



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:40 PM UTC

PDB ID : 8QMC / pdb_00008qmc
Title : High resolution structure of the Streptococcus pneumoniae topoisomerase IV-complex with the V-site 18mer dsDNA and novel fluoroquinolone Delafloxacin
Authors : Najmudin, S.; Pan, X.S.; Wang, B.; Chayen, N.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2023-09-21
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

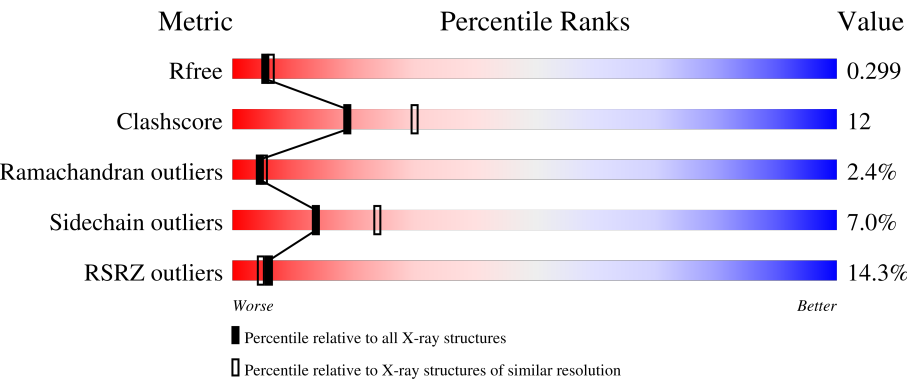
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	742	15% 71% 22% 5% .
1	B	742	12% 70% 25% . .
2	E	7	57% 29% 14%
3	F	11	9% 64% 36%

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Mol	Chain	Length	Quality of chain
4	H	11	27% 36% 55% 9%
5	G	7	14% 14% 86%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 24995 atoms, of which 12198 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 (ATP-hydrolyzing), DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	724	Total 11662	C 3651	H 5882	N 1007	O 1097	S 25	325	3	0
1	B	724	Total 11620	C 3641	H 5859	N 1000	O 1096	S 24	321	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	initiating methionine	UNP J0V1V8
A	404	LYS	-	expression tag	UNP J0V1V8
A	405	ASN	-	expression tag	UNP J0V1V8
A	406	LYS	-	expression tag	UNP J0V1V8
A	407	LYS	-	expression tag	UNP J0V1V8
A	408	ASP	-	expression tag	UNP J0V1V8
A	409	LYS	-	expression tag	UNP J0V1V8
A	410	GLY	-	expression tag	UNP J0V1V8
A	411	LEU	-	expression tag	UNP J0V1V8
A	648	HIS	-	linker	UNP J0V1V8
A	1257	THR	ILE	conflict	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	-	initiating methionine	UNP J0V1V8
B	404	LYS	-	expression tag	UNP J0V1V8
B	405	ASN	-	expression tag	UNP J0V1V8
B	406	LYS	-	expression tag	UNP J0V1V8
B	407	LYS	-	expression tag	UNP J0V1V8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	ASP	-	expression tag	UNP J0V1V8
B	409	LYS	-	expression tag	UNP J0V1V8
B	410	GLY	-	expression tag	UNP J0V1V8
B	411	LEU	-	expression tag	UNP J0V1V8
B	648	HIS	-	linker	UNP J0V1V8
B	1257	THR	ILE	conflict	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 DNA (5'-D(*T)-R(P*G)-D(P*T)-R(P*GP*GP*A)-D(P*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	7	Total	C	H	N	O	P	1	0	0
			225	70	81	26	42	6			

- Molecule 3 is a DNA chain called DNA/RNA (5'-R(P*GP*G)-D(P*TP*T)-R(P*A)-D(P*T)-R(P*CP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	11	Total	C	H	N	O	P	1	0	0
			349	107	125	40	66	11			

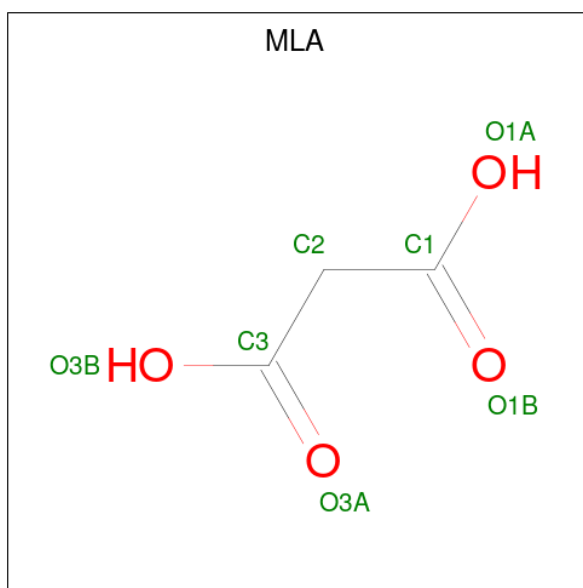
- Molecule 4 is a DNA chain called DNA/RNA (5'-R(P*AP*AP*CP*CP*G)-D(P*T)-R(P*A)-D(P*TP*T)-R(P*AP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	11	Total	C	H	N	O	P	1	0	0
			348	107	125	40	65	11			

- Molecule 5 is a DNA chain called DNA/RNA (5'-R(*G)-D(P*T)-R(P*AP*A)-D(P*T)-R(P*AP*C)-3').

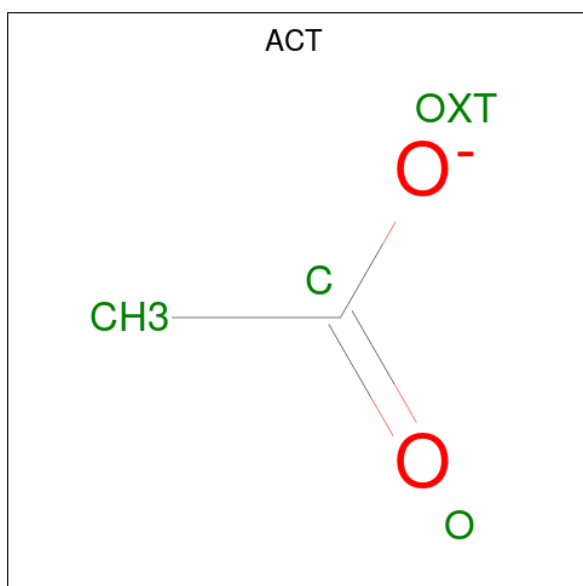
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	G	7	Total	C	H	N	O	P	1	0	0
			221	69	80	27	39	6			

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			9	3	2	4		
6	A	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		

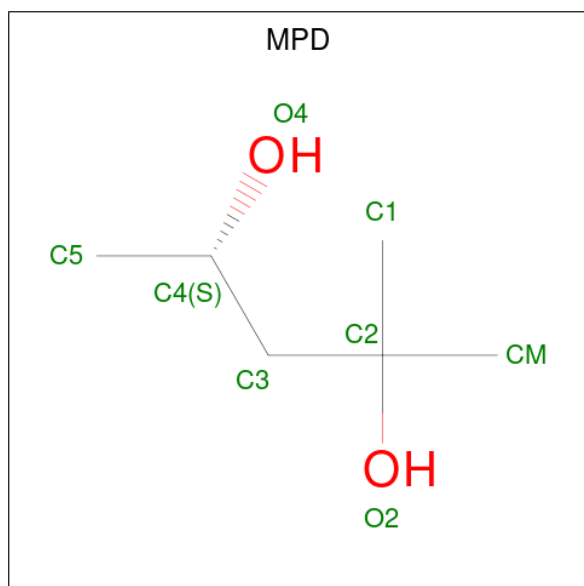
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	Mg	0	0
			3	3		
8	B	3	Total	Mg	0	0
			3	3		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	B	1	Total	Cl	0	0
			1	1		

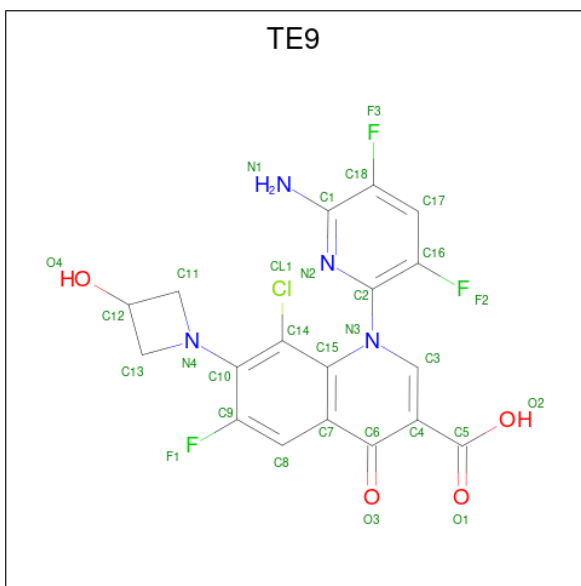
- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	1	0
			22	6	14	2		

- Molecule 11 is delafloxacin (CCD ID: TE9) (formula: C₁₈H₁₂ClF₃N₄O₄) (labeled as "Ligand

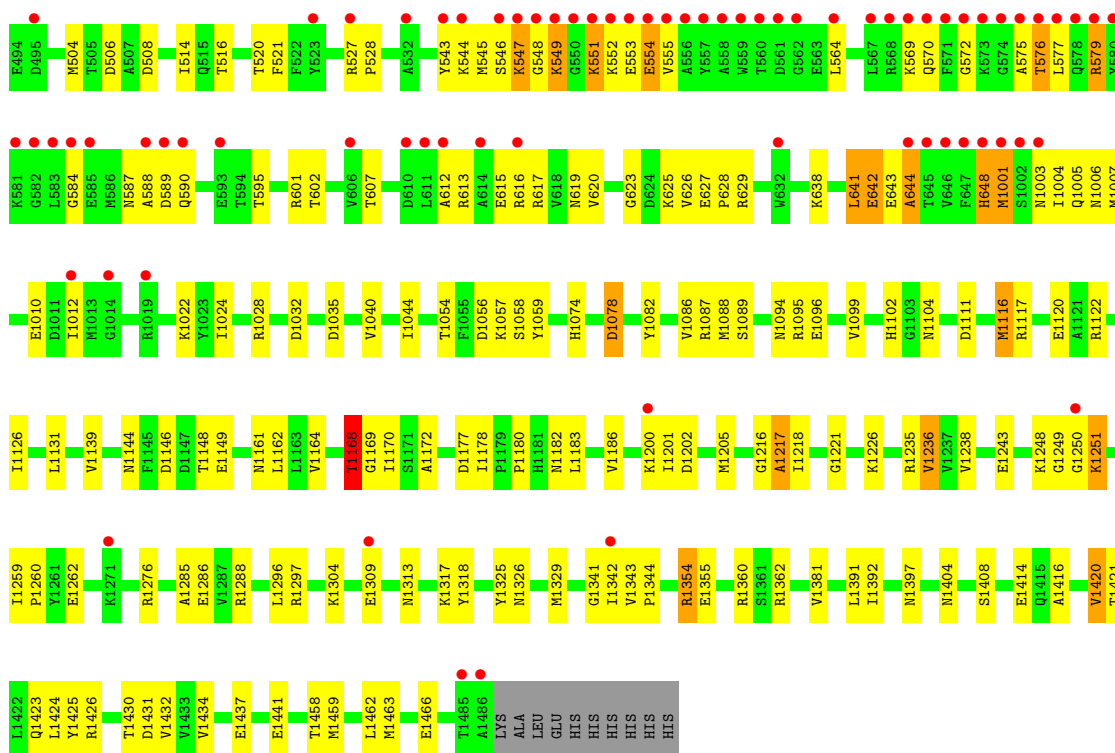
of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
11	F	1	Total 41	C 18	Cl 1	F 3	H 11	N 4	O 4	1	0
11	H	1	Total 41	C 18	Cl 1	F 3	H 11	N 4	O 4	1	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	193	Total O 193 193	0	0
12	B	199	Total O 199 199	0	0
12	E	8	Total O 8 8	0	0
12	F	9	Total O 9 9	0	0
12	H	10	Total O 10 10	0	0
12	G	7	Total O 7 7	0	0



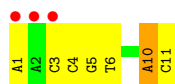
- Molecule 2: DNA (5'-D(*T)-R(P*G)-D(P*T)-R(P*GP*GP*A)-D(P*T)-3')



- Molecule 3: DNA/RNA (5'-R(P*GP*G)-D(P*TP*T)-R(P*A)-D(P*T)-R(P*CP*CP*AP*CP*A)-3')



- Molecule 4: DNA/RNA (5'-R(P*AP*AP*CP*CP*G)-D(P*T)-R(P*A)-D(P*TP*T)-R(P*AP*C)-3')



- Molecule 5: DNA/RNA (5'-R(*G)-D(P*T)-R(P*AP*A)-D(P*T)-R(P*AP*C)-3')



G9
T10
A11
A12
T13
A14
G15

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.14Å 157.14Å 211.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.86 – 2.40 64.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	50.9 (64.86-2.40) 50.9 (64.86-2.40)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PDB-REDO	Depositor
R, R_{free}	0.241 , 0.299 0.241 , 0.299	Depositor DCC
R_{free} test set	3070 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24995	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MLA, ACT, TE9, CL, MG

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	0.54	0/5880	1.06	3/7927 (0.0%)
1	B	0.53	0/5858	1.03	5/7900 (0.1%)
2	E	0.54	0/161	1.22	1/248 (0.4%)
3	F	0.63	0/250	1.21	1/383 (0.3%)
4	H	0.53	0/249	1.30	6/381 (1.6%)
5	G	0.54	0/158	1.26	0/242
All	All	0.54	0/12556	1.06	16/17081 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	2
All	All	0	8

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	ASP	CA-CB-CG	8.93	121.53	112.60
4	H	10	DA	P-O3'-C3'	-6.92	109.82	120.20
1	B	1111	ASP	CB-CA-C	6.91	120.27	109.42
4	H	3	DC	P-O3'-C3'	-6.79	110.02	120.20
4	H	4	DC	P-O3'-C3'	-6.51	110.43	120.20
4	H	5	DG	P-O3'-C3'	-5.82	111.48	120.20
1	B	1168	THR	CB-CA-C	5.77	119.37	110.14
1	B	506	ASP	CA-CB-CG	5.50	118.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	DG	P-O3'-C3'	-5.40	112.11	120.20
2	E	14	DA	P-O3'-C3'	-5.25	112.33	120.20
1	A	508	ASP	CA-CB-CG	5.22	117.83	112.60
4	H	5	DG	C4-N9-C1'	-5.21	119.19	127.00
1	A	1367	LYS	CB-CA-C	-5.17	102.54	110.81
1	A	506	ASP	CA-CB-CG	5.15	117.75	112.60
4	H	5	DG	C8-N9-C1'	5.08	134.62	127.00
1	B	1111	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1276	ARG	Sidechain
1	A	1353	ARG	Sidechain
1	A	1426	ARG	Sidechain
1	A	537	ILE	Peptide
1	A	550	GLY	Peptide
1	A	551	LYS	Peptide
1	B	1117	ARG	Sidechain
1	B	1354	ARG	Sidechain

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	5780	5882	5871	136	0
1	B	5761	5859	5848	137	0
2	E	144	81	82	6	0
3	F	224	125	125	3	0
4	H	223	125	125	6	0
5	G	141	80	81	11	0
6	A	14	4	4	1	0
7	A	8	6	6	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
9	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	1	0	0	0	0
10	B	8	14	14	3	0
11	F	30	11	0	4	0
11	H	30	11	0	4	0
12	A	193	0	0	27	0
12	B	199	0	0	21	0
12	E	8	0	0	1	0
12	F	9	0	0	1	0
12	G	7	0	0	0	0
12	H	10	0	0	0	0
All	All	12797	12198	12156	289	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 12.

All (289) 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)
11:H:101:TE9:CL1	11:H:101:TE9:N2	2.25	1.05
1:B:623:GLY:O	1:B:629:ARG:NH2	1.94	0.99
11:F:101:TE9:CL1	11:F:101:TE9:N2	2.33	0.98
1:B:1001:MET:HB3	1:B:1005:GLN:HE21	1.26	0.98
11:F:101:TE9:CL1	11:F:101:TE9:C2	2.54	0.93
11:H:101:TE9:CL1	11:H:101:TE9:C2	2.57	0.89
1:A:528:PRO:HA	12:A:1620:HOH:O	1.75	0.87
1:A:623:GLY:O	1:A:629:ARG:NH2	2.09	0.84
1:B:1408:SER:HB2	12:B:1602:HOH:O	1.76	0.84
1:B:1430:THR:HG22	10:B:1501:MPD:H52	1.61	0.81
1:A:1443[A]:ARG:NH1	6:A:1502:MLA:O1A	2.14	0.81
1:A:461:ASN:ND2	1:A:622[B]:MET:HE3	2.03	0.73
5:G:10:DT:H2''	5:G:11:DA:O5'	1.88	0.73
1:B:1202:ASP:OD1	1:B:1226:LYS:HE3	1.91	0.70
1:A:545:MET:HB3	1:A:567:LEU:HD23	1.74	0.69
1:B:555:VAL:HA	12:B:1725:HOH:O	1.91	0.69
1:A:531:GLU:HB2	12:A:1620:HOH:O	1.94	0.68
1:B:1054:THR:OG1	1:B:1056:ASP:OD1	2.12	0.68
1:A:1055:PHE:HA	1:A:1122:ARG:HD2	1.78	0.66
1:B:1178:ILE:HG23	1:B:1329:MET:HE2	1.76	0.66
1:A:546:SER:HB3	1:A:554:GLU:HB3	1.75	0.66
1:B:1423:GLN:NE2	1:B:1425:TYR:HE2	1.94	0.66
1:B:1003:ASN:HB3	1:B:1004:ILE:HD12	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1286:GLU:OE1	1:B:1288:ARG:NH1	2.30	0.65
1:B:612:ALA:HA	12:B:1701:HOH:O	1.96	0.65
2:E:9:DT:H5''	2:E:9:DT:H6	1.62	0.65
11:H:101:TE9:CL1	11:H:101:TE9:C13	2.82	0.64
1:A:461:ASN:HD21	1:A:622[B]:MET:HB3	1.62	0.64
1:B:527:ARG:N	1:B:528:PRO:HD2	2.13	0.64
1:B:1423:GLN:HE21	1:B:1425:TYR:HE2	1.44	0.64
1:B:1010:GLU:HA	12:B:1735:HOH:O	1.98	0.64
1:B:1243:GLU:HB3	12:B:1714:HOH:O	1.98	0.64
1:A:1391:LEU:HD21	1:A:1404:ASN:HB2	1.79	0.63
1:A:1431:ASP:OD2	1:A:1434:VAL:HG23	1.99	0.63
1:B:615:GLU:O	1:B:619:ASN:ND2	2.31	0.63
1:A:463:ALA:HB2	12:A:1627:HOH:O	1.98	0.63
1:B:1341:GLY:O	1:B:1344:PRO:HD2	1.99	0.63
2:E:9:DT:H6	2:E:9:DT:C5'	2.12	0.63
1:A:647:PHE:O	1:A:1001:MET:HE2	1.99	0.62
1:A:1308:THR:HB	12:A:1736:HOH:O	1.98	0.62
1:A:1044:ILE:O	1:A:1048:MET:HG3	1.99	0.61
1:B:1001:MET:CB	1:B:1005:GLN:HE21	2.09	0.60
11:F:101:TE9:CL1	11:F:101:TE9:C13	2.87	0.60
11:H:101:TE9:CL1	11:H:101:TE9:C1	2.87	0.60
1:A:584:GLY:HA2	12:A:1770:HOH:O	2.02	0.60
1:A:528:PRO:CA	12:A:1620:HOH:O	2.41	0.60
1:A:609:GLU:O	1:A:610:ASP:CB	2.50	0.59
1:B:1216:GLY:O	1:B:1217:ALA:HB3	2.03	0.59
1:B:1004:ILE:HD12	1:B:1004:ILE:H	1.68	0.59
1:A:506:ASP:C	1:A:508:ASP:H	2.11	0.59
1:B:1326:ASN:ND2	4:H:11:DC:H4'	2.17	0.58
1:A:1420:VAL:HG13	1:B:1425:TYR:HB3	1.83	0.58
1:B:1024[A]:ILE:HD11	1:B:1172:ALA:HB2	1.84	0.58
1:B:432:VAL:HG22	1:B:504:MET:HE2	1.85	0.58
1:B:607:THR:HG21	1:B:1006:ASN:HD22	1.68	0.58
1:A:1070:MET:HE1	1:A:1078:ASP:HB3	1.84	0.58
1:B:548:GLY:HA2	1:B:551:LYS:CG	2.34	0.58
1:A:590:GLN:HG3	12:A:1735:HOH:O	2.04	0.58
1:A:616:ARG:O	1:A:620:VAL:HG12	2.03	0.57
1:A:1222:ARG:HH11	1:A:1484:ASP:CG	2.12	0.57
1:B:1360:ARG:HD3	12:B:1691:HOH:O	2.03	0.57
1:B:1431:ASP:CG	1:B:1434:VAL:HG23	2.28	0.57
1:B:1296:LEU:HD23	1:B:1297:ARG:N	2.20	0.57
1:B:548:GLY:HA2	1:B:551:LYS:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:TRP:HA	1:A:596:MET:HB2	1.87	0.57
1:A:1411:PHE:HZ	12:A:1700:HOH:O	1.87	0.57
5:G:12:DA:H2'	5:G:12:DA:O5'	2.05	0.57
1:B:587:ASN:O	1:B:589:ASP:N	2.38	0.56
1:B:1362:ARG:HD3	12:B:1674:HOH:O	2.05	0.56
1:A:609:GLU:O	1:A:610:ASP:HB2	2.05	0.56
2:E:12:DG:H8	12:E:103:HOH:O	1.88	0.56
1:B:584:GLY:HA2	12:B:1765:HOH:O	2.04	0.56
1:A:579:ARG:HH11	1:A:579:ARG:HB3	1.70	0.56
1:A:1173:GLY:O	1:A:1174:TYR:CG	2.59	0.56
1:A:1116:MET:HE2	12:B:1704:HOH:O	2.05	0.56
1:A:1293:ARG:HG2	1:A:1293:ARG:HH11	1.71	0.55
1:B:613:ARG:HG2	1:B:613:ARG:HH11	1.71	0.55
1:A:1383:SER:HB2	12:A:1673:HOH:O	2.06	0.55
1:A:531:GLU:CB	12:A:1620:HOH:O	2.50	0.55
11:F:101:TE9:CL1	11:F:101:TE9:C1	2.92	0.55
1:A:1274:ASP:O	1:A:1278:ASN:ND2	2.40	0.55
1:B:491:PHE:CD2	1:B:528:PRO:HG2	2.42	0.55
1:B:638:LYS:CG	1:B:641:LEU:HD23	2.37	0.54
1:B:1004:ILE:HD12	1:B:1004:ILE:N	2.23	0.54
1:A:1293:ARG:HD3	1:B:589:ASP:OD1	2.08	0.54
1:B:1326:ASN:HD21	4:H:11:DC:H4'	1.71	0.54
1:B:415:LYS:O	1:B:454:PRO:HD2	2.07	0.54
1:A:594:THR:OG1	1:A:595:THR:HG22	2.08	0.53
1:A:1308:THR:HG23	12:A:1723:HOH:O	2.08	0.53
1:B:1235:ARG:HB2	12:B:1630:HOH:O	2.08	0.53
1:A:1117:ARG:NH1	12:A:1603:HOH:O	2.37	0.53
1:B:1168:THR:HG22	12:B:1692:HOH:O	2.07	0.53
1:A:1371:ARG:O	1:A:1375:VAL:HG23	2.09	0.53
4:H:10:DA:H61	5:G:10:DT:H3	1.57	0.52
1:B:627:GLU:N	1:B:628:PRO:HD2	2.24	0.52
1:A:1182:ASN:O	1:A:1186:VAL:HG23	2.10	0.52
1:B:1216:GLY:O	1:B:1217:ALA:CB	2.57	0.52
1:A:503:ILE:O	1:A:538:ALA:HB2	2.10	0.52
1:B:1170:ILE:HD11	5:G:11:DA:C2	2.45	0.52
1:B:1205:MET:CE	1:B:1226:LYS:HA	2.40	0.52
1:A:464:LYS:O	1:A:465:ALA:C	2.52	0.51
1:B:643:GLU:O	1:B:644:ALA:C	2.53	0.51
1:B:615:GLU:HG3	1:B:619:ASN:HD21	1.74	0.51
1:B:1035:ASP:O	1:B:1161:ASN:HB3	2.11	0.51
1:A:1001:MET:HG3	1:A:1005:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1381:VAL:HA	12:A:1700:HOH:O	2.11	0.51
1:A:504:MET:HA	1:A:538:ALA:HB2	1.92	0.51
1:A:1296:LEU:HD23	1:A:1297:ARG:N	2.26	0.51
1:B:626:VAL:HG11	4:H:10:DA:OP2	2.11	0.51
1:B:1391:LEU:HD11	1:B:1404:ASN:HB3	1.93	0.51
12:B:1617:HOH:O	4:H:1:DA:H8	1.94	0.51
1:B:1001:MET:HB3	1:B:1005:GLN:NE2	2.10	0.50
1:A:1333:ASP:OD2	1:A:1338:ARG:NH1	2.43	0.50
1:A:1384:ILE:HD13	1:A:1409:TYR:CD1	2.47	0.50
1:B:641:LEU:O	1:B:1022:LYS:NZ	2.44	0.50
1:A:524:ARG:O	1:A:525:TYR:CD1	2.65	0.50
1:B:1182:ASN:O	1:B:1186:VAL:HG23	2.11	0.50
1:B:1205:MET:HE1	1:B:1226:LYS:HA	1.92	0.50
1:A:597:ASN:ND2	1:A:599:GLU:HB2	2.27	0.50
1:A:1334:ASN:O	1:A:1336:THR:HG23	2.12	0.50
1:B:1218:ILE:O	1:B:1238:VAL:HA	2.10	0.50
1:B:1458:THR:HA	12:B:1671:HOH:O	2.11	0.50
1:B:602:THR:HG21	1:B:648:HIS:NE2	2.26	0.50
5:G:9:DG:H4'	5:G:10:DT:O5'	2.12	0.50
1:A:1381:VAL:O	1:A:1382:ILE:C	2.55	0.50
1:A:465:ALA:O	1:A:470:ILE:HD11	2.11	0.50
1:B:547:LYS:HB3	1:B:575:ALA:HB2	1.94	0.49
1:B:1088:MET:HA	1:B:1094:ASN:ND2	2.27	0.49
1:B:1354:ARG:HG3	1:B:1459:MET:CE	2.41	0.49
1:A:1400:ASP:OD2	1:A:1404:ASN:ND2	2.37	0.49
1:B:1144:ASN:ND2	1:B:1149:GLU:HB3	2.26	0.49
1:A:488:GLY:O	1:A:489:ALA:CB	2.61	0.49
1:A:1354:ARG:HG3	1:A:1459:MET:HE2	1.93	0.49
1:B:416:LEU:HD22	1:B:482:THR:HG23	1.95	0.49
1:A:463:ALA:O	1:A:464:LYS:C	2.55	0.49
1:A:1173:GLY:O	1:A:1174:TYR:CD2	2.66	0.49
1:A:490:ASP:OD1	1:A:490:ASP:N	2.45	0.49
1:B:1082:TYR:O	1:B:1086:VAL:HG23	2.13	0.49
1:B:1087:ARG:HG2	1:B:1087:ARG:HH11	1.76	0.49
1:B:1169:GLY:C	1:B:1170:ILE:HG13	2.38	0.49
1:B:1317:LYS:HD3	1:B:1318:TYR:CE2	2.48	0.49
1:B:1028:ARG:CZ	5:G:14:DA:H4'	2.43	0.49
1:A:481:TYR:CD1	1:A:481:TYR:C	2.91	0.49
1:B:547:LYS:HG2	1:B:554:GLU:HG3	1.95	0.49
1:B:642:GLU:C	1:B:643:GLU:HG3	2.38	0.49
1:B:1146:ASP:OD1	1:B:1148:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:HG2	1:A:568:ARG:HH11	1.78	0.48
1:A:1273:ASP:OD1	1:A:1276:ARG:NH1	2.46	0.48
1:B:638:LYS:HG3	1:B:641:LEU:HD23	1.95	0.48
1:A:543:TYR:HB3	1:A:577:LEU:HD11	1.94	0.48
1:A:1011:ASP:OD1	1:A:1011:ASP:N	2.45	0.48
1:A:1028:ARG:CZ	2:E:14:DA:H4'	2.44	0.48
1:A:1258:GLU:HA	12:A:1658:HOH:O	2.14	0.48
1:A:1259:ILE:HB	1:A:1260:PRO:CD	2.44	0.48
1:B:1420:VAL:HG12	1:B:1421:THR:HG23	1.96	0.48
1:A:467:MET:O	1:A:468:ALA:HB3	2.12	0.47
1:B:1397:ASN:HB2	12:B:1652:HOH:O	2.14	0.47
1:A:463:ALA:CB	12:A:1627:HOH:O	2.57	0.47
1:A:546:SER:HB3	1:A:554:GLU:CB	2.44	0.47
1:B:460:ILE:HA	4:H:6:DT:O3'	2.14	0.47
1:B:1249:GLY:O	1:B:1304:LYS:HE2	2.14	0.47
1:A:478:THR:O	1:A:482:THR:OG1	2.32	0.47
1:B:1262:GLU:HG3	5:G:11:DA:H4'	1.96	0.47
1:A:414:GLY:HA3	1:A:454:PRO:O	2.15	0.47
1:A:1333:ASP:O	1:A:1334:ASN:C	2.58	0.47
1:B:1057:LYS:O	1:B:1122:ARG:NH1	2.45	0.47
1:B:1355:GLU:HA	1:B:1355:GLU:OE1	2.13	0.47
1:B:1360:ARG:HH22	1:B:1466:GLU:CD	2.23	0.47
12:B:1779:HOH:O	5:G:9:DG:H5'	2.15	0.47
1:B:1096:GLU:HG2	1:B:1126:ILE:HD13	1.97	0.47
1:B:1164:VAL:HG21	1:B:1183:LEU:HD12	1.97	0.47
1:B:1262:GLU:CG	5:G:11:DA:H4'	2.45	0.47
1:A:1007:MET:HE2	1:A:1012:ILE:CD1	2.45	0.47
1:A:1007:MET:HE2	1:A:1012:ILE:HD13	1.97	0.47
1:B:1259:ILE:HB	1:B:1260:PRO:CD	2.45	0.47
5:G:12:DA:H4'	5:G:13:DT:OP1	2.15	0.47
1:A:509:THR:HB	12:A:1791:HOH:O	2.15	0.47
1:B:446:ASP:O	1:B:450:GLN:HB2	2.14	0.47
1:A:605:ARG:HH11	1:A:605:ARG:CB	2.28	0.46
1:B:481:TYR:CD1	1:B:481:TYR:C	2.93	0.46
1:B:1056:ASP:OD1	1:B:1056:ASP:N	2.48	0.46
1:B:579:ARG:HB3	1:B:579:ARG:HH11	1.80	0.46
1:A:531:GLU:CG	12:A:1620:HOH:O	2.64	0.46
1:A:1216:GLY:O	1:A:1217:ALA:HB3	2.16	0.46
1:A:1419:ILE:O	1:B:1424:LEU:HD12	2.15	0.46
1:B:520:THR:O	1:B:521:PHE:C	2.59	0.46
1:A:461:ASN:O	1:A:465:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:ILE:HG12	1:B:1329:MET:HG2	1.97	0.46
1:A:627:GLU:N	1:A:628:PRO:CD	2.78	0.46
1:B:1095:ARG:HG3	1:B:1095:ARG:HH11	1.81	0.46
1:B:1082:TYR:CD1	1:B:1116:MET:HB3	2.51	0.46
1:A:1382:ILE:HG22	12:A:1663:HOH:O	2.16	0.46
1:B:475:GLU:O	1:B:479:MET:HG3	2.16	0.46
1:B:1326:ASN:HB2	12:B:1655:HOH:O	2.15	0.46
1:A:1201:ILE:HG13	1:A:1230:GLU:HG3	1.97	0.45
1:A:591:LEU:HD12	1:A:595:THR:HG23	1.97	0.45
1:B:1078:ASP:CG	12:B:1704:HOH:O	2.59	0.45
1:B:1200:LYS:HB2	12:B:1616:HOH:O	2.16	0.45
1:A:548:GLY:O	1:A:549:LYS:HB3	2.16	0.45
1:A:1391:LEU:HD23	1:A:1391:LEU:C	2.42	0.45
1:B:638:LYS:HG2	1:B:641:LEU:HD23	1.97	0.45
1:B:1040:VAL:O	1:B:1044:ILE:HG13	2.16	0.45
1:B:1040:VAL:HG23	1:B:1074:HIS:CD2	2.51	0.45
1:B:1205:MET:HE1	1:B:1226:LYS:CA	2.47	0.45
5:G:10:DT:H2'	5:G:11:DA:C8	2.52	0.45
1:A:474:GLU:O	1:A:478:THR:HG23	2.16	0.45
1:B:1426:ARG:O	10:B:1501:MPD:H31	2.17	0.45
1:B:1296:LEU:HD23	1:B:1296:LEU:C	2.42	0.45
1:A:611:LEU:C	1:A:611:LEU:HD23	2.42	0.45
1:B:547:LYS:HG3	1:B:572:GLY:HA3	1.98	0.45
1:B:1459:MET:SD	1:B:1459:MET:C	3.00	0.45
1:A:1431:ASP:HB2	12:A:1745:HOH:O	2.16	0.45
2:E:9:DT:C5'	2:E:9:DT:C6	2.97	0.45
1:A:528:PRO:C	12:A:1620:HOH:O	2.61	0.44
1:A:610:ASP:OD2	1:A:613:ARG:HD3	2.18	0.44
1:A:1192:TYR:CE1	1:A:1196:HIS:CE1	3.06	0.44
1:B:1408:SER:CB	12:B:1602:HOH:O	2.52	0.44
1:A:595:THR:O	1:A:595:THR:OG1	2.32	0.44
1:A:1102:HIS:CE1	1:B:590:GLN:HE22	2.35	0.44
1:B:1205:MET:HE1	1:B:1226:LYS:CB	2.48	0.44
1:A:1036:GLY:HA2	1:A:1162:LEU:HD13	1.99	0.43
1:B:1416:ALA:O	1:B:1420:VAL:HB	2.18	0.43
1:B:545:MET:HA	1:B:576:THR:O	2.18	0.43
1:B:617:ARG:HA	12:B:1627:HOH:O	2.18	0.43
1:B:1236:VAL:HG12	1:B:1325:TYR:HB3	2.00	0.43
1:A:626:VAL:HG11	3:F:10:DC:OP2	2.19	0.43
1:A:527:ARG:N	1:A:528:PRO:CD	2.81	0.43
1:B:460:ILE:HD12	1:B:473:ASN:ND2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1276:ARG:HD2	1:B:1285:ALA:O	2.17	0.43
1:A:1023:TYR:HE2	1:A:1028:ARG:HH21	1.66	0.43
1:A:1193:MET:CE	1:A:1347:SER:HB3	2.49	0.43
1:B:481:TYR:C	1:B:481:TYR:HD1	2.26	0.43
1:A:625:LYS:HB2	1:A:628:PRO:HD2	2.01	0.42
1:A:1107:SER:OG	1:A:1111:ASP:OD1	2.33	0.42
1:B:411:LEU:O	1:B:456:ARG:NH1	2.51	0.42
1:B:430:TYR:OH	1:B:601:ARG:NH1	2.52	0.42
1:B:1089:SER:HA	1:B:1099:VAL:O	2.19	0.42
1:B:1426:ARG:HD2	10:B:1501:MPD:HM3	2.00	0.42
1:B:1462:LEU:O	1:B:1463:MET:C	2.61	0.42
1:A:1397:ASN:HB2	12:A:1633:HOH:O	2.19	0.42
1:B:474:GLU:O	1:B:478:THR:HG23	2.19	0.42
1:B:1004:ILE:HG22	1:B:1005:GLN:N	2.35	0.42
1:A:556:ALA:HB3	1:A:567:LEU:HD21	2.01	0.42
1:A:1060:ARG:HD3	12:A:1744:HOH:O	2.20	0.42
1:A:1060:ARG:NH2	12:A:1621:HOH:O	2.53	0.42
1:A:1015:GLU:O	1:A:1019[A]:ARG:HB2	2.20	0.42
1:B:544:LYS:O	1:B:577:LEU:HA	2.20	0.42
1:B:1177:ASP:HB3	1:B:1325:TYR:OH	2.20	0.42
1:A:458:LYS:HD3	1:A:458:LYS:HA	1.93	0.42
1:A:1464:LYS:O	1:A:1465:LYS:C	2.63	0.42
1:B:527:ARG:N	1:B:528:PRO:CD	2.81	0.42
1:B:1095:ARG:HB2	1:B:1180:PRO:HB3	2.02	0.42
1:A:481:TYR:C	1:A:481:TYR:HD1	2.26	0.41
1:A:1033:ILE:HA	1:A:1162:LEU:HD22	2.02	0.41
1:A:543:TYR:HB2	1:A:558:ALA:HB3	2.03	0.41
1:A:545:MET:O	1:A:546:SER:HB2	2.21	0.41
1:A:1028:ARG:NH1	2:E:14:DA:H4'	2.34	0.41
1:B:1001:MET:H	1:B:1005:GLN:NE2	2.18	0.41
1:B:1250:GLY:O	1:B:1251:LYS:O	2.38	0.41
1:A:589:ASP:HB2	12:A:1735:HOH:O	2.21	0.41
1:B:1201:ILE:O	1:B:1202:ASP:C	2.64	0.41
1:A:1220:GLN:HG2	1:A:1483:GLU:HB2	2.03	0.41
1:A:1386:ASP:OD1	1:A:1386:ASP:N	2.47	0.41
1:B:1425:TYR:CD1	1:B:1425:TYR:C	2.98	0.41
1:A:544:LYS:O	1:A:577:LEU:HD12	2.20	0.41
1:A:579:ARG:HB3	12:A:1616:HOH:O	2.21	0.41
1:A:1344:PRO:O	1:A:1348:SER:OG	2.26	0.41
1:B:625:LYS:HB3	1:B:628:PRO:CG	2.50	0.41
1:B:1414:GLU:HG2	12:B:1787:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:C	1:A:525:TYR:CD1	2.99	0.41
1:A:1051:ASP:HB3	1:A:1060:ARG:HH12	1.86	0.41
1:A:1308:THR:CG2	12:A:1723:HOH:O	2.66	0.41
1:A:1402:LYS:O	1:A:1405:LEU:HB2	2.21	0.41
1:B:543:TYR:HB3	1:B:577:LEU:HD21	2.01	0.41
1:B:616:ARG:O	1:B:620:VAL:HG12	2.21	0.41
1:A:1082:TYR:O	1:A:1086:VAL:HG23	2.20	0.41
1:A:1174:TYR:C	3:F:9:DA:H4'	2.46	0.41
1:A:548:GLY:O	1:A:549:LYS:CB	2.69	0.40
1:A:1183:LEU:HD13	1:A:1183:LEU:C	2.45	0.40
1:A:1245:GLU:CD	1:A:1255:VAL:HG21	2.46	0.40
1:A:1428:THR:HG22	1:B:1392:ILE:O	2.22	0.40
1:A:1008:SER:HB2	12:A:1778:HOH:O	2.20	0.40
1:B:625:LYS:HE2	1:B:625:LYS:HA	2.02	0.40
1:A:597:ASN:HD21	1:A:599:GLU:HB2	1.87	0.40
1:A:621:LEU:HB3	1:A:622[A]:MET:HE3	2.03	0.40
1:A:1203:LYS:HA	1:A:1203:LYS:HD2	1.88	0.40
1:A:626:VAL:O	1:A:629:ARG:HB3	2.22	0.40
1:A:1219:ILE:HB	1:A:1482:LEU:HD23	2.03	0.40
3:F:7:DC:H1'	12:F:203:HOH:O	2.20	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	725/742 (98%)	657 (91%)	49 (7%)	19 (3%)	4	4
1	B	723/742 (97%)	660 (91%)	47 (6%)	16 (2%)	5	6
All	All	1448/1484 (98%)	1317 (91%)	96 (7%)	35 (2%)	4	5

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ALA
1	A	549	LYS
1	A	610	ASP
1	B	569	LYS
1	B	588	ALA
1	B	1217	ALA
1	B	1251	LYS
1	A	464	LYS
1	A	488	GLY
1	A	526	MET
1	A	546	SER
1	A	1003	ASN
1	A	1217	ALA
1	A	1410	ASP
1	B	466	LYS
1	B	552	LYS
1	B	553	GLU
1	B	554	GLU
1	B	570	GLN
1	B	644	ALA
1	A	424	PRO
1	A	463	ALA
1	A	507	ALA
1	A	1174	TYR
1	B	642	GLU
1	B	648	HIS
1	B	1059	TYR
1	A	467	MET
1	B	467	MET
1	A	538	ALA
1	B	549	LYS
1	A	1075	PRO
1	A	550	GLY
1	A	1221	GLY
1	B	1221	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/635 (98%)	574 (92%)	48 (8%)	12	20
1	B	620/635 (98%)	580 (94%)	40 (6%)	15	27
All	All	1242/1270 (98%)	1154 (93%)	88 (7%)	14	23

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	LEU
1	A	415	LYS
1	A	462	THR
1	A	466	LYS
1	A	472	LYS
1	A	490	ASP
1	A	492	SER
1	A	493	ILE
1	A	499	ASP
1	A	509	THR
1	A	516	THR
1	A	539	LEU
1	A	555	VAL
1	A	570	GLN
1	A	573	LYS
1	A	579	ARG
1	A	593	GLU
1	A	595	THR
1	A	602	THR
1	A	605	ARG
1	A	616	ARG
1	A	622[A]	MET
1	A	622[B]	MET
1	A	645	THR
1	A	1011	ASP
1	A	1027	ASP
1	A	1048	MET
1	A	1102	HIS
1	A	1111	ASP
1	A	1139	VAL
1	A	1168	THR
1	A	1177	ASP
1	A	1187	ILE
1	A	1222	ARG
1	A	1236	VAL

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Mol	Chain	Res	Type
1	A	1275	VAL
1	A	1279	ASN
1	A	1281	VAL
1	A	1301	GLU
1	A	1308	THR
1	A	1336	THR
1	A	1367	LYS
1	A	1381	VAL
1	A	1382	ILE
1	A	1383	SER
1	A	1386	ASP
1	A	1403	GLU
1	A	1420	VAL
1	B	422	LYS
1	B	472	LYS
1	B	482	THR
1	B	492	SER
1	B	514	ILE
1	B	516	THR
1	B	546	SER
1	B	547	LYS
1	B	549	LYS
1	B	551	LYS
1	B	564	LEU
1	B	576	THR
1	B	579	ARG
1	B	595	THR
1	B	641	LEU
1	B	1001	MET
1	B	1007	MET
1	B	1012	ILE
1	B	1032	ASP
1	B	1058	SER
1	B	1078	ASP
1	B	1102	HIS
1	B	1104	ASN
1	B	1116	MET
1	B	1120	GLU
1	B	1131	LEU
1	B	1139	VAL
1	B	1162	LEU
1	B	1168	THR

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Mol	Chain	Res	Type
1	B	1236	VAL
1	B	1248	LYS
1	B	1309	GLU
1	B	1313	ASN
1	B	1342	ILE
1	B	1343	VAL
1	B	1381	VAL
1	B	1420	VAL
1	B	1432	VAL
1	B	1437	GLU
1	B	1441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	477	ASN
1	A	597	ASN
1	A	1003	ASN
1	A	1005	GLN
1	A	1102	HIS
1	A	1267	ASN
1	A	1278	ASN
1	B	427	ASN
1	B	473	ASN
1	B	497	ASN
1	B	515	GLN
1	B	578	GLN
1	B	590	GLN
1	B	619	ASN
1	B	636	ASN
1	B	1005	GLN
1	B	1006	ASN
1	B	1053	ASN
1	B	1094	ASN
1	B	1132	GLN
1	B	1397	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\# Z > 2$
6	MLA	A	1501	-	6,6,6	1.28	0	7,7,7	1.12	0
10	MPD	B	1501	-	7,7,7	0.21	0	9,10,10	0.57	0
7	ACT	A	1503	-	3,3,3	1.04	0	3,3,3	1.09	0
11	TE9	F	101	8	32,33,33	1.10	3 (9%)	38,51,51	1.22	3 (7%)
7	ACT	A	1504	-	3,3,3	1.20	0	3,3,3	0.91	0
11	TE9	H	101	8	32,33,33	1.13	2 (6%)	38,51,51	1.21	2 (5%)
6	MLA	A	1502	-	6,6,6	1.32	0	7,7,7	1.09	0

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
6	MLA	A	1501	-	-	0/4/4/4	-
10	MPD	B	1501	-	-	0/5/5/5	-
11	TE9	F	101	8	-	3/11/20/20	0/4/4/4
11	TE9	H	101	8	-	6/11/20/20	0/4/4/4
6	MLA	A	1502	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	101	TE9	C2-C16	-2.83	1.39	1.42
11	H	101	TE9	C1-C18	2.51	1.42	1.39
11	F	101	TE9	C2-C16	-2.34	1.39	1.42
11	F	101	TE9	C1-C18	2.29	1.42	1.39
11	F	101	TE9	O1-C5	2.25	1.28	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	101	TE9	C17-C18-C1	-3.23	119.56	121.68
11	F	101	TE9	C17-C18-C1	-3.19	119.59	121.68
11	H	101	TE9	C4-C3-N3	-2.76	120.55	123.81
11	F	101	TE9	C4-C3-N3	-2.55	120.80	123.81
11	F	101	TE9	C1-N2-C2	2.10	122.34	116.99

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	101	TE9	N2-C2-N3-C3
11	H	101	TE9	N2-C2-N3-C3
6	A	1502	MLA	C1-C2-C3-O3A
11	H	101	TE9	C6-C4-C5-O2
6	A	1502	MLA	C1-C2-C3-O3B
11	H	101	TE9	C3-C4-C5-O2
11	H	101	TE9	C6-C4-C5-O1
11	H	101	TE9	C3-C4-C5-O1
11	F	101	TE9	C16-C2-N3-C15
11	H	101	TE9	C16-C2-N3-C15
11	F	101	TE9	C6-C4-C5-O1

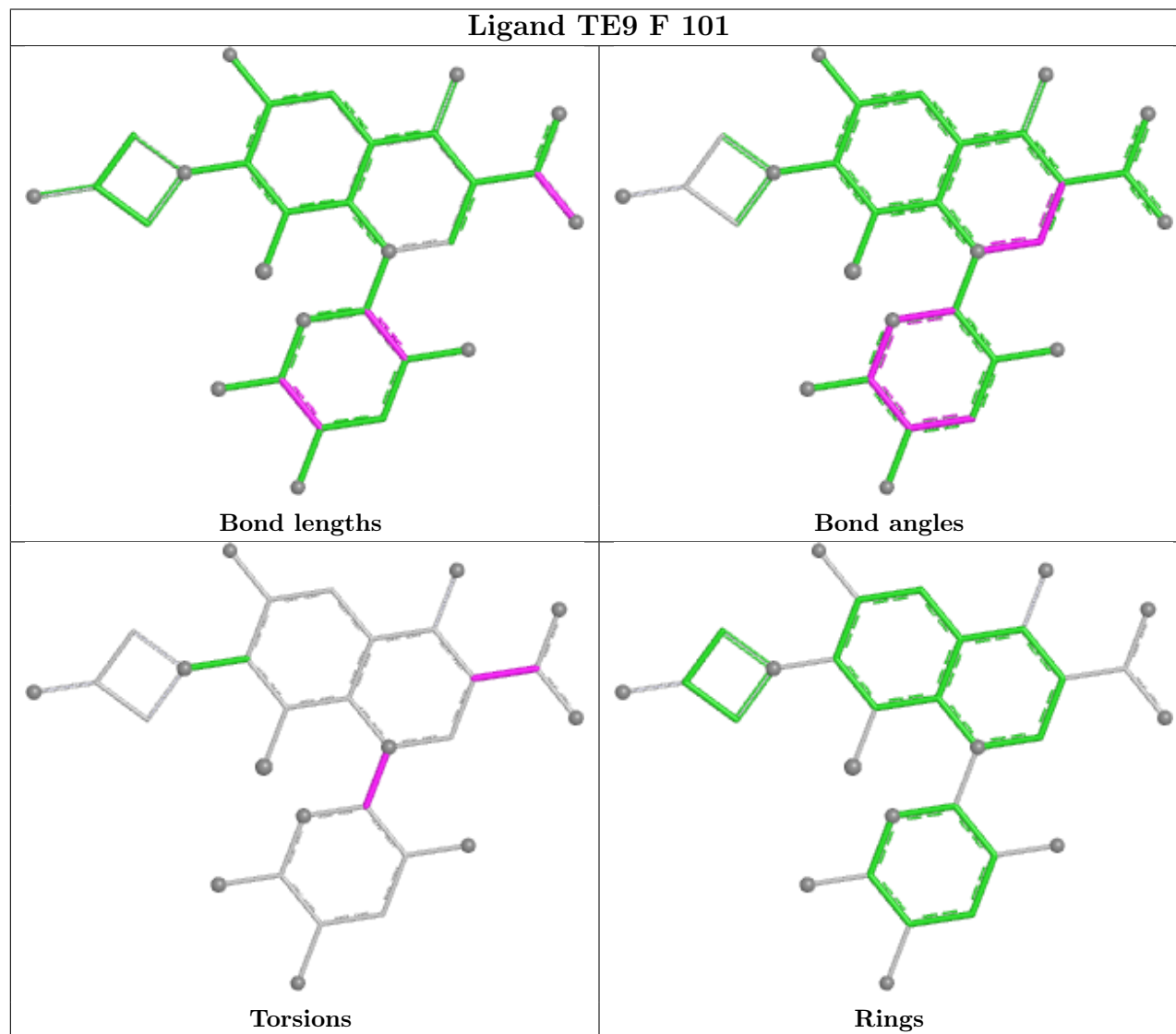
There are no ring outliers.

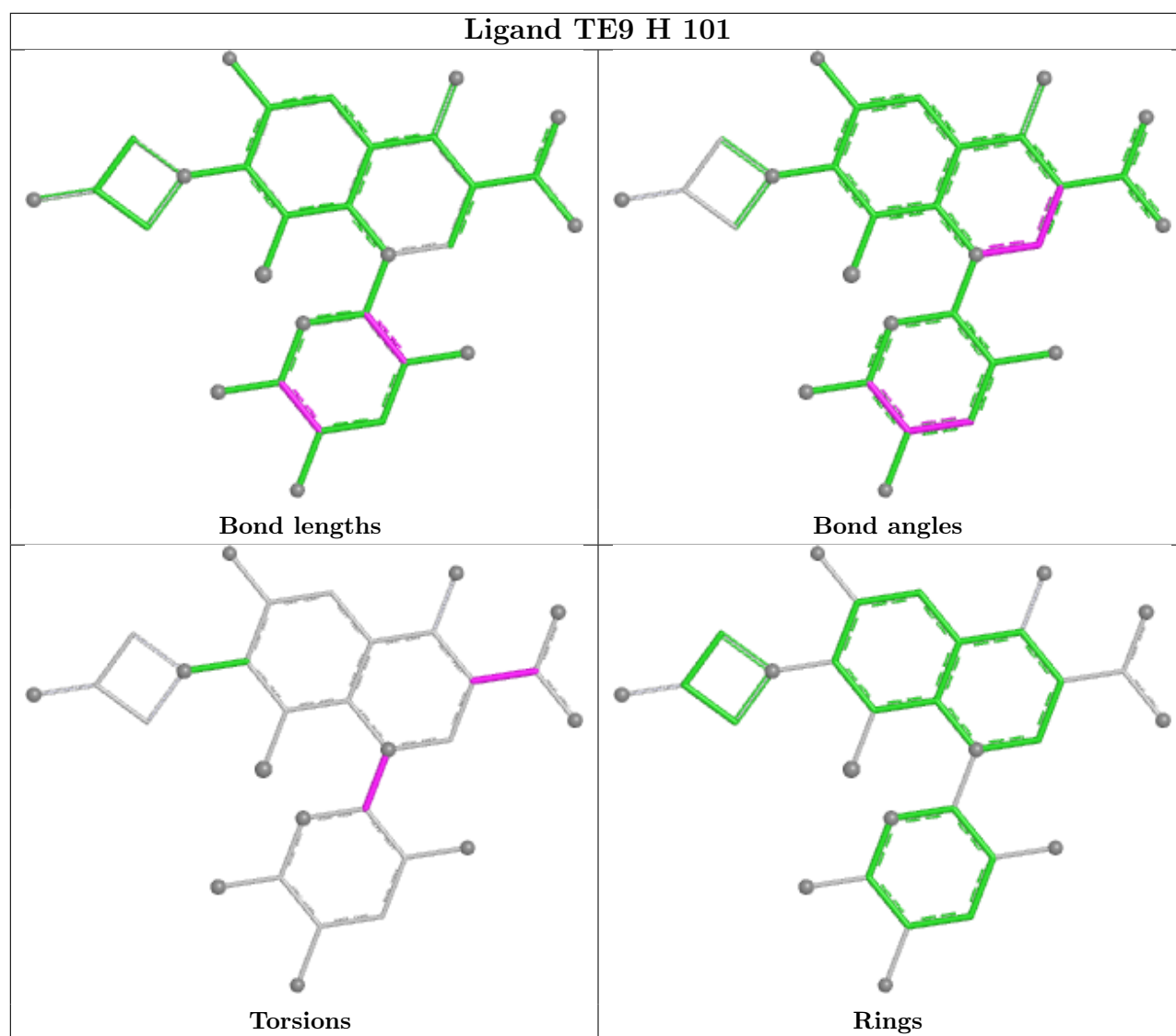
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1501	MPD	3	0
11	F	101	TE9	4	0
11	H	101	TE9	4	0
6	A	1502	MLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	724/742 (97%)	0.77	115 (15%) 5 4	6, 21, 65, 93	3 (0%)
1	B	724/742 (97%)	0.60	92 (12%) 8 6	6, 19, 57, 87	1 (0%)
2	E	7/7 (100%)	0.36	0 100 100	16, 16, 36, 52	0
3	F	11/11 (100%)	0.77	1 (9%) 15 12	20, 28, 51, 55	0
4	H	11/11 (100%)	1.39	3 (27%) 1 1	37, 47, 64, 65	0
5	G	7/7 (100%)	0.11	1 (14%) 6 5	12, 14, 36, 54	0
All	All	1484/1520 (97%)	0.69	212 (14%) 6 5	6, 21, 61, 93	4 (0%)

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	555	VAL	8.5
1	A	644	ALA	8.1
1	A	646	VAL	8.0
1	B	571	PHE	7.7
1	B	644	ALA	7.6
1	A	647	PHE	7.5
1	A	571	PHE	7.4
1	A	551	LYS	7.3
1	A	574	GLY	7.0
1	B	1001	MET	6.8
1	B	646	VAL	6.7
1	B	550	GLY	6.5
1	B	570	GLN	6.4
1	B	549	LYS	6.4
1	B	572	GLY	6.3
1	A	572	GLY	6.0
1	B	647	PHE	5.8
1	A	645	THR	5.8
1	A	466	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	553	GLU	5.7
1	A	567	LEU	5.7
1	B	551	LYS	5.7
1	B	552	LYS	5.4
1	A	570	GLN	5.4
1	A	549	LYS	5.4
1	A	411	LEU	5.4
1	B	645	THR	5.3
1	A	576	THR	5.3
1	A	547	LYS	5.0
1	A	575	ALA	5.0
1	A	578	GLN	4.9
1	A	471	LEU	4.9
1	A	641	LEU	4.9
1	B	548	GLY	4.9
1	B	569	LYS	4.8
1	B	411	LEU	4.8
1	A	1485	THR	4.7
1	A	565	GLU	4.7
1	A	560	THR	4.7
1	B	574	GLY	4.6
1	A	1002	SER	4.6
1	A	467	MET	4.6
1	B	556	ALA	4.5
1	A	564	LEU	4.5
1	A	1003	ASN	4.5
1	B	413	SER	4.4
1	A	1001	MET	4.4
1	A	553	GLU	4.4
1	A	562	GLY	4.3
1	B	466	LYS	4.3
1	A	484	GLY	4.3
1	B	611	LEU	4.3
1	A	468	ALA	4.3
1	B	584	GLY	4.2
1	A	425	ALA	4.2
1	B	576	THR	4.2
1	A	555	VAL	4.2
1	B	1003	ASN	4.2
1	B	648	HIS	4.1
1	A	469	ASP	4.1
1	A	573	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1486	ALA	4.1
1	A	415	LYS	4.1
1	B	554	GLU	4.0
1	A	525	TYR	4.0
1	B	557	TYR	4.0
1	A	550	GLY	3.9
1	A	568	ARG	3.9
1	A	556	ALA	3.8
1	A	488	GLY	3.8
1	A	606	VAL	3.8
1	B	414	GLY	3.8
1	A	493	ILE	3.8
1	B	412	LEU	3.8
1	B	523	TYR	3.7
1	B	1486	ALA	3.7
1	A	607	THR	3.7
1	A	648	HIS	3.6
1	B	546	SER	3.6
1	A	569	LYS	3.6
1	B	468	ALA	3.5
1	B	471	LEU	3.5
1	A	481	TYR	3.5
1	A	487	VAL	3.4
1	A	554	GLU	3.4
1	A	557	TYR	3.4
1	A	616	ARG	3.4
1	A	465	ALA	3.3
1	A	480	ILE	3.3
1	A	496	ALA	3.3
1	B	489	ALA	3.3
1	A	534	HIS	3.3
1	B	575	ALA	3.3
1	B	1485	THR	3.2
1	A	563	GLU	3.2
1	B	415	LYS	3.2
1	B	562	GLY	3.2
1	A	561	ASP	3.2
1	B	612	ALA	3.1
1	A	611	LEU	3.1
1	B	467	MET	3.1
1	A	1484	ASP	3.1
1	A	543	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	544	LYS	3.1
1	A	412	LEU	3.1
1	B	579	ARG	3.1
1	A	552	LYS	3.0
1	B	547	LYS	3.0
1	A	643	GLU	3.0
1	B	573	LYS	3.0
1	B	581	LYS	3.0
1	A	546	SER	3.0
1	B	578	GLN	3.0
1	A	476	ILE	2.9
1	A	559	TRP	2.9
1	B	559	TRP	2.9
1	B	543	TYR	2.9
1	A	470	ILE	2.9
1	A	485	ALA	2.9
1	A	533	GLY	2.9
1	B	1002	SER	2.9
1	A	615	GLU	2.9
1	A	422	LYS	2.9
1	A	536	TYR	2.9
1	A	584	GLY	2.9
1	A	472	LYS	2.9
1	A	642	GLU	2.9
1	A	424	PRO	2.8
1	B	465	ALA	2.8
1	A	539	LEU	2.8
1	A	577	LEU	2.8
1	B	588	ALA	2.8
1	A	1295	GLY	2.7
1	B	582	GLY	2.7
1	A	523	TYR	2.7
1	A	614	ALA	2.7
1	A	622[A]	MET	2.7
1	B	590	GLN	2.7
1	A	414	GLY	2.7
1	B	472	LYS	2.7
1	A	494	GLU	2.7
1	A	489	ALA	2.7
1	A	1005	GLN	2.7
1	A	580	TYR	2.6
1	B	614	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	H	3	DC	2.6
5	G	9	DG	2.6
1	A	625	LYS	2.6
1	B	568	ARG	2.6
1	A	605	ARG	2.5
1	B	469	ASP	2.5
1	A	420	GLN	2.5
1	B	486	GLY	2.5
1	B	593	GLU	2.5
1	B	532	ALA	2.5
1	B	560	THR	2.5
1	A	499	ASP	2.5
4	H	2	DA	2.5
1	B	418	PRO	2.5
1	B	585	GLU	2.4
1	B	476	ILE	2.4
1	A	586	MET	2.4
1	A	585	GLU	2.4
1	B	580	TYR	2.4
1	A	544	LYS	2.4
1	B	1271	LYS	2.4
1	A	413	SER	2.3
1	B	567	LEU	2.3
1	B	475	GLU	2.3
1	A	603	LEU	2.3
1	A	608	ILE	2.3
1	B	495	ASP	2.3
1	B	558	ALA	2.3
1	A	640	THR	2.3
1	B	1014	GLY	2.3
1	A	475	GLU	2.3
1	A	566	GLU	2.3
1	B	527	ARG	2.3
3	F	1	DG	2.2
1	B	1012	ILE	2.2
1	B	589	ASP	2.2
1	B	1309	GLU	2.2
1	B	606	VAL	2.2
1	A	497	ASN	2.2
1	B	1200	LYS	2.2
1	A	501	ILE	2.2
1	B	493	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	561	ASP	2.2
1	B	1250	GLY	2.2
1	B	616	ARG	2.2
1	A	423	ASN	2.2
1	A	490	ASP	2.2
1	B	632	TRP	2.2
1	A	500	LYS	2.1
1	A	491	PHE	2.1
1	B	583	LEU	2.1
1	A	483	ILE	2.1
1	B	470	ILE	2.1
1	B	1019	ARG	2.1
4	H	1	DA	2.1
1	A	474	GLU	2.1
1	B	610	ASP	2.1
1	A	521	PHE	2.1
1	A	538	ALA	2.1
1	A	477	ASN	2.1
1	B	564	LEU	2.0
1	B	577	LEU	2.0
1	A	1304	LYS	2.0
1	B	1342	ILE	2.0
1	A	589	ASP	2.0
1	B	421	SER	2.0
1	A	594	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

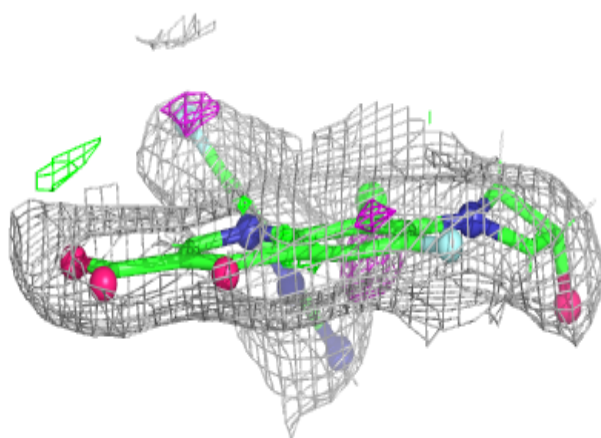
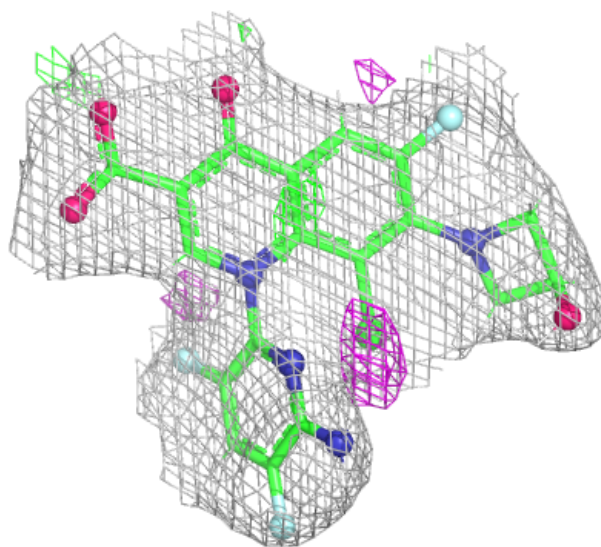
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MLA	A	1502	7/7	0.81	0.14	24,26,28,28	0
7	ACT	A	1504	4/4	0.81	0.14	22,22,23,23	0
8	MG	B	1502	1/1	0.81	0.10	15,15,15,15	0
8	MG	B	1504	1/1	0.84	0.10	9,9,9,9	0
9	CL	A	1508	1/1	0.84	0.15	17,17,17,17	0
6	MLA	A	1501	7/7	0.88	0.11	23,23,24,24	0
11	TE9	F	101	30/30	0.89	0.13	22,25,29,30	1
11	TE9	H	101	30/30	0.89	0.14	30,42,45,45	1
8	MG	A	1505	1/1	0.90	0.05	11,11,11,11	0
9	CL	B	1505	1/1	0.90	0.06	15,15,15,15	0
8	MG	A	1507	1/1	0.91	0.07	17,17,17,17	0
7	ACT	A	1503	4/4	0.92	0.12	13,13,13,14	0
8	MG	A	1506	1/1	0.93	0.11	8,8,8,8	0
10	MPD	B	1501	8/8	0.93	0.11	11,12,14,30	1
8	MG	B	1503	1/1	0.96	0.08	12,12,12,12	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.

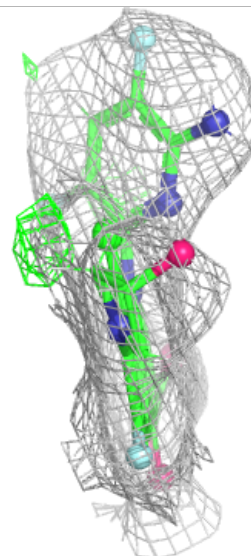
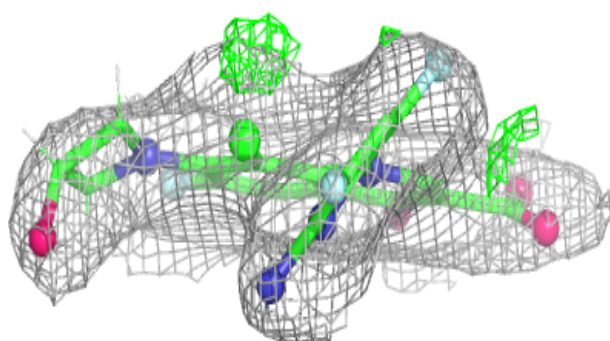
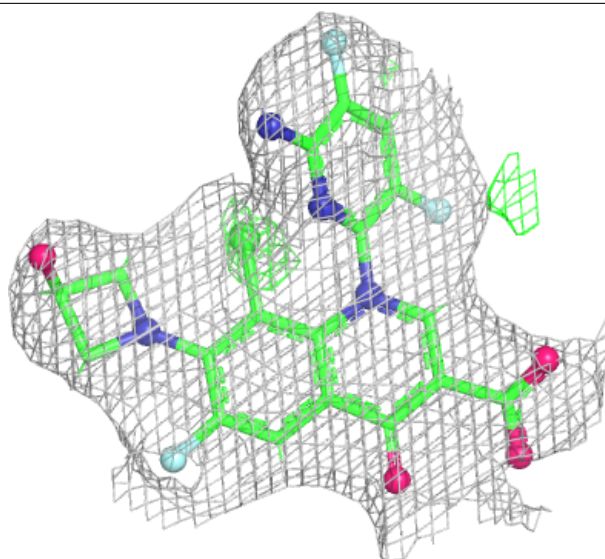
Electron density around TE9 F 101:

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



Electron density around TE9 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 [i](#)

There are no such residues in this entry.