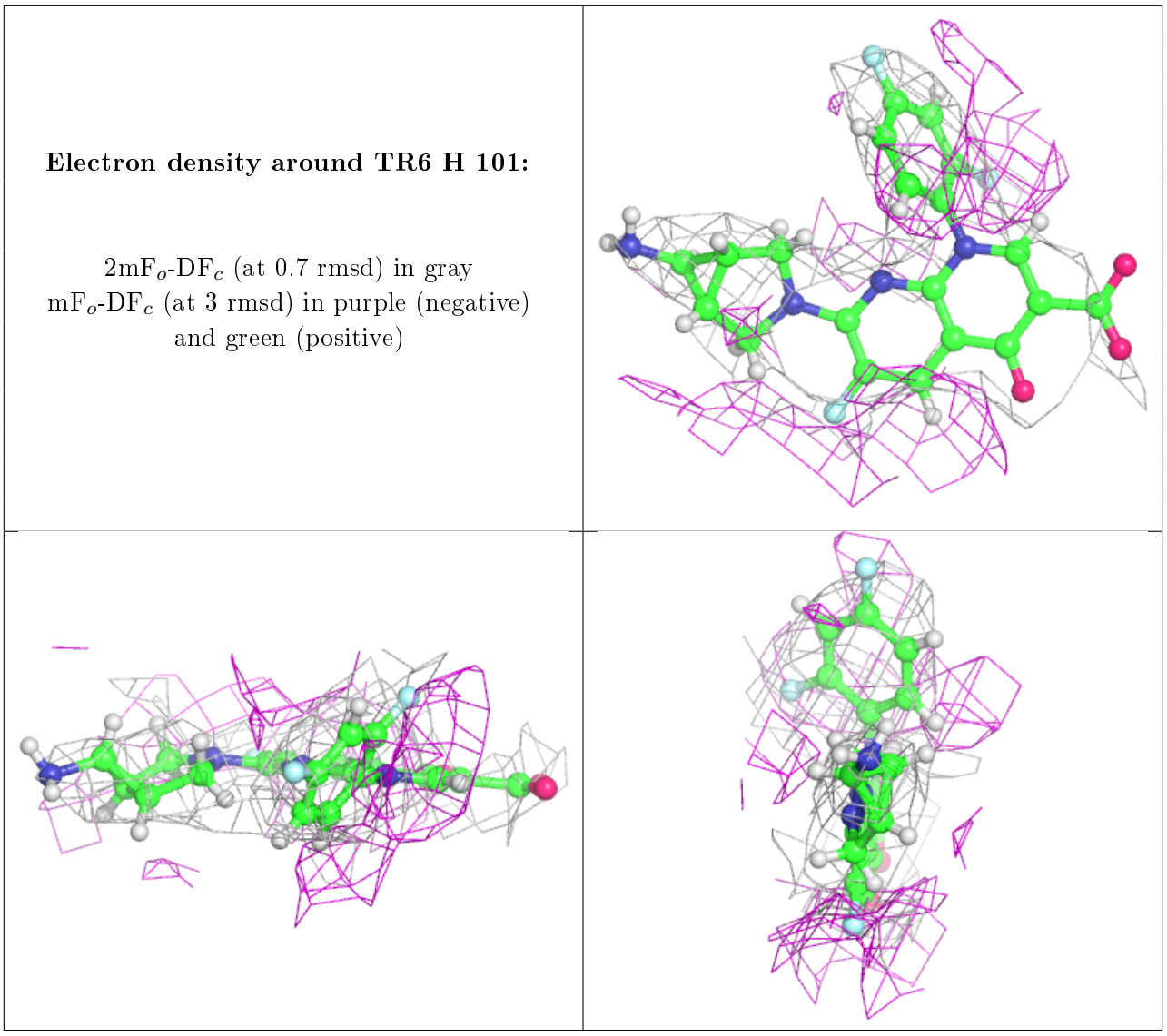
Electron density around TR6 F 101:

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



Electron density around TR6 H 101:

$2mF_o$-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.