



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:14 PM UTC

PDB ID : 9GEF / pdb_00009gef
Title : Experimental localization of metal-binding sites reveals the role of metal ions in the delafloxacin-stabilized *Streptococcus pneumoniae* topoisomerase IV DNA cleavage complex
Authors : Wang, B.; Najmudin, S.; Pan, X.-S.; Mykhaylyk, V.; Orr, C.; Wagner, A.; Govada, L.; Chayen, N.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2024-08-08
Resolution : 2.62 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](#) ①) were used in the production of this report:

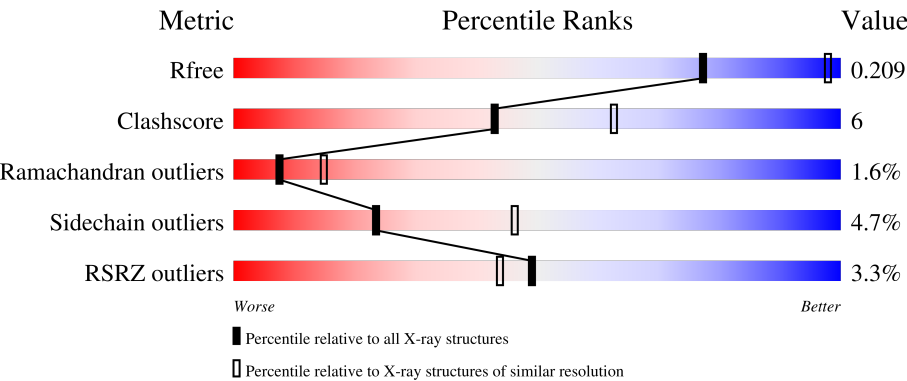
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	723	5% 81% 14% .
1	B	723	2% 84% 13% .
2	E	7	14% 86% 14%
3	F	11	73% 27%
4	G	7	57% 43%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	H	11	 82% 18%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA TOPOISOMERASE (ATP-HYDROLYZING),DNA TOPOISOMERASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5752	3633	999	1096	24			
1	B	723	Total	C	N	O	S	0	0	0
			5752	3633	999	1096	24			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*GP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			144	70	26	42	6			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	11	Total	C	N	O	P	0	0	0
			224	107	40	66	11			

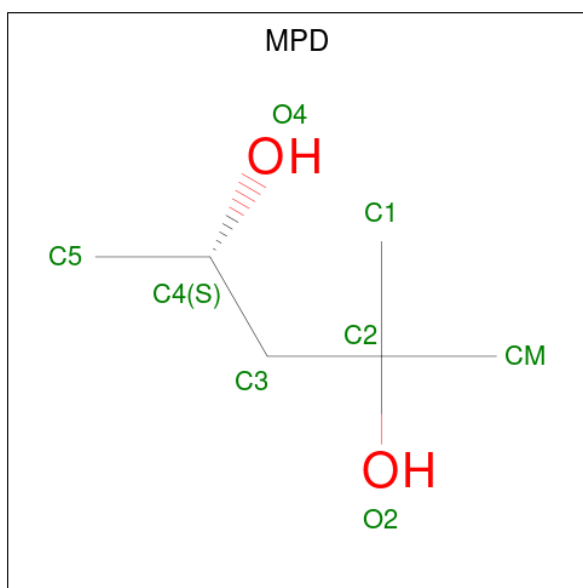
- Molecule 4 is a DNA chain called DNA (5'-D(*GP*TP*AP*AP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	P	0	0	0
			141	69	27	39	6			

- Molecule 5 is a DNA chain called DNA (5'-D(P*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	11	Total	C	N	O	P	0	0	0
			223	107	40	65	11			

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		
7	B	1	Total	Mg	0	0
			1	1		
7	H	1	Total	Mg	0	0
			1	1		

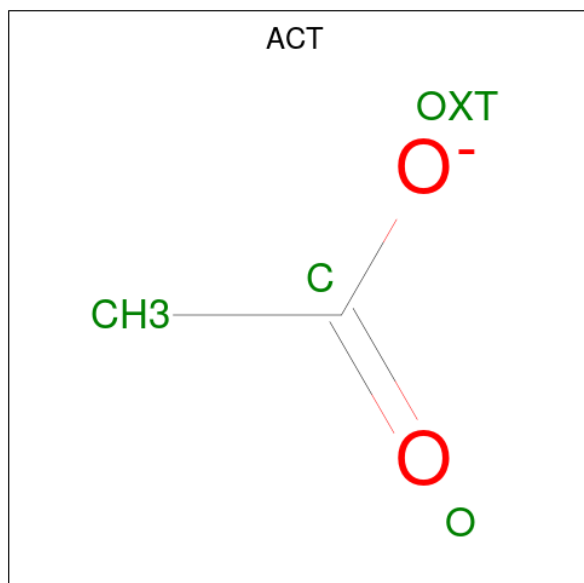
- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	K	0	0
			3	3		
8	B	5	Total	K	0	0
			5	5		

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

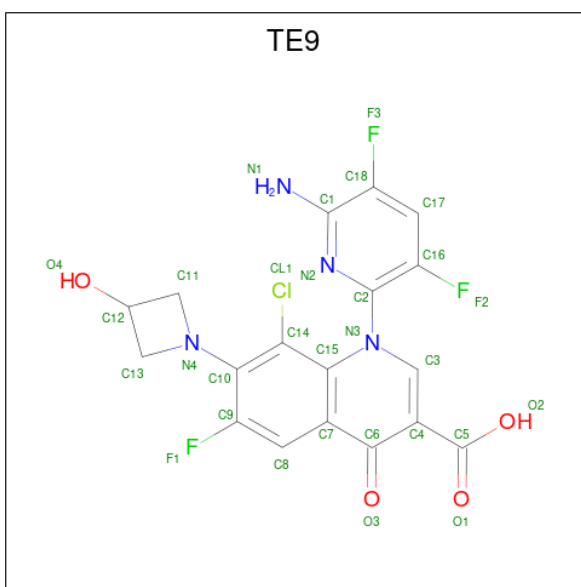
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	B	1	Total	Cl	0	0
			1	1		

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is delafloxacin (CCD ID: TE9) (formula: C₁₈H₁₂ClF₃N₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	Cl	F	N	O	
			30	18	1	3	4	4	0
11	H	1	Total	C	Cl	F	N	O	
			30	18	1	3	4	4	0

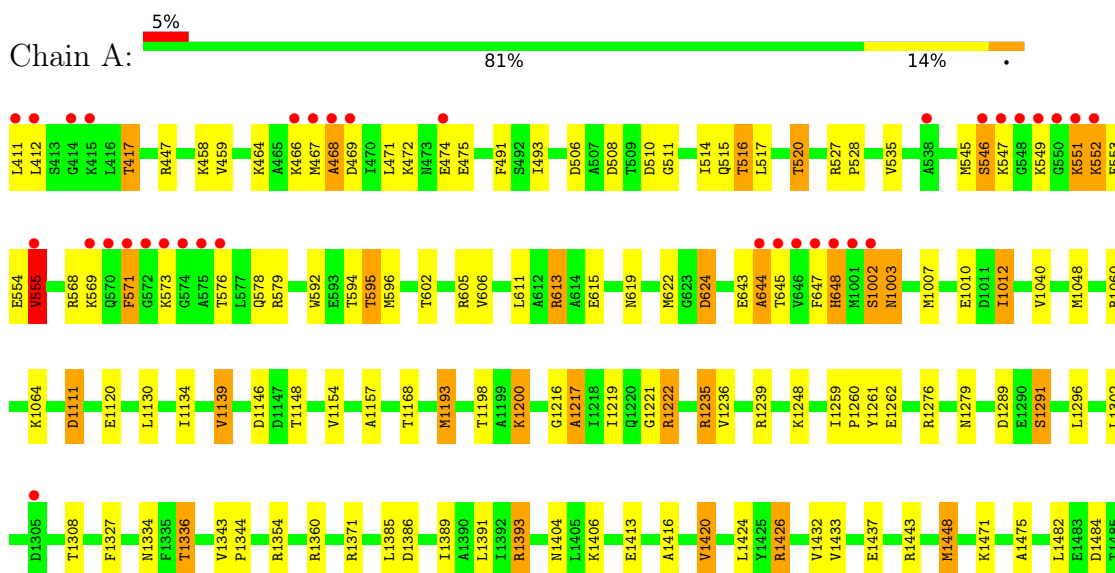
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	47	Total	O		
			47	47	0	0
12	B	45	Total	O		
			45	45	0	0
12	E	3	Total	O		
			3	3	0	0
12	F	6	Total	O		
			6	6	0	0
12	G	2	Total	O		
			2	2	0	0
12	H	5	Total	O		
			5	5	0	0

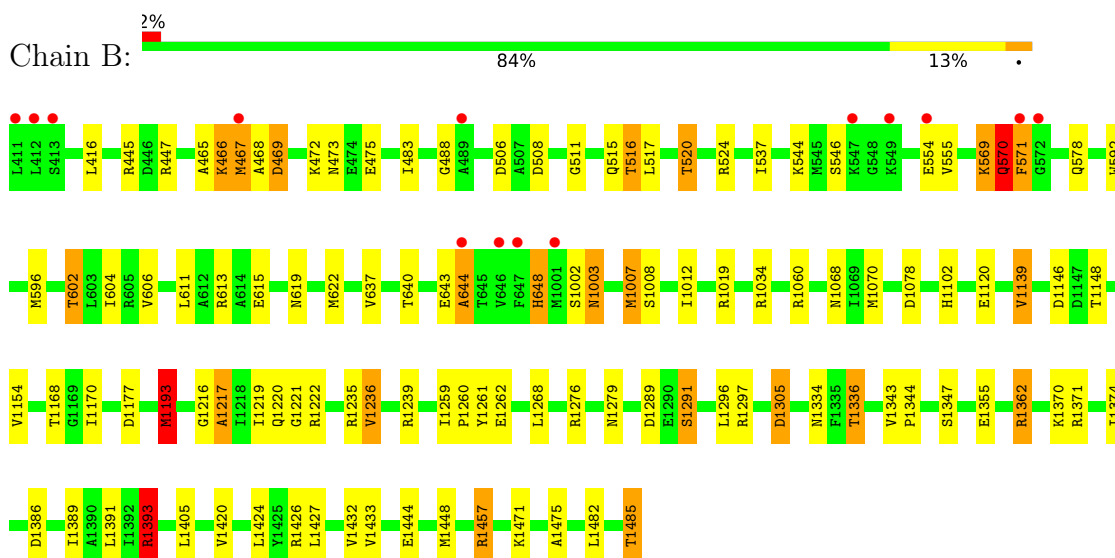
3 Residue-property plots

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.

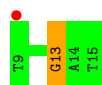
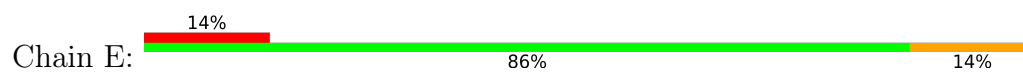
- Molecule 1: DNA TOPOISOMERASE (ATP-HYDROLYZING),DNA TOPOISOMERASE 4



- Molecule 1: DNA TOPOISOMERASE (ATP-HYDROLYZING),DNA TOPOISOMERASE 4



- Molecule 2: DNA (5'-D(*TP*GP*TP*GP*GP*AP*T)-3')



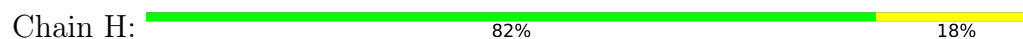
- Molecule 3: DNA (5'-D(P*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*A)-3')



- Molecule 4: DNA (5'-D(*GP*TP*AP*AP*TP*AP*C)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.53Å 158.53Å 210.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.39 – 2.62 79.39 – 2.62	Depositor EDS
% Data completeness (in resolution range)	69.5 (79.39-2.62) 69.5 (79.39-2.62)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.62Å)	Xtriage
Refinement program	PDB-REDO 8.11, PHENIX 4.4.7	Depositor
R, R_{free}	0.180 , 0.208 0.189 , 0.209	Depositor DCC
R_{free} test set	1109 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12454	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.73	2/5846 (0.0%)	1.01	8/7882 (0.1%)
1	B	0.71	3/5846 (0.1%)	1.01	7/7882 (0.1%)
2	E	0.31	0/161	1.12	1/248 (0.4%)
3	F	0.36	0/250	1.09	1/383 (0.3%)
4	G	0.32	0/158	1.26	1/242 (0.4%)
5	H	0.34	0/249	1.00	0/381
All	All	0.70	5/12510 (0.0%)	1.02	18/17018 (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	13
1	B	0	15
All	All	0	28

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1448	MET	SD-CE	8.90	2.01	1.79
1	B	1193	MET	SD-CE	7.59	1.98	1.79
1	B	1007	MET	SD-CE	5.96	1.94	1.79
1	A	1048	MET	SD-CE	-5.83	1.65	1.79
1	B	1448	MET	SD-CE	5.04	1.92	1.79

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ASP	CA-CB-CG	7.83	120.43	112.60
1	B	1305	ASP	CA-CB-CG	7.50	120.11	112.60
1	B	1432	VAL	N-CA-C	7.28	118.04	110.62
3	F	5	DA	P-O5'-C5'	-6.58	110.14	120.00
1	B	466	LYS	N-CA-C	6.35	120.88	111.04
4	G	9	DG	O3'-P-O5'	-5.97	95.04	104.00
1	A	1386	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	506	ASP	CA-CB-CG	5.80	118.40	112.60
2	E	13	DG	O3'-P-O5'	-5.78	95.33	104.00
1	A	508	ASP	CA-CB-CG	5.74	118.33	112.60
1	B	508	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	506	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	571	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	1111	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	571	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	417	THR	CB-CA-C	5.17	115.91	110.17
1	A	1327	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	1236	VAL	N-CA-CB	-5.06	105.44	112.52

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1060	ARG	Sidechain
1	A	1222	ARG	Sidechain
1	A	1235	ARG	Sidechain
1	A	1239	ARG	Sidechain
1	A	1276	ARG	Sidechain
1	A	1354	ARG	Sidechain
1	A	1360	ARG	Sidechain
1	A	1393	ARG	Sidechain
1	A	1426	ARG	Sidechain
1	A	447	ARG	Sidechain
1	A	579	ARG	Sidechain
1	A	605	ARG	Sidechain
1	A	613	ARG	Sidechain
1	B	1019	ARG	Sidechain
1	B	1034	ARG	Sidechain
1	B	1060	ARG	Sidechain
1	B	1222	ARG	Sidechain
1	B	1235	ARG	Sidechain
1	B	1239	ARG	Sidechain
1	B	1276	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	1297	ARG	Sidechain
1	B	1362	ARG	Sidechain
1	B	1393	ARG	Sidechain
1	B	1426	ARG	Sidechain
1	B	445	ARG	Sidechain
1	B	465	ALA	Peptide
1	B	467	MET	Peptide
1	B	613	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	5752	0	5832	80	1
1	B	5752	0	5832	69	1
2	E	144	0	82	1	0
3	F	224	0	125	2	0
4	G	141	0	81	2	0
5	H	223	0	125	1	0
6	A	16	0	28	4	0
6	B	16	0	28	3	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	H	1	0	0	1	0
8	A	3	0	0	0	0
8	B	5	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	1	0
10	B	4	0	3	0	0
11	F	30	0	0	4	0
11	H	30	0	0	5	0
12	A	47	0	0	0	0
12	B	45	0	0	1	0
12	E	3	0	0	0	0
12	F	6	0	0	0	0
12	G	2	0	0	0	0
12	H	5	0	0	2	0
All	All	12454	0	12136	152	1

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 6.

All (152) 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:1448:MET:SD	1:A:1448:MET:CE	2.01	1.48
11:H:101:TE9:CL1	11:H:101:TE9:N2	2.32	0.98
1:A:546:SER:O	1:A:554:GLU:HG2	1.71	0.91
11:F:101:TE9:CL1	11:F:101:TE9:N2	2.41	0.90
11:H:101:TE9:CL1	11:H:101:TE9:C2	2.58	0.88
11:F:101:TE9:CL1	11:F:101:TE9:C2	2.60	0.87
11:F:101:TE9:CL1	11:F:101:TE9:C13	2.64	0.83
11:H:101:TE9:CL1	11:H:101:TE9:C13	2.66	0.81
1:A:411:LEU:HB3	1:A:412:LEU:HD12	1.60	0.81
1:A:546:SER:OG	1:A:549:LYS:HB2	1.82	0.79
1:B:1457:ARG:HG2	1:B:1457:ARG:HH11	1.47	0.78
1:A:594:THR:OG1	1:A:595:THR:HG22	1.92	0.70
7:H:102:MG:MG	12:H:201:HOH:O	1.37	0.68
1:A:1235:ARG:NH2	3:F:11:DA:O3'	2.26	0.68
1:B:1371:ARG:HH22	6:B:1501:MPD:H4	1.59	0.67
1:A:1291:SER:HB3	1:A:1296:LEU:HA	1.78	0.66
1:B:1291:SER:HB3	1:B:1296:LEU:HA	1.79	0.65
1:B:466:LYS:HB2	1:B:468:ALA:O	1.97	0.65
1:A:554:GLU:O	1:A:555:VAL:C	2.40	0.64
4:G:10:DT:H2''	4:G:11:DA:C8	2.34	0.63
1:A:547:LYS:HD3	1:B:1102:HIS:NE2	2.15	0.61
1:A:613:ARG:NH2	1:A:1010:GLU:OE2	2.33	0.61
1:B:516:THR:O	1:B:520:THR:HG23	2.00	0.60
1:B:611:LEU:O	1:B:611:LEU:HD13	2.02	0.60
1:A:516:THR:O	1:A:520:THR:HG23	2.01	0.60
1:B:1362:ARG:HD3	12:B:1620:HOH:O	2.02	0.60
1:A:611:LEU:HD13	1:A:611:LEU:O	2.02	0.59
1:A:474:GLU:CD	1:A:474:GLU:H	2.11	0.58
1:A:1289:ASP:OD1	1:A:1291:SER:OG	2.22	0.58
1:A:1007:MET:HB3	1:A:1012:ILE:HD13	1.86	0.57
1:A:520:THR:HG21	1:A:622:MET:HG3	1.87	0.57
1:A:1426:ARG:HD2	6:A:1508:MPD:H13	1.86	0.57
1:A:527:ARG:N	1:A:528:PRO:HD2	2.20	0.56
1:A:535:VAL:HG23	1:A:606:VAL:HB	1.88	0.56
1:A:1002:SER:O	1:A:1003:ASN:HB2	2.05	0.56
1:B:520:THR:HG21	1:B:622:MET:HG3	1.87	0.56
11:H:101:TE9:O1	12:H:201:HOH:O	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:ARG:HH12	6:A:1501:MPD:H31	1.71	0.56
1:B:1289:ASP:OD1	1:B:1291:SER:OG	2.23	0.55
1:A:549:LYS:O	1:A:549:LYS:HD3	2.06	0.55
1:B:1007:MET:SD	1:B:1012:ILE:HD11	2.47	0.55
1:B:1170:ILE:HD11	4:G:11:DA:C2	2.42	0.54
1:B:468:ALA:O	1:B:469:ASP:HB2	2.07	0.54
1:B:1002:SER:O	1:B:1003:ASN:HB2	2.07	0.54
1:B:1457:ARG:HH11	1:B:1457:ARG:CG	2.18	0.53
1:A:1007:MET:SD	1:A:1012:ILE:HD11	2.48	0.53
1:A:510:ASP:O	1:A:514:ILE:HG12	2.08	0.52
1:B:1193:MET:HE1	1:B:1347:SER:HB3	1.91	0.52
11:H:101:TE9:CL1	11:H:101:TE9:C1	2.94	0.52
1:A:546:SER:HB3	1:A:576:THR:O	2.08	0.52
1:A:474:GLU:OE1	1:A:474:GLU:N	2.37	0.52
1:B:569:LYS:O	1:B:571:PHE:N	2.43	0.52
6:B:1501:MPD:H52	6:B:1501:MPD:H11	1.94	0.50
1:B:473:ASN:OD1	1:B:475:GLU:HB2	2.12	0.50
1:B:569:LYS:O	1:B:570:GLN:C	2.55	0.50
1:A:1406:LYS:HE2	1:A:1413:GLU:HA	1.94	0.49
1:A:555:VAL:O	1:A:555:VAL:HG12	2.11	0.49
1:B:602:THR:HG21	1:B:648:HIS:ND1	2.28	0.49
1:B:1393:ARG:HG3	1:B:1393:ARG:HH11	1.77	0.49
1:A:1393:ARG:NH1	1:B:1386:ASP:OD2	2.46	0.48
1:B:1343:VAL:HB	1:B:1344:PRO:HD3	1.95	0.48
1:B:1471:LYS:O	1:B:1475:ALA:HB2	2.13	0.48
1:B:602:THR:HG21	1:B:648:HIS:CE1	2.49	0.48
1:B:1393:ARG:HG3	1:B:1393:ARG:NH1	2.28	0.48
1:B:537:ILE:HB	1:B:604:ILE:HG12	1.96	0.48
1:B:643:GLU:O	1:B:644:ALA:HB3	2.15	0.47
1:A:1433:VAL:O	1:A:1437:GLU:HG3	2.15	0.47
1:A:552:LYS:O	1:A:554:GLU:HB3	2.14	0.47
1:A:1259:ILE:HB	1:A:1260:PRO:CD	2.45	0.47
1:A:1471:LYS:O	1:A:1475:ALA:HB2	2.15	0.47
1:B:1259:ILE:HB	1:B:1260:PRO:CD	2.45	0.47
1:A:643:GLU:O	1:A:644:ALA:HB3	2.13	0.46
1:A:1139:VAL:HG22	1:A:1154:VAL:HG13	1.97	0.46
1:B:1216:GLY:O	1:B:1217:ALA:HB3	2.15	0.46
1:A:1193:MET:HE1	1:A:1343:VAL:HA	1.97	0.46
1:A:615:GLU:O	1:A:619:ASN:ND2	2.49	0.46
1:B:615:GLU:O	1:B:619:ASN:ND2	2.49	0.46
1:A:458:LYS:HD3	1:A:514:ILE:HD13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:THR:HG21	1:A:648:HIS:CE1	2.51	0.46
1:A:1343:VAL:HB	1:A:1344:PRO:HD3	1.98	0.46
1:B:1371:ARG:NH2	6:B:1501:MPD:H4	2.29	0.46
1:A:1216:GLY:O	1:A:1217:ALA:HB3	2.16	0.45
1:B:469:ASP:H	1:B:472:LYS:HD3	1.81	0.45
1:B:1334:ASN:O	1:B:1336:THR:HG23	2.15	0.45
1:B:1391:LEU:HD23	1:B:1405:LEU:HD23	1.98	0.45
1:A:1064:LYS:HE3	1:B:1068:ASN:HD22	1.80	0.45
1:B:611:LEU:HD13	1:B:611:LEU:C	2.41	0.45
1:A:602:THR:HG21	1:A:648:HIS:HE1	1.82	0.45
1:A:511:GLY:O	1:A:515:GLN:HG3	2.16	0.45
1:B:570:GLN:HE21	1:B:570:GLN:HB2	1.63	0.45
1:B:1070:MET:HE1	1:B:1078:ASP:HB3	1.98	0.45
1:A:458:LYS:HD3	1:A:514:ILE:CD1	2.47	0.45
1:B:571:PHE:CD1	1:B:571:PHE:O	2.70	0.45
5:H:1:DA:H2"	5:H:2:DA:C8	2.52	0.45
1:A:578:GLN:NE2	1:B:1120:GLU:OE2	2.48	0.44
1:B:1007:MET:CB	1:B:1012:ILE:HD11	2.47	0.44
1:B:511:GLY:O	1:B:515:GLN:HG3	2.17	0.44
11:F:101:TE9:CL1	11:F:101:TE9:C1	3.02	0.44
1:B:1457:ARG:CG	1:B:1457:ARG:NH1	2.78	0.44
1:B:1370:LYS:O	1:B:1374:ILE:HD13	2.18	0.44
1:A:547:LYS:HD3	1:B:1102:HIS:CE1	2.53	0.44
1:A:1334:ASN:O	1:A:1336:THR:HG23	2.17	0.43
1:A:1130:LEU:HD23	1:A:1157:ALA:HA	2.00	0.43
1:A:1146:ASP:OD1	1:A:1148:THR:HG23	2.18	0.43
1:A:1222:ARG:HB3	1:A:1484:ASP:CG	2.42	0.43
1:B:468:ALA:O	1:B:469:ASP:CB	2.66	0.43
1:B:1389:ILE:HD11	1:B:1427:LEU:HD13	2.00	0.43
1:A:467:MET:O	1:A:468:ALA:HB2	2.18	0.43
1:A:546:SER:CB	1:A:549:LYS:HB2	2.48	0.43
1:A:1393:ARG:NH1	1:B:1386:ASP:CG	2.77	0.43
1:B:520:THR:O	1:B:524:ARG:HG3	2.19	0.43
1:A:491:PHE:CD2	1:A:528:PRO:HG2	2.54	0.42
1:A:1002:SER:O	1:A:1003:ASN:CB	2.66	0.42
1:B:544:LYS:HG3	1:B:555:VAL:HG13	2.00	0.42
1:B:1219:ILE:HB	1:B:1482:LEU:HD23	2.02	0.42
1:B:516:THR:HG22	1:B:517:LEU:N	2.35	0.42
1:B:1139:VAL:HG22	1:B:1154:VAL:HG13	2.01	0.42
1:A:1007:MET:SD	1:A:1012:ILE:CD1	3.07	0.42
1:A:1424:LEU:HD23	1:B:1424:LEU:HD23	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:HD13	1:A:611:LEU:C	2.43	0.42
1:A:1219:ILE:HB	1:A:1482:LEU:HD23	2.02	0.42
1:B:1002:SER:O	1:B:1003:ASN:CB	2.67	0.42
1:A:547:LYS:CD	1:B:1102:HIS:NE2	2.81	0.42
1:A:1385:LEU:O	1:A:1389:ILE:HG12	2.20	0.42
1:A:464:LYS:HE2	3:F:8:DC:OP2	2.20	0.41
1:A:1040:VAL:HG11	2:E:13:DG:H5'	2.00	0.41
1:A:594:THR:OG1	1:A:595:THR:CG2	2.67	0.41
1:A:1198:THR:O	1:A:1200:LYS:HD3	2.21	0.41
1:A:516:THR:HG22	1:A:517:LEU:N	2.36	0.41
1:A:1120:GLU:OE2	1:B:578:GLN:NE2	2.50	0.41
1:B:1008:SER:HB2	9:B:1509:CL:CL	2.57	0.41
1:A:1371:ARG:NH1	6:A:1501:MPD:H31	2.34	0.41
1:B:1220:GLN:HB3	1:B:1485:THR:O	2.20	0.41
1:A:468:ALA:O	1:A:472:LYS:HD3	2.20	0.41
1:A:592:TRP:HA	1:A:596:MET:HB2	2.02	0.41
1:A:1443:ARG:HH11	1:A:1443:ARG:HG2	1.86	0.41
1:B:1261:TYR:CD2	1:B:1262:GLU:HG3	2.55	0.41
1:A:1391:LEU:HD21	1:A:1404:ASN:HB3	2.02	0.41
1:B:1007:MET:SD	1:B:1012:ILE:CD1	3.09	0.41
1:A:551:LYS:CG	1:A:551:LYS:O	2.69	0.41
1:A:1426:ARG:CD	6:A:1508:MPD:H13	2.51	0.41
1:B:416:LEU:HD13	1:B:416:LEU:C	2.46	0.41
1:B:1007:MET:HB3	1:B:1012:ILE:HD11	2.01	0.41
1:B:1070:MET:CE	1:B:1078:ASP:HB3	2.51	0.41
1:B:1355:GLU:HA	1:B:1355:GLU:OE1	2.21	0.41
1:A:1291:SER:O	1:B:447:ARG:NH1	2.52	0.41
1:B:592:TRP:HA	1:B:596:MET:HB2	2.02	0.41
1:B:1146:ASP:OD1	1:B:1148:THR:HG23	2.21	0.41
1:A:466:LYS:HD3	1:A:466:LYS:H	1.86	0.40
1:A:554:GLU:CD	1:A:554:GLU:C	2.90	0.40
1:A:1261:TYR:CD2	1:A:1262:GLU:HG3	2.56	0.40
1:A:1416:ALA:O	1:A:1420:VAL:HB	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1393:ARG:NH2	1:B:1279:ASN:O[4_455]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	721/723 (100%)	684 (95%)	24 (3%)	13 (2%)	6	13
1	B	721/723 (100%)	685 (95%)	26 (4%)	10 (1%)	9	17
All	All	1442/1446 (100%)	1369 (95%)	50 (4%)	23 (2%)	7	15

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	ALA
1	A	553	GLU
1	A	555	VAL
1	A	573	LYS
1	A	1003	ASN
1	B	467	MET
1	B	554	GLU
1	B	570	GLN
1	B	1003	ASN
1	A	552	LYS
1	A	647	PHE
1	A	1248	LYS
1	A	1217	ALA
1	B	1217	ALA
1	A	546	SER
1	B	1305	ASP
1	B	644	ALA
1	A	571	PHE
1	A	644	ALA
1	B	469	ASP
1	B	1221	GLY
1	A	1221	GLY
1	B	488	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	619/619 (100%)	586 (95%)	33 (5%)	20	41
1	B	619/619 (100%)	594 (96%)	25 (4%)	28	53
All	All	1238/1238 (100%)	1180 (95%)	58 (5%)	23	46

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	THR
1	A	459	VAL
1	A	469	ASP
1	A	471	LEU
1	A	475	GLU
1	A	493	ILE
1	A	516	THR
1	A	520	THR
1	A	545	MET
1	A	551	LYS
1	A	555	VAL
1	A	568	ARG
1	A	569	LYS
1	A	595	THR
1	A	624	ASP
1	A	645	THR
1	A	648	HIS
1	A	1002	SER
1	A	1012	ILE
1	A	1111	ASP
1	A	1134	ILE
1	A	1139	VAL
1	A	1168	THR
1	A	1193	MET
1	A	1200	LYS
1	A	1236	VAL
1	A	1279	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1291	SER
1	A	1302	LEU
1	A	1308	THR
1	A	1336	THR
1	A	1420	VAL
1	A	1432	VAL
1	B	483	ILE
1	B	516	THR
1	B	520	THR
1	B	546	SER
1	B	569	LYS
1	B	570	GLN
1	B	602	THR
1	B	606	VAL
1	B	637	VAL
1	B	640	THR
1	B	648	HIS
1	B	1139	VAL
1	B	1168	THR
1	B	1177	ASP
1	B	1193	MET
1	B	1236	VAL
1	B	1268	LEU
1	B	1291	SER
1	B	1336	THR
1	B	1393	ARG
1	B	1420	VAL
1	B	1433	VAL
1	B	1444	GLU
1	B	1457	ARG
1	B	1485	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	477	ASN
1	A	619	ASN
1	A	1006	ASN
1	A	1102	HIS
1	A	1196	HIS
1	A	1326	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1423	GLN
1	B	570	GLN
1	B	619	ASN
1	B	1003	ASN
1	B	1068	ASN
1	B	1094	ASN
1	B	1132	GLN
1	B	1196	HIS
1	B	1324	ASN
1	B	1326	ASN
1	B	1461	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 14 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	$\# Z > 2$
11	TE9	H	101	7	32,33,33	1.23	4 (12%)	38,51,51	1.56	8 (21%)
6	MPD	B	1502	-	7,7,7	0.25	0	9,10,10	0.54	0
10	ACT	B	1510	-	3,3,3	1.30	0	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MPD	A	1501	-	7,7,7	0.24	0	9,10,10	0.46	0
11	TE9	F	101	7	32,33,33	1.26	5 (15%)	38,51,51	1.45	7 (18%)
6	MPD	A	1508	-	7,7,7	0.13	0	9,10,10	0.35	0
6	MPD	B	1501	-	7,7,7	0.33	0	9,10,10	0.95	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
11	TE9	H	101	7	-	5/11/20/20	0/4/4/4
6	MPD	B	1502	-	-	4/5/5/5	-
6	MPD	A	1501	-	-	3/5/5/5	-
11	TE9	F	101	7	-	1/11/20/20	0/4/4/4
6	MPD	A	1508	-	-	1/5/5/5	-
6	MPD	B	1501	-	-	5/5/5/5	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	101	TE9	C10-C14	-3.15	1.35	1.40
11	F	101	TE9	C2-C16	-3.14	1.38	1.42
11	H	101	TE9	C2-C16	-3.04	1.38	1.42
11	F	101	TE9	C10-C14	-2.84	1.35	1.40
11	F	101	TE9	C11-C12	2.34	1.57	1.53
11	F	101	TE9	C1-C18	2.16	1.42	1.39
11	F	101	TE9	O1-C5	2.12	1.27	1.22
11	H	101	TE9	C1-C18	2.05	1.41	1.39
11	H	101	TE9	C11-C12	2.01	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	101	TE9	C17-C18-C1	-3.79	119.20	121.68
11	H	101	TE9	C4-C3-N3	-3.49	119.68	123.81
11	F	101	TE9	C13-N4-C11	-3.24	91.86	94.52
11	F	101	TE9	C4-C3-N3	-3.04	120.22	123.81
11	H	101	TE9	O1-C5-C4	-2.85	116.77	122.67
11	H	101	TE9	C13-N4-C11	-2.74	92.27	94.52
11	F	101	TE9	C17-C18-C1	-2.56	120.00	121.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	101	TE9	N1-C1-N2	2.56	120.48	117.03
11	F	101	TE9	C15-N3-C2	2.43	123.50	119.11
11	H	101	TE9	C3-C4-C6	2.36	121.67	119.94
11	F	101	TE9	O1-C5-C4	-2.18	118.16	122.67
11	H	101	TE9	N1-C1-N2	2.17	119.96	117.03
11	H	101	TE9	C8-C9-C10	-2.14	120.16	123.34
11	H	101	TE9	C15-N3-C2	2.13	122.96	119.11
11	F	101	TE9	C3-C4-C6	2.01	121.41	119.94

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1501	MPD	C1-C2-C3-C4
6	B	1501	MPD	O2-C2-C3-C4
11	F	101	TE9	N2-C2-N3-C3
11	H	101	TE9	N2-C2-N3-C3
11	H	101	TE9	C6-C4-C5-O1
11	H	101	TE9	C6-C4-C5-O2
11	H	101	TE9	C3-C4-C5-O2
6	A	1501	MPD	C2-C3-C4-O4
6	A	1508	MPD	C2-C3-C4-O4
6	B	1501	MPD	CM-C2-C3-C4
6	B	1502	MPD	C1-C2-C3-C4
6	B	1501	MPD	C2-C3-C4-C5
11	H	101	TE9	C3-C4-C5-O1
6	B	1502	MPD	O2-C2-C3-C4
6	B	1501	MPD	C2-C3-C4-O4
6	B	1502	MPD	C2-C3-C4-O4
6	A	1501	MPD	C1-C2-C3-C4
6	A	1501	MPD	CM-C2-C3-C4
6	B	1502	MPD	CM-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 16 short contacts:

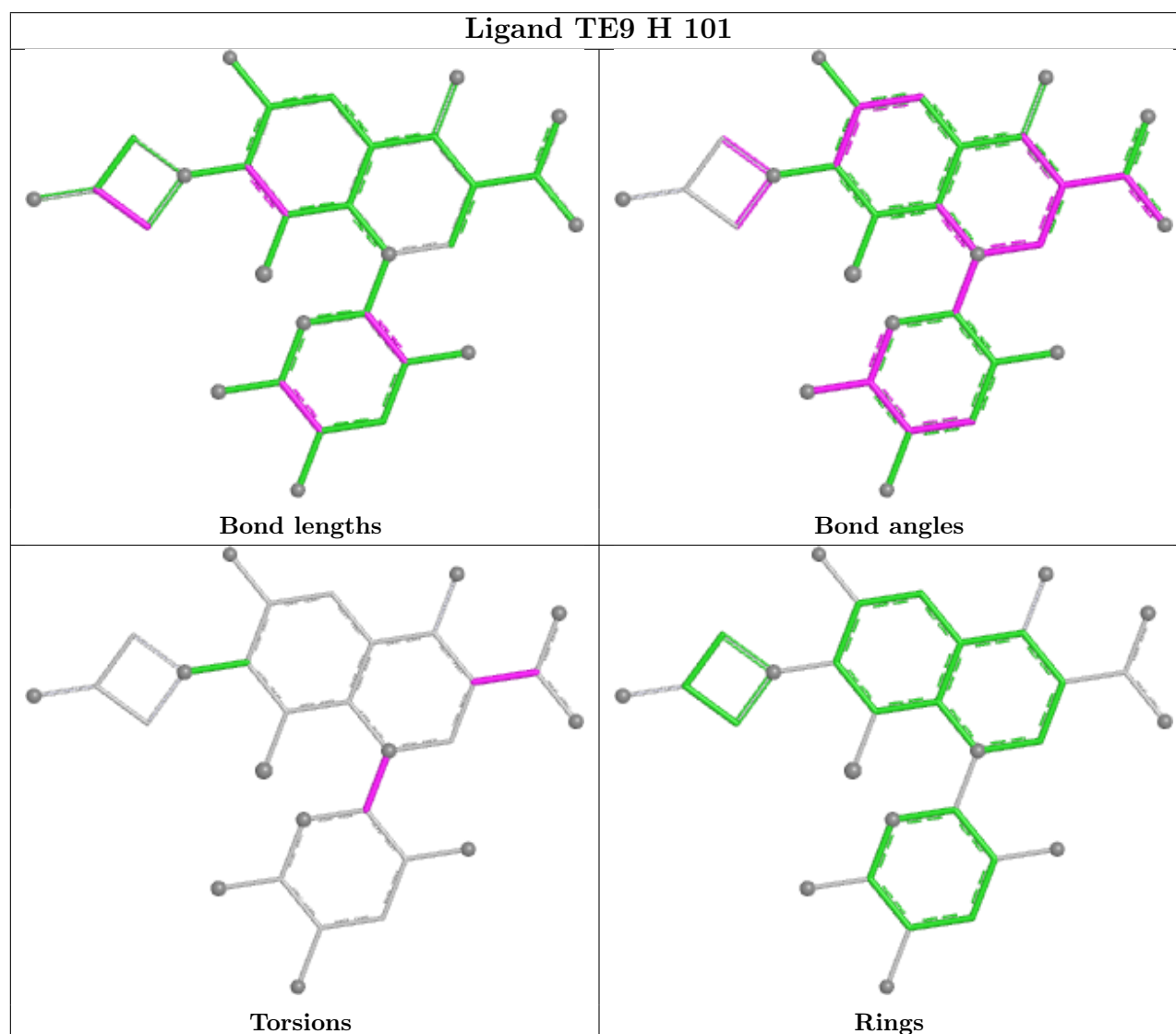
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	101	TE9	5	0
6	A	1501	MPD	2	0
11	F	101	TE9	4	0
6	A	1508	MPD	2	0

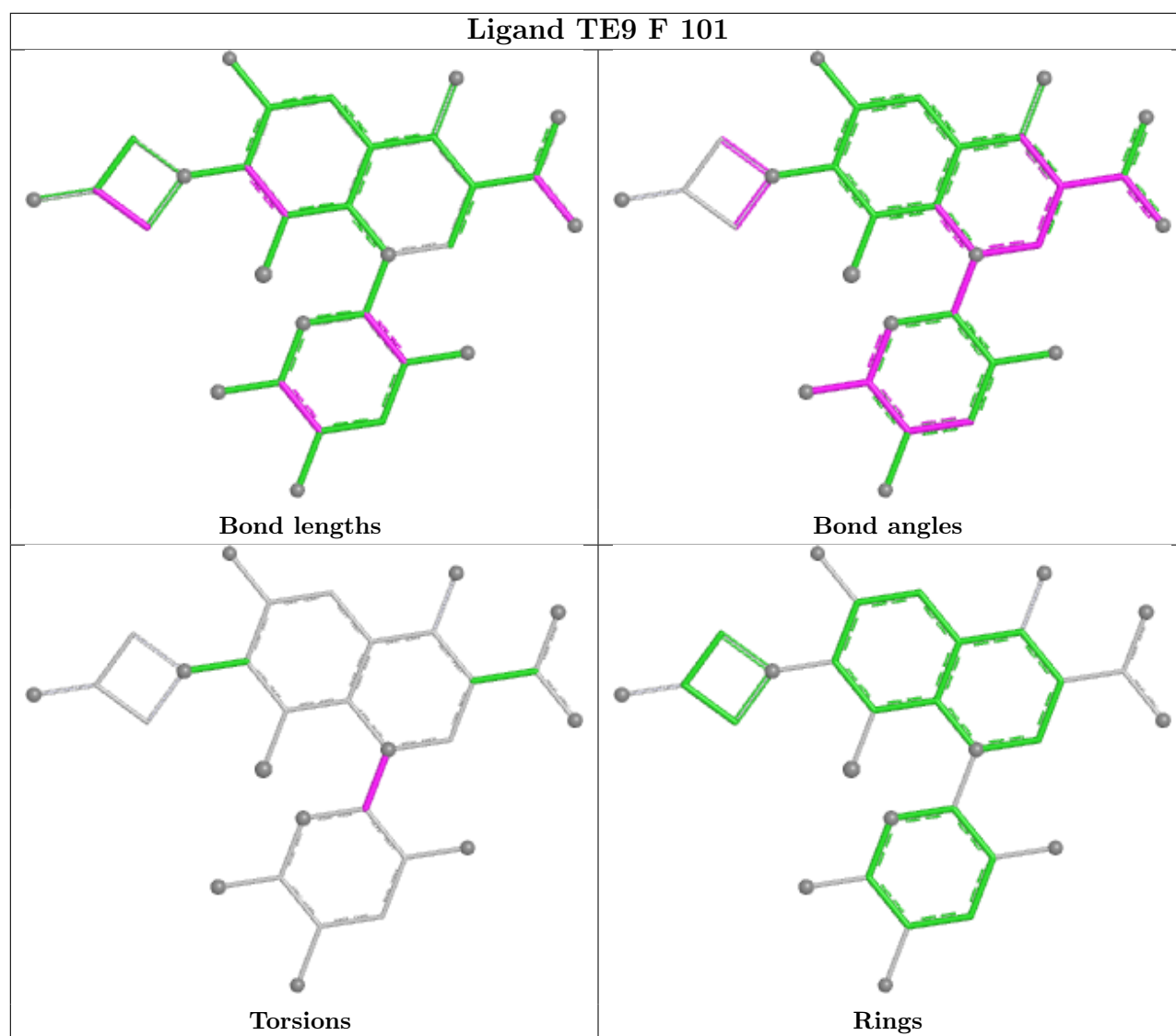
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1501	MPD	3	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	723/723 (100%)	-0.08	34 (4%) 36 31	24, 41, 87, 142	0
1	B	723/723 (100%)	-0.15	14 (1%) 66 62	23, 40, 87, 131	0
2	E	7/7 (100%)	0.16	1 (14%) 6 5	34, 36, 62, 84	0
3	F	11/11 (100%)	-0.02	0 100 100	42, 57, 68, 86	0
4	G	7/7 (100%)	-0.26	0 100 100	33, 35, 64, 82	0
5	H	11/11 (100%)	-0.09	0 100 100	41, 53, 66, 84	0
All	All	1482/1482 (100%)	-0.12	49 (3%) 49 44	23, 41, 87, 142	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	LYS	7.6
1	A	411	LEU	6.1
1	A	548	GLY	5.6
1	A	555	VAL	5.5
1	A	646	VAL	5.5
1	A	571	PHE	5.3
1	B	411	LEU	5.2
1	B	646	VAL	4.9
1	A	644	ALA	4.5
1	A	1001	MET	4.4
1	A	551	LYS	4.4
1	A	546	SER	4.2
1	B	644	ALA	4.1
1	A	647	PHE	4.0
1	B	571	PHE	4.0
1	A	574	GLY	3.9
1	A	575	ALA	3.7
1	A	550	GLY	3.5
1	B	647	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	552	LYS	3.4
1	A	412	LEU	3.3
1	A	466	LYS	3.3
1	B	547	LYS	3.3
1	A	645	THR	3.2
1	A	549	LYS	3.2
1	A	648	HIS	2.9
1	A	468	ALA	2.9
1	B	412	LEU	2.7
1	B	1001	MET	2.7
1	B	467	MET	2.7
1	A	474	GLU	2.6
1	A	467	MET	2.6
1	B	572	GLY	2.6
1	A	573	LYS	2.5
1	B	413	SER	2.5
1	B	554	GLU	2.5
1	A	414	GLY	2.5
1	A	1002	SER	2.4
1	A	576	THR	2.4
1	A	572	GLY	2.4
1	B	549	LYS	2.3
1	A	538	ALA	2.3
1	A	469	ASP	2.2
1	A	569	LYS	2.2
1	A	1305	ASP	2.2
2	E	9	DT	2.1
1	A	570	GLN	2.1
1	B	489	ALA	2.0
1	A	415	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

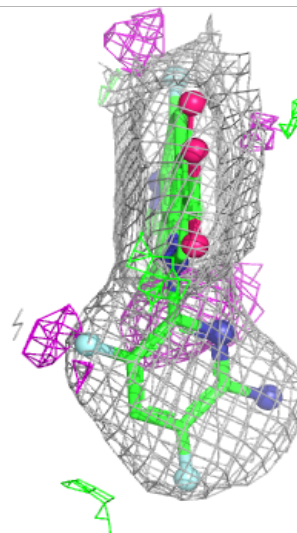
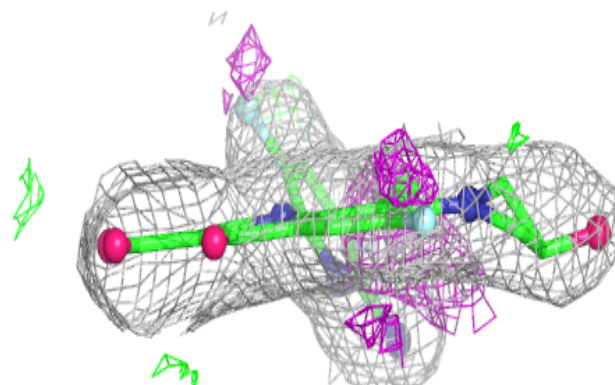
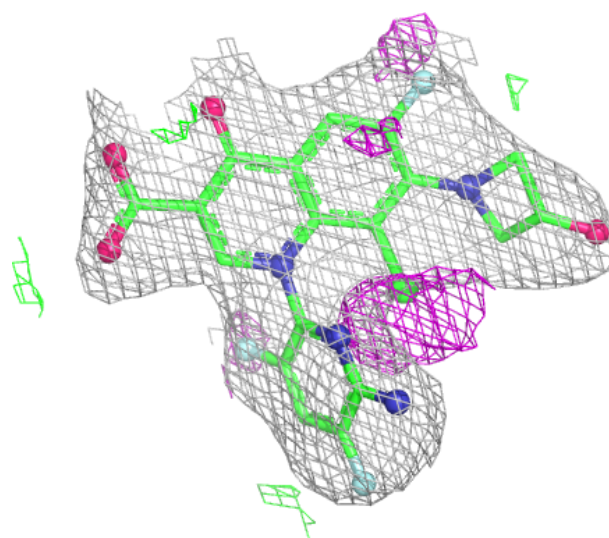
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
10	ACT	B	1510	4/4	0.74	0.21	45,53,55,56	0
6	MPD	B	1501	8/8	0.83	0.18	48,52,57,58	0
6	MPD	A	1501	8/8	0.84	0.20	47,53,63,70	0
8	K	B	1507	1/1	0.89	0.21	79,79,79,79	0
8	K	A	1505	1/1	0.89	0.21	67,67,67,67	0
6	MPD	A	1508	8/8	0.90	0.13	43,51,54,54	0
8	K	B	1505	1/1	0.91	0.11	68,68,68,68	0
9	CL	B	1509	1/1	0.92	0.11	76,76,76,76	0
6	MPD	B	1502	8/8	0.94	0.13	44,45,51,54	0
9	CL	A	1507	1/1	0.94	0.09	75,75,75,75	0
8	K	B	1504	1/1	0.95	0.15	45,45,45,45	0
8	K	B	1506	1/1	0.95	0.08	68,68,68,68	0
11	TE9	F	101	30/30	0.95	0.08	32,38,45,87	0
11	TE9	H	101	30/30	0.95	0.07	31,35,42,83	0
8	K	A	1504	1/1	0.96	0.19	39,39,39,39	0
7	MG	A	1502	1/1	0.96	0.07	45,45,45,45	0
8	K	A	1506	1/1	0.96	0.15	34,34,34,34	0
7	MG	H	102	1/1	0.96	0.05	54,54,54,54	0
8	K	B	1508	1/1	0.97	0.17	29,29,29,29	0
7	MG	A	1503	1/1	0.99	0.04	21,21,21,21	0
7	MG	B	1503	1/1	1.00	0.03	22,22,22,22	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.

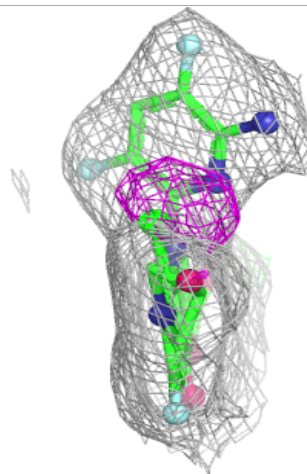
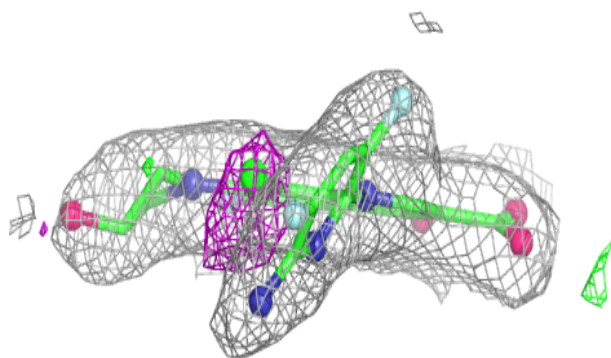
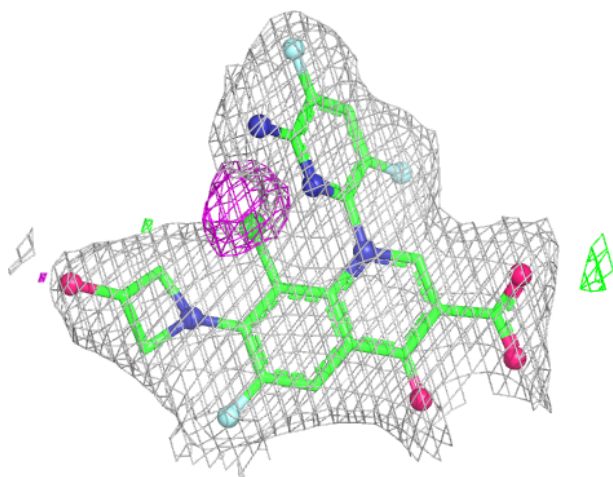
Electron density around TE9 F 101:

$2mF_o-DF_c$ (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.