



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:51 PM UTC

PDB ID : 5VIL / pdb_00005vil
Title : Crystal structure of ASK1 kinase domain with a potent inhibitor (analog 6)
Authors : Jasti, J.; Chang, J.; Kurumbail, R.
Deposited on : 2017-04-17
Resolution : 2.64 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

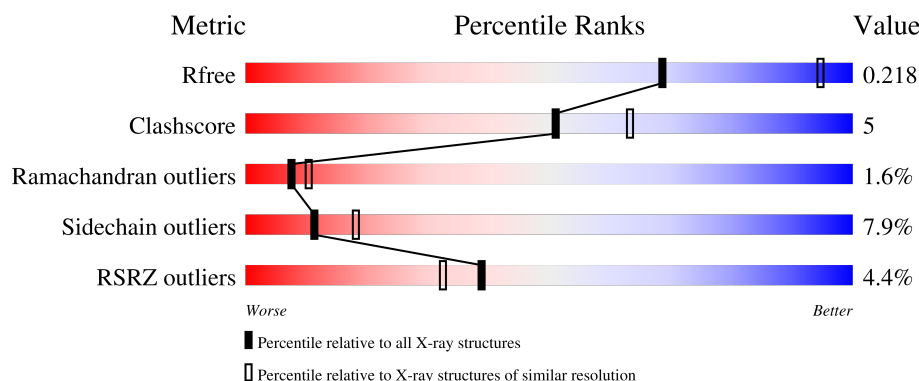
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	293	3% 72% 17% • 8%
1	B	293	3% 75% 15% • 8%
1	C	293	3% 76% 14% • 8%
1	D	293	7% 71% 18% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMS	B	1003	-	-	X	-

2 Entry composition [i](#)

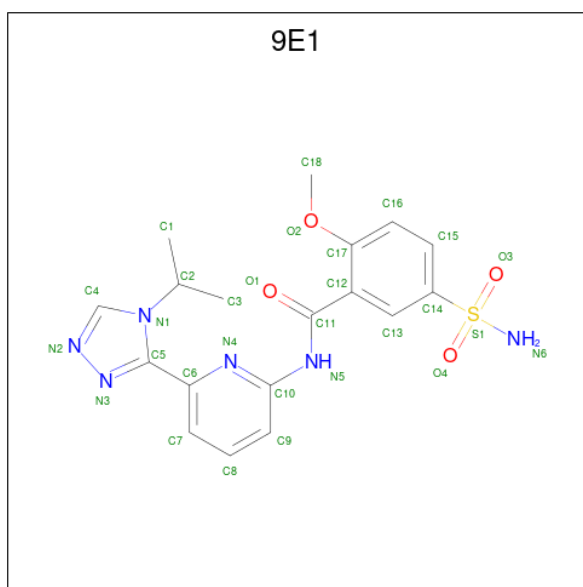
There are 4 unique types of molecules in this entry. The entry contains 8958 atoms, of which 104 are hydrogens and 0 are deuteriums.

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 Mitogen-activated protein kinase kinase kinase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2146	1376	358	402	10			
1	B	271	Total	C	N	O	S	0	0	0
			2146	1376	358	402	10			
1	C	271	Total	C	N	O	S	0	0	0
			2146	1376	358	402	10			
1	D	271	Total	C	N	O	S	0	0	0
			2146	1376	358	402	10			

- Molecule 2 is 2-methoxy-N-{6-[4-(propan-2-yl)-4H-1,2,4-triazol-3-yl]pyridin-2-yl}-5-sulfamoylbenzamide (CCD ID: 9E1) (formula: C₁₈H₂₀N₆O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O S	20	0
			49	18	20	6	4 1		
2	B	1	Total	C	H	N	O S	20	0
			49	18	20	6	4 1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	S	20	0
			49	18	20	6	4	1		
2	D	1	Total	C	H	N	O	S	20	0
			49	18	20	6	4	1		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
3	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	63	Total	O	0	0
			63	63		
4	C	9	Total	O	0	0
			9	9		

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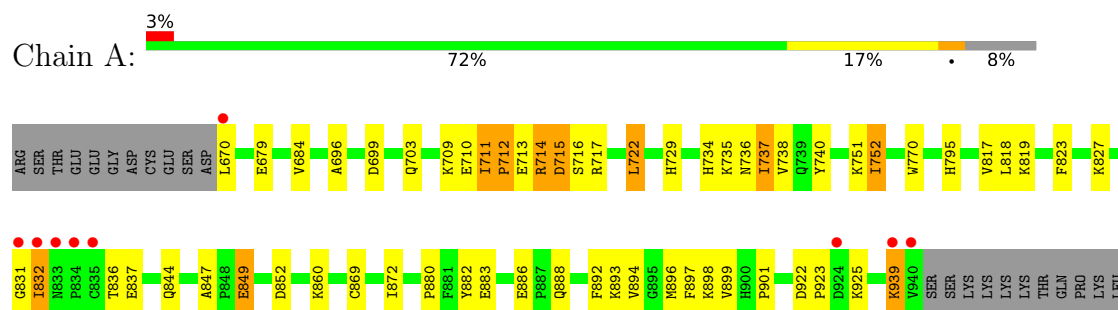
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	14	Total	O	0	0
			14	14		

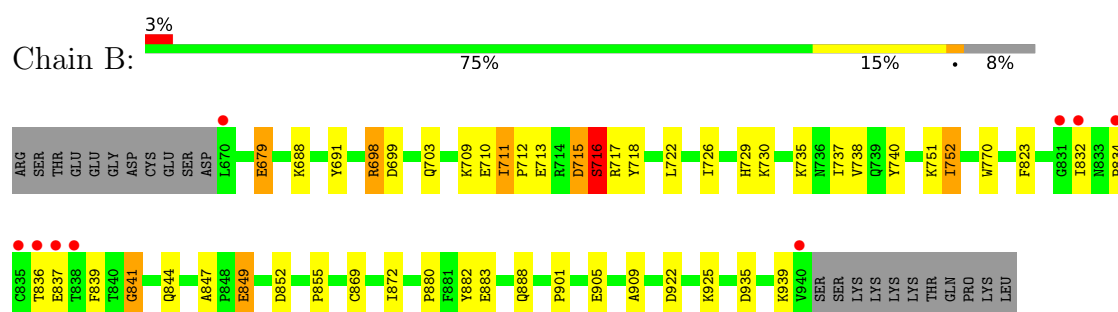
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

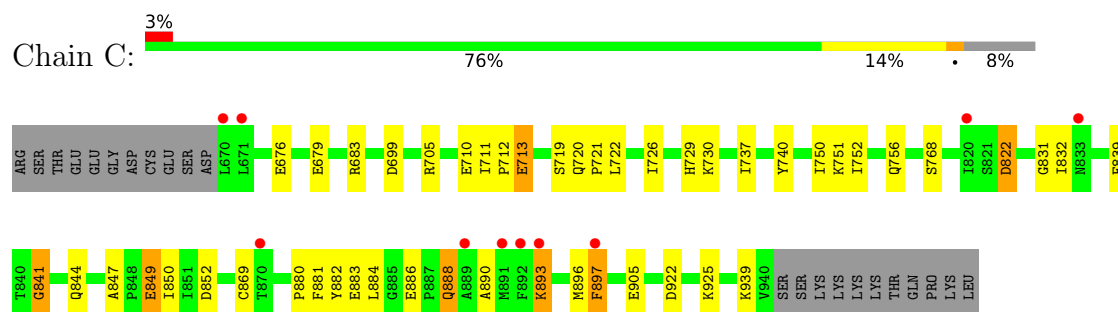
- Molecule 1: Mitogen-activated protein kinase kinase kinase 5



- Molecule 1: Mitogen-activated protein kinase kinase kinase 5

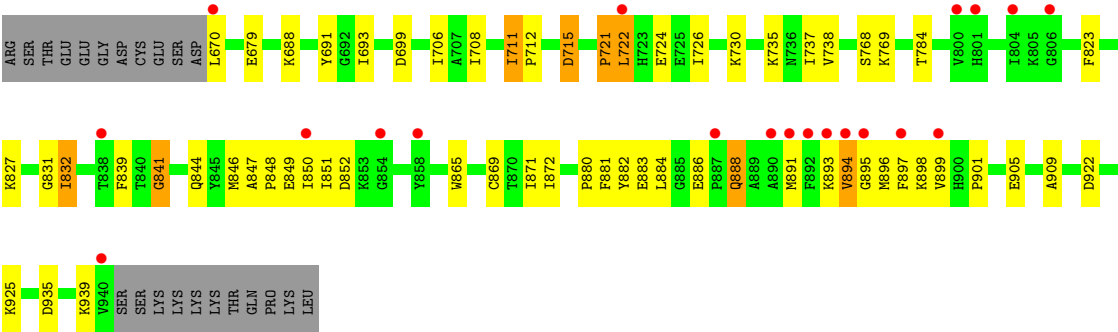


- Molecule 1: Mitogen-activated protein kinase kinase kinase 5



- Molecule 1: Mitogen-activated protein kinase kinase kinase 5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.54Å 132.09Å 135.22Å 90.00° 92.82° 90.00°	Depositor
Resolution (Å)	135.00 – 2.64 135.00 – 2.64	Depositor EDS
% Data completeness (in resolution range)	82.7 (135.00-2.64) 82.7 (135.00-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.180 , 0.213 0.189 , 0.218	Depositor DCC
R_{free} test set	1773 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 116.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.012 for -h,-l,-k 0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8958	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: 9E1, DMS

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	0.92	2/2195 (0.1%)	1.41	10/2963 (0.3%)
1	B	0.91	0/2195	1.37	9/2963 (0.3%)
1	C	0.78	0/2195	1.37	9/2963 (0.3%)
1	D	0.79	1/2195 (0.0%)	1.38	15/2963 (0.5%)
All	All	0.85	3/8780 (0.0%)	1.38	43/11852 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	832	ILE	CA-C	5.67	1.57	1.53
1	D	832	ILE	CA-C	5.46	1.57	1.53
1	A	737	ILE	CA-CB	5.27	1.61	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	897	PHE	N-CA-C	-9.71	102.05	112.93
1	D	722	LEU	N-CA-C	-7.92	103.42	113.23
1	C	893	LYS	CA-C-N	7.72	130.88	120.77
1	C	893	LYS	C-N-CA	7.72	130.88	120.77
1	B	717	ARG	N-CA-C	-7.08	102.77	111.40
1	D	897	PHE	CA-C-N	7.00	132.56	122.40
1	D	897	PHE	C-N-CA	7.00	132.56	122.40
1	A	715	ASP	CA-CB-CG	6.89	119.50	112.60
1	B	699	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	882	TYR	CA-C-N	6.24	128.93	120.38
1	A	882	TYR	C-N-CA	6.24	128.93	120.38
1	B	882	TYR	CA-C-N	6.03	128.63	120.38
1	B	882	TYR	C-N-CA	6.03	128.63	120.38
1	D	882	TYR	CA-C-N	6.02	128.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	882	TYR	C-N-CA	6.02	128.63	120.38
1	C	882	TYR	CA-C-N	5.96	128.55	120.38
1	C	882	TYR	C-N-CA	5.96	128.55	120.38
1	B	823	PHE	CA-CB-CG	-5.84	107.96	113.80
1	C	719	SER	CA-C-N	5.81	127.35	120.09
1	C	719	SER	C-N-CA	5.81	127.35	120.09
1	A	823	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	712	PRO	CA-C-N	5.60	128.06	120.38
1	A	712	PRO	C-N-CA	5.60	128.06	120.38
1	D	899	VAL	CA-C-N	5.58	130.85	121.92
1	D	899	VAL	C-N-CA	5.58	130.85	121.92
1	A	716	SER	CA-C-N	5.34	127.69	120.38
1	A	716	SER	C-N-CA	5.34	127.69	120.38
1	B	909	ALA	CA-C-N	5.33	127.38	120.44
1	B	909	ALA	C-N-CA	5.33	127.38	120.44
1	A	699	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	699	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	713	GLU	N-CA-C	5.14	117.55	111.33
1	C	712	PRO	CA-C-N	5.13	131.33	121.54
1	C	712	PRO	C-N-CA	5.13	131.33	121.54
1	D	699	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	909	ALA	CA-C-N	5.09	127.06	120.44
1	D	909	ALA	C-N-CA	5.09	127.06	120.44
1	D	935	ASP	CA-C-N	5.06	127.77	120.38
1	D	935	ASP	C-N-CA	5.06	127.77	120.38
1	B	935	ASP	CA-C-N	5.06	127.77	120.38
1	B	935	ASP	C-N-CA	5.06	127.77	120.38
1	D	823	PHE	CA-C-N	5.04	125.68	119.99
1	D	823	PHE	C-N-CA	5.04	125.68	119.99

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	2146	0	2136	24	0
1	B	2146	0	2136	24	0
1	C	2146	0	2136	19	0
1	D	2146	0	2136	25	0
2	A	29	20	0	0	0
2	B	29	20	0	0	0
2	C	29	20	0	1	0
2	D	29	20	0	0	0
3	A	4	6	6	0	0
3	B	12	18	18	8	0
4	A	52	0	0	0	0
4	B	63	0	0	0	0
4	C	9	0	0	0	0
4	D	14	0	0	0	0
All	All	8854	104	8568	90	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 5.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ASP:O	1:B:716:SER:HB3	1.51	1.11
1:A:711:ILE:HD13	1:A:712:PRO:HD2	1.34	1.03
1:B:711:ILE:HD13	1:B:712:PRO:HD2	1.42	1.02
1:B:770:TRP:HE1	3:B:1002:DMS:H12	1.24	1.00
1:D:848:PRO:HB3	1:D:895:GLY:HA3	1.55	0.88
1:D:846:MET:O	1:D:894:VAL:HG11	1.88	0.74
1:A:711:ILE:HD13	1:A:712:PRO:CD	2.17	0.71
1:B:711:ILE:HD13	1:B:712:PRO:CD	2.21	0.68
1:C:705:ARG:HH22	1:D:769:LYS:HZ3	1.42	0.68
1:D:896:MET:C	1:D:898:LYS:H	2.01	0.68
1:B:836:THR:O	1:B:839:PHE:HB3	1.98	0.63
1:A:893:LYS:HG2	1:A:899:VAL:HG21	1.81	0.61
1:A:849:GLU:HG2	1:A:923:PRO:HG3	1.84	0.59
1:C:713:GLU:O	1:C:750:ILE:HD11	2.03	0.59
1:A:703:GLN:O	3:B:1002:DMS:H11	2.04	0.58
1:D:688:LYS:HG3	1:D:693:ILE:HG13	1.85	0.58
1:D:712:PRO:HB2	1:D:715:ASP:HB3	1.84	0.58
1:C:884:LEU:HD12	1:C:890:ALA:HA	1.85	0.57
1:D:884:LEU:HD11	1:D:893:LYS:HD3	1.85	0.57
1:D:886:GLU:HB3	1:D:888:GLN:HE21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LYS:HB3	1:A:752:ILE:HG23	1.86	0.57
1:B:710:GLU:HG2	1:B:751:LYS:HG2	1.87	0.56
1:B:709:LYS:HB3	1:B:752:ILE:HG23	1.88	0.56
1:A:710:GLU:HG2	1:A:751:LYS:HG2	1.87	0.55
1:B:847:ALA:HB1	1:B:849:GLU:OE2	2.05	0.55
1:D:721:PRO:HB2	1:D:724:GLU:HB2	1.90	0.54
1:D:848:PRO:HB3	1:D:895:GLY:CA	2.35	0.54
1:B:715:ASP:O	1:B:716:SER:CB	2.33	0.53
1:D:895:GLY:HA2	1:D:898:LYS:HA	1.90	0.53
1:B:839:PHE:CZ	1:B:841:GLY:HA2	2.43	0.53
1:D:922:ASP:HB3	1:D:925:LYS:HB2	1.91	0.52
1:C:839:PHE:CZ	1:C:841:GLY:HA2	2.45	0.52
1:D:869:CYS:HB3	1:D:880:PRO:HG3	1.92	0.52
1:A:888:GLN:O	1:A:892:PHE:HD1	1.92	0.52
1:B:770:TRP:HE1	3:B:1002:DMS:C1	2.09	0.52
1:D:851:ILE:HG23	1:D:891:MET:HE3	1.92	0.51
1:D:784:THR:CG2	1:D:871:ILE:HG12	2.41	0.51
1:A:872:ILE:HG21	1:A:901:PRO:HB2	1.92	0.51
1:B:691:TYR:HD1	1:B:718:TYR:CD1	2.28	0.51
1:C:896:MET:HA	1:C:896:MET:HE2	1.93	0.51
1:A:847:ALA:HB1	1:A:849:GLU:OE2	2.10	0.51
1:B:922:ASP:HB3	1:B:925:LYS:HB2	1.93	0.50
1:C:881:PHE:CB	1:C:890:ALA:HB1	2.41	0.50
1:B:869:CYS:HB3	1:B:880:PRO:HG3	1.94	0.50
1:C:847:ALA:HB3	1:C:850:ILE:HG12	1.94	0.50
1:A:817:VAL:HG12	1:A:819:LYS:HD3	1.94	0.50
1:B:740:TYR:HD2	1:B:752:ILE:HD11	1.77	0.50
1:C:881:PHE:HB3	1:C:890:ALA:HB1	1.94	0.49
1:C:922:ASP:HB3	1:C:925:LYS:HB2	1.93	0.48
1:A:922:ASP:HB3	1:A:925:LYS:HB2	1.95	0.48
1:B:872:ILE:HG21	1:B:901:PRO:HB2	1.94	0.48
1:D:847:ALA:HB3	1:D:850:ILE:HG12	1.96	0.48
1:A:770:TRP:HE1	3:B:1003:DMS:H22	1.78	0.48
1:D:691:TYR:C	1:D:711:ILE:HD12	2.39	0.48
1:C:886:GLU:C	1:C:888:GLN:H	2.22	0.47
1:D:839:PHE:CZ	1:D:841:GLY:HA2	2.49	0.47
1:A:684:VAL:HB	1:A:696:ALA:HB3	1.96	0.47
1:A:770:TRP:HE1	3:B:1003:DMS:C2	2.27	0.47
1:C:847:ALA:HB1	1:C:849:GLU:OE2	2.16	0.46
1:A:894:VAL:O	1:A:898:LYS:HA	2.16	0.45
1:C:710:GLU:HG2	1:C:751:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:869:CYS:HB3	1:C:880:PRO:HG3	1.99	0.45
1:A:714:ARG:HB3	1:A:715:ASP:H	1.65	0.45
1:B:703:GLN:O	3:B:1003:DMS:C2	2.66	0.44
1:C:822:ASP:HA	2:C:4000:9E1:N2	2.32	0.44
1:A:869:CYS:HB3	1:A:880:PRO:HG3	2.00	0.44
1:A:795:HIS:O	1:A:860:LYS:HE2	2.18	0.44
1:B:726:ILE:O	1:B:730:LYS:HB2	2.18	0.44
1:D:784:THR:HG21	1:D:871:ILE:HG12	1.99	0.44
1:D:865:TRP:CZ2	1:D:894:VAL:HG13	2.52	0.43
1:D:872:ILE:HG21	1:D:901:PRO:HB2	2.00	0.43
1:C:893:LYS:HB3	1:C:897:PHE:CE1	2.54	0.43
1:C:705:ARG:HH22	1:D:769:LYS:NZ	2.15	0.43
1:B:729:HIS:CD2	1:B:740:TYR:HB2	2.54	0.42
1:B:703:GLN:O	3:B:1003:DMS:H21	2.20	0.42
1:A:736:ASN:HA	1:A:818:LEU:O	2.19	0.42
1:B:834:PRO:HD2	1:B:837:GLU:HB2	2.02	0.42
1:A:729:HIS:CD2	1:A:740:TYR:HB2	2.55	0.42
1:D:881:PHE:CE2	1:D:894:VAL:HG22	2.55	0.41
1:C:726:ILE:O	1:C:730:LYS:HB2	2.20	0.41
1:A:734:HIS:HB3	1:A:737:ILE:HD13	2.02	0.41
1:B:698:ARG:HD3	3:B:1003:DMS:H11	2.01	0.41
1:B:837:GLU:O	1:B:855:PRO:HB3	2.21	0.41
1:D:726:ILE:O	1:D:730:LYS:HB2	2.20	0.41
1:C:729:HIS:CD2	1:C:740:TYR:HB2	2.55	0.41
1:B:679:GLU:CD	1:B:679:GLU:H	2.29	0.41
1:C:720:GLN:N	1:C:721:PRO:HD2	2.36	0.41
1:D:784:THR:HG22	1:D:871:ILE:HG12	2.03	0.40
1:A:897:PHE:HB2	1:A:899:VAL:HG13	2.03	0.40
1:A:711:ILE:HG22	1:A:722:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

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	269/293 (92%)	249 (93%)	18 (7%)	2 (1%)	18	27
1	B	269/293 (92%)	254 (94%)	11 (4%)	4 (2%)	8	11
1	C	269/293 (92%)	237 (88%)	27 (10%)	5 (2%)	6	8
1	D	269/293 (92%)	241 (90%)	22 (8%)	6 (2%)	5	7
All	All	1076/1172 (92%)	981 (91%)	78 (7%)	17 (2%)	7	10

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	939	LYS
1	B	715	ASP
1	B	939	LYS
1	C	713	GLU
1	D	894	VAL
1	A	831	GLY
1	B	716	SER
1	C	831	GLY
1	C	822	ASP
1	C	939	LYS
1	D	715	ASP
1	D	939	LYS
1	B	841	GLY
1	C	841	GLY
1	D	831	GLY
1	D	841	GLY
1	D	721	PRO

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	231/252 (92%)	211 (91%)	20 (9%)	9	15
1	B	231/252 (92%)	213 (92%)	18 (8%)	11	18
1	C	231/252 (92%)	214 (93%)	17 (7%)	13	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	231/252 (92%)	213 (92%)	18 (8%)	11	18
All	All	924/1008 (92%)	851 (92%)	73 (8%)	11	18

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	670	LEU
1	A	679	GLU
1	A	711	ILE
1	A	714	ARG
1	A	717	ARG
1	A	722	LEU
1	A	735	LYS
1	A	738	VAL
1	A	752	ILE
1	A	827	LYS
1	A	832	ILE
1	A	836	THR
1	A	837	GLU
1	A	844	GLN
1	A	849	GLU
1	A	852	ASP
1	A	883	GLU
1	A	886	GLU
1	A	896	MET
1	A	939	LYS
1	B	679	GLU
1	B	688	LYS
1	B	698	ARG
1	B	711	ILE
1	B	713	GLU
1	B	716	SER
1	B	722	LEU
1	B	735	LYS
1	B	737	ILE
1	B	738	VAL
1	B	752	ILE
1	B	832	ILE
1	B	844	GLN
1	B	849	GLU
1	B	852	ASP
1	B	883	GLU

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Mol	Chain	Res	Type
1	B	888	GLN
1	B	905	GLU
1	C	676	GLU
1	C	679	GLU
1	C	683	ARG
1	C	711	ILE
1	C	722	LEU
1	C	737	ILE
1	C	752	ILE
1	C	756	GLN
1	C	768	SER
1	C	832	ILE
1	C	844	GLN
1	C	849	GLU
1	C	852	ASP
1	C	883	GLU
1	C	888	GLN
1	C	897	PHE
1	C	905	GLU
1	D	670	LEU
1	D	679	GLU
1	D	706	ILE
1	D	708	ILE
1	D	711	ILE
1	D	722	LEU
1	D	735	LYS
1	D	737	ILE
1	D	738	VAL
1	D	768	SER
1	D	827	LYS
1	D	832	ILE
1	D	844	GLN
1	D	849	GLU
1	D	852	ASP
1	D	883	GLU
1	D	888	GLN
1	D	905	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	776	ASN

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Mol	Chain	Res	Type
1	A	888	GLN
1	B	731	HIS
1	C	703	GLN
1	C	720	GLN
1	C	756	GLN
1	C	808	ASN
1	D	703	GLN
1	D	888	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DMS	A	1002	-	3,3,3	0.30	0	3,3,3	0.71	0
2	9E1	C	4000	-	31,31,31	1.77	5 (16%)	43,45,45	1.26	5 (11%)
3	DMS	B	1004	-	3,3,3	0.28	0	3,3,3	0.76	0
3	DMS	B	1002	-	3,3,3	0.23	0	3,3,3	0.60	0
2	9E1	D	4000	-	31,31,31	1.78	5 (16%)	43,45,45	1.29	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	9E1	B	1001	-	31,31,31	1.75	5 (16%)	43,45,45	1.34	5 (11%)
2	9E1	A	1001	-	31,31,31	1.77	5 (16%)	43,45,45	1.28	5 (11%)
3	DMS	B	1003	-	3,3,3	0.92	0	3,3,3	1.48	1 (33%)

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
2	9E1	B	1001	-	-	4/24/24/24	0/3/3/3
2	9E1	A	1001	-	-	4/24/24/24	0/3/3/3
2	9E1	C	4000	-	-	4/24/24/24	0/3/3/3
2	9E1	D	4000	-	-	6/24/24/24	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	9E1	C14-S1	-6.88	1.66	1.77
2	B	1001	9E1	C14-S1	-6.80	1.66	1.77
2	D	4000	9E1	C14-S1	-6.77	1.66	1.77
2	C	4000	9E1	C14-S1	-6.74	1.66	1.77
2	D	4000	9E1	C5-N3	3.47	1.37	1.32
2	C	4000	9E1	C5-N3	3.46	1.37	1.32
2	A	1001	9E1	C5-N3	3.28	1.37	1.32
2	B	1001	9E1	C5-N1	3.20	1.40	1.37
2	B	1001	9E1	C5-N3	3.17	1.37	1.32
2	A	1001	9E1	C5-N1	2.99	1.40	1.37
2	C	4000	9E1	C5-N1	2.91	1.40	1.37
2	D	4000	9E1	C5-N1	2.89	1.40	1.37
2	C	4000	9E1	C4-N2	2.86	1.37	1.31
2	D	4000	9E1	C4-N2	2.82	1.37	1.31
2	B	1001	9E1	C4-N2	2.81	1.37	1.31
2	A	1001	9E1	C4-N2	2.79	1.37	1.31
2	B	1001	9E1	N2-N3	-2.58	1.33	1.39
2	A	1001	9E1	N2-N3	-2.55	1.34	1.39
2	C	4000	9E1	N2-N3	-2.53	1.34	1.39
2	D	4000	9E1	N2-N3	-2.52	1.34	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4000	9E1	N1-C5-N3	-4.33	108.29	110.31
2	B	1001	9E1	N1-C5-N3	-4.29	108.31	110.31
2	A	1001	9E1	N1-C5-N3	-4.17	108.36	110.31
2	C	4000	9E1	N1-C5-N3	-4.10	108.39	110.31
2	B	1001	9E1	C14-S1-N6	-3.47	103.57	108.40
2	A	1001	9E1	C14-S1-N6	-3.06	104.14	108.40
2	C	4000	9E1	C14-S1-N6	-3.04	104.17	108.40
2	D	4000	9E1	C13-C14-S1	2.97	124.71	119.34
2	D	4000	9E1	C14-S1-N6	-2.94	104.31	108.40
2	B	1001	9E1	C16-C15-C14	2.86	122.23	119.44
2	A	1001	9E1	C16-C15-C14	2.79	122.15	119.44
2	C	4000	9E1	C13-C14-S1	2.67	124.16	119.34
2	C	4000	9E1	C16-C15-C14	2.63	122.00	119.44
2	B	1001	9E1	C15-C14-C13	-2.63	117.42	120.68
2	D	4000	9E1	C16-C15-C14	2.62	121.99	119.44
2	B	1001	9E1	C13-C14-S1	2.60	124.03	119.34
2	A	1001	9E1	C13-C14-S1	2.59	124.01	119.34
2	C	4000	9E1	C15-C14-C13	-2.54	117.53	120.68
2	A	1001	9E1	C15-C14-C13	-2.51	117.58	120.68
2	D	4000	9E1	C15-C14-C13	-2.50	117.59	120.68
3	B	1003	DMS	O-S-C1	2.39	118.44	106.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	9E1	C15-C14-S1-O3
2	C	4000	9E1	C15-C14-S1-O3
2	A	1001	9E1	C13-C14-S1-N6
2	B	1001	9E1	C13-C14-S1-N6
2	C	4000	9E1	C13-C14-S1-O3
2	A	1001	9E1	C13-C14-S1-O3
2	A	1001	9E1	C15-C14-S1-O3
2	B	1001	9E1	C13-C14-S1-O3
2	A	1001	9E1	C15-C14-S1-N6
2	B	1001	9E1	C15-C14-S1-N6
2	C	4000	9E1	C13-C14-S1-N6
2	C	4000	9E1	C15-C14-S1-N6
2	D	4000	9E1	C13-C14-S1-N6
2	D	4000	9E1	C15-C14-S1-N6
2	D	4000	9E1	C15-C14-S1-O3
2	D	4000	9E1	C13-C14-S1-O3
2	D	4000	9E1	O1-C11-C12-C17

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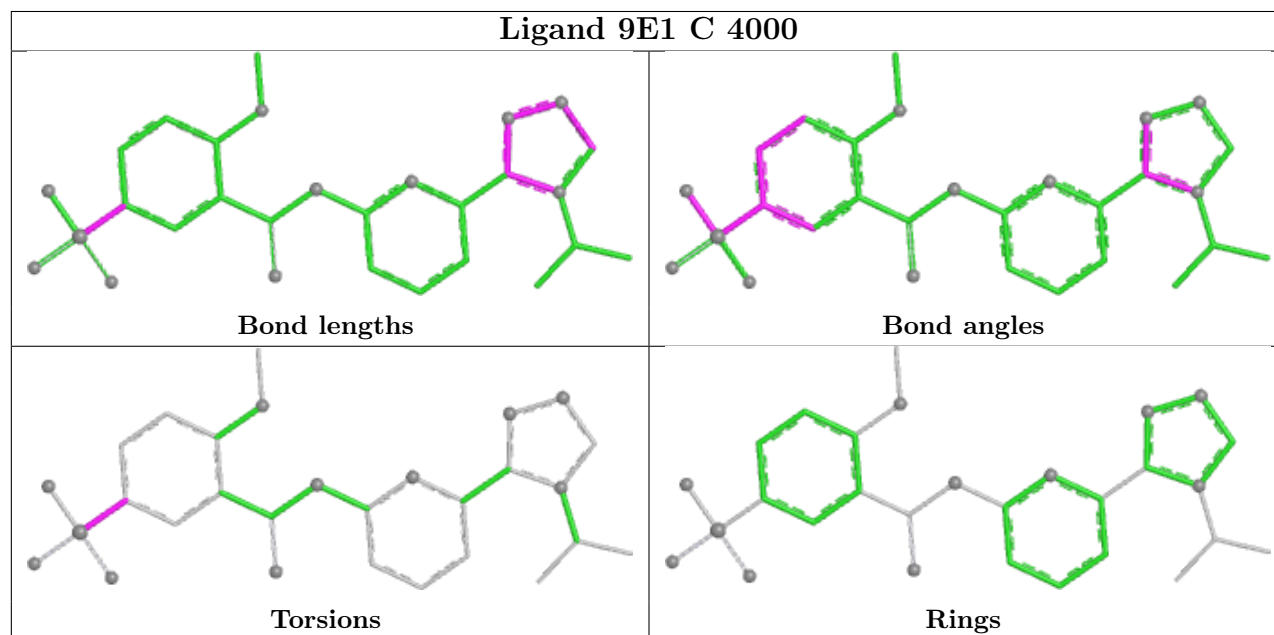
Mol	Chain	Res	Type	Atoms
2	D	4000	9E1	N5-C11-C12-C17

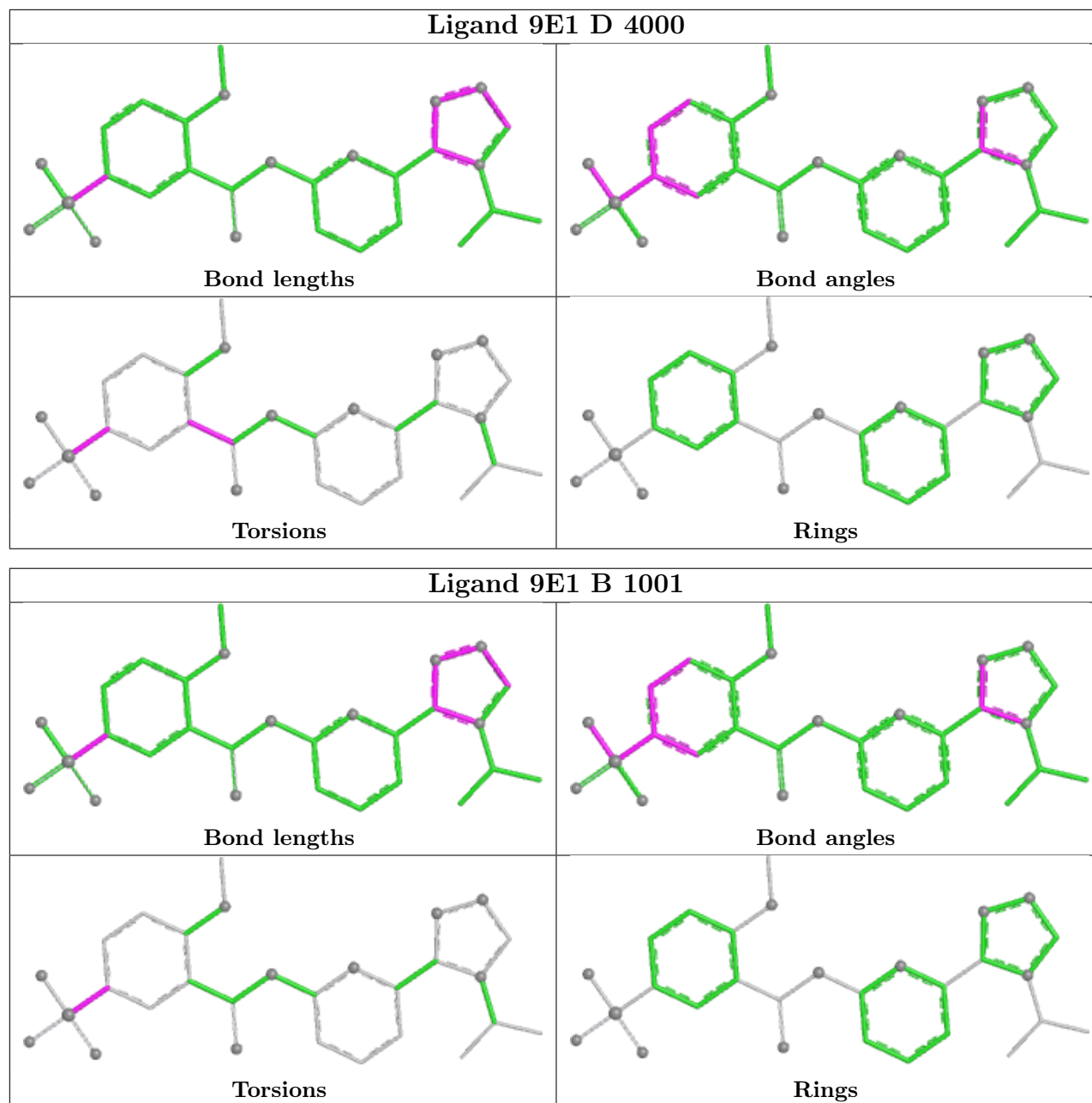
There are no ring outliers.

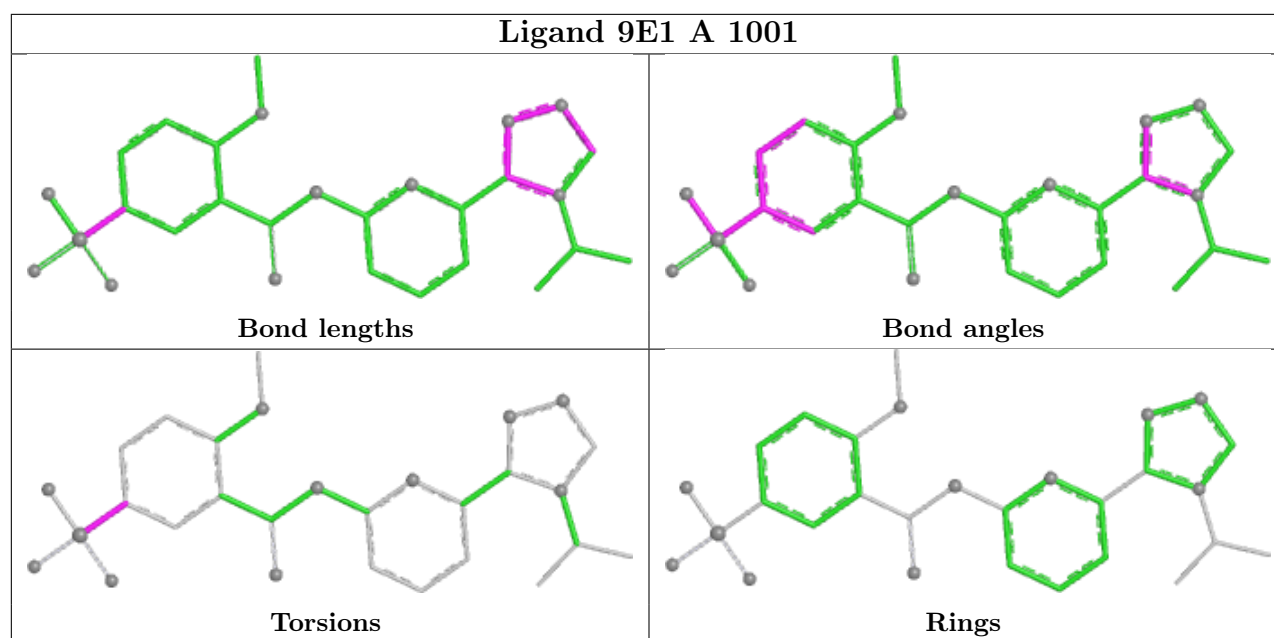
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4000	9E1	1	0
3	B	1002	DMS	3	0
3	B	1003	DMS	5	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	271/293 (92%)	-0.21	9 (3%)	49	43	46, 84, 143, 197	0
1	B	271/293 (92%)	-0.35	9 (3%)	49	43	46, 78, 136, 173	0
1	C	271/293 (92%)	0.34	10 (3%)	45	39	93, 165, 230, 243	0
1	D	271/293 (92%)	0.42	20 (7%)	20	17	96, 161, 208, 229	0
All	All	1084/1172 (92%)	0.05	48 (4%)	39	32	46, 117, 207, 243	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	894	VAL	4.6
1	B	836	THR	4.1
1	A	940	VAL	3.8
1	C	670	LEU	3.7
1	C	889	ALA	3.6
1	C	897	PHE	3.6
1	D	887	PRO	3.6
1	C	892	PHE	3.2
1	C	891	MET	3.1
1	B	831	GLY	3.1
1	C	893	LYS	3.0
1	A	834	PRO	2.9
1	D	804	ILE	2.9
1	B	832	ILE	2.9
1	D	801	HIS	2.8
1	D	897	PHE	2.8
1	D	722	LEU	2.8
1	D	890	ALA	2.8
1	A	831	GLY	2.7
1	B	834	PRO	2.7
1	D	838	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	820	ILE	2.6
1	D	854	GLY	2.6
1	A	835	CYS	2.5
1	D	670	LEU	2.5
1	D	895	GLY	2.5
1	B	940	VAL	2.5
1	A	833	ASN	2.4
1	D	806	GLY	2.4
1	B	838	THR	2.4
1	D	800	VAL	2.4
1	C	671	LEU	2.3
1	A	939	LYS	2.3
1	B	835	CYS	2.3
1	A	670	LEU	2.3
1	A	832	ILE	2.3
1	D	893	LYS	2.2
1	D	899	VAL	2.2
1	D	850	ILE	2.2
1	B	837	GLU	2.2
1	A	924	ASP	2.2
1	B	670	LEU	2.2
1	D	891	MET	2.2
1	D	892	PHE	2.1
1	C	870	THR	2.1
1	C	833	ASN	2.1
1	D	858	TYR	2.1
1	D	940	VAL	2.1

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.

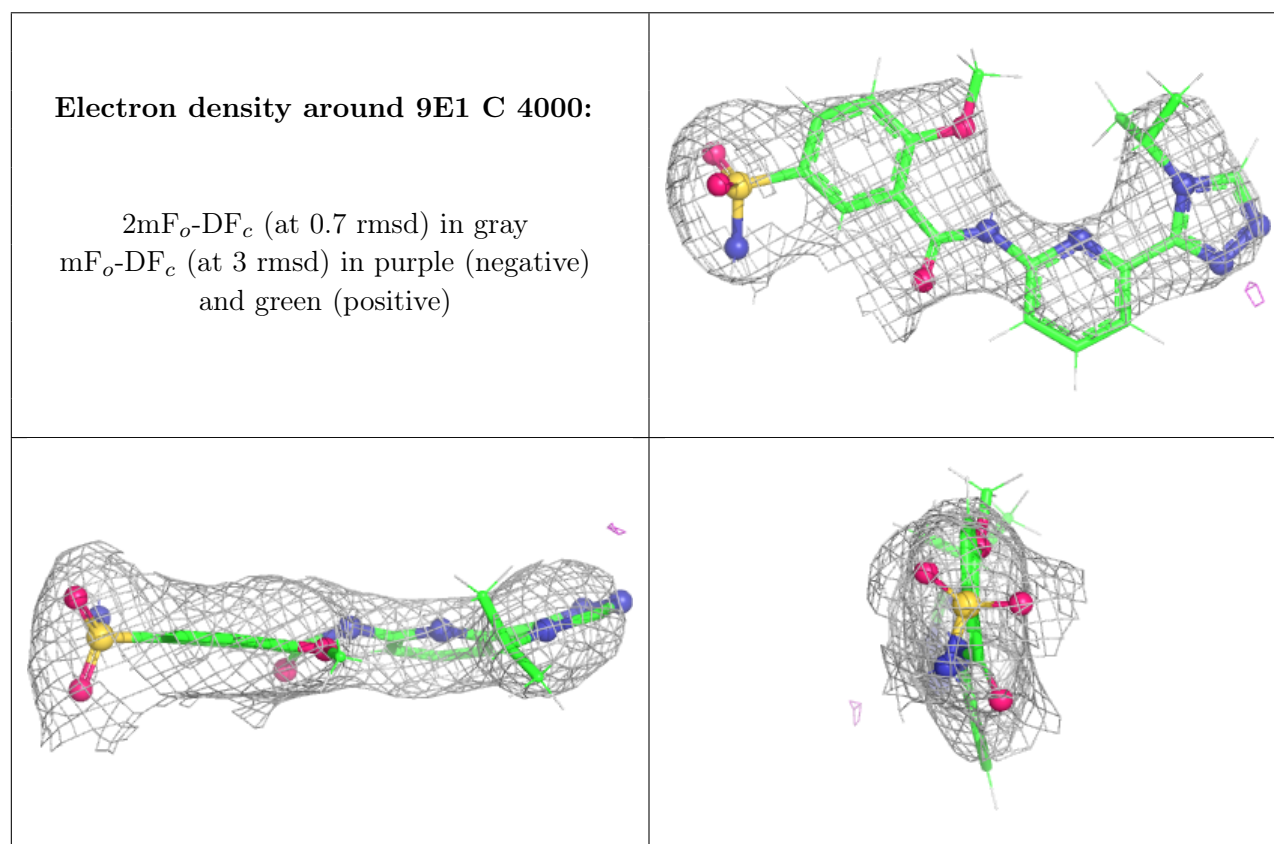
6.4 Ligands [i](#)

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, 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.

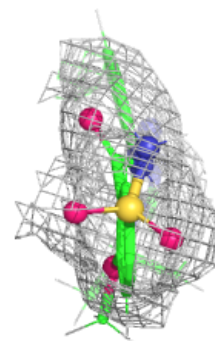
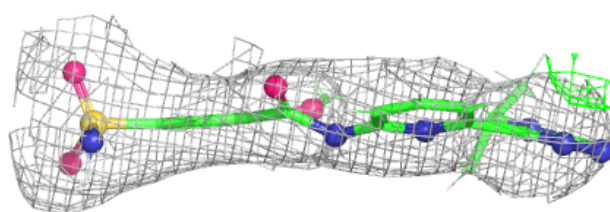
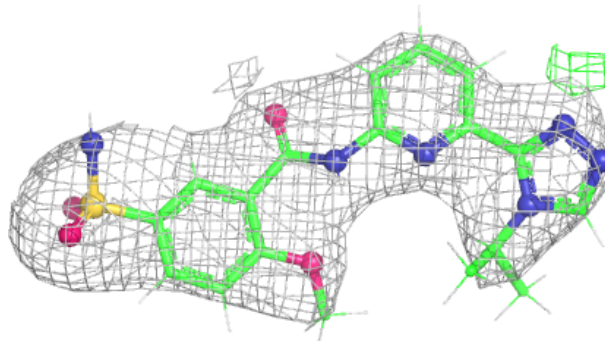
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DMS	B	1002	4/4	0.92	0.12	98,100,103,104	0
3	DMS	B	1003	4/4	0.92	0.14	63,75,77,84	0
2	9E1	C	4000	29/29	0.95	0.08	102,123,139,143	20
3	DMS	A	1002	4/4	0.95	0.19	78,86,88,90	0
2	9E1	D	4000	29/29	0.96	0.07	104,114,131,135	20
3	DMS	B	1004	4/4	0.96	0.15	80,86,89,90	0
2	9E1	A	1001	29/29	0.98	0.05	50,58,63,66	20
2	9E1	B	1001	29/29	0.98	0.06	35,47,55,59	20

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.

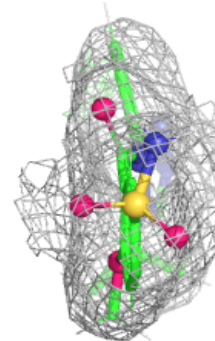
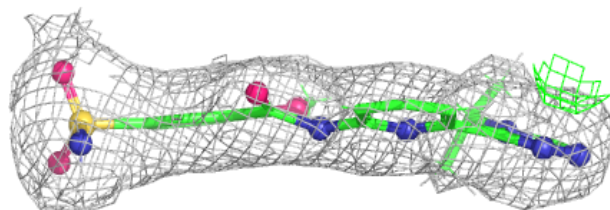
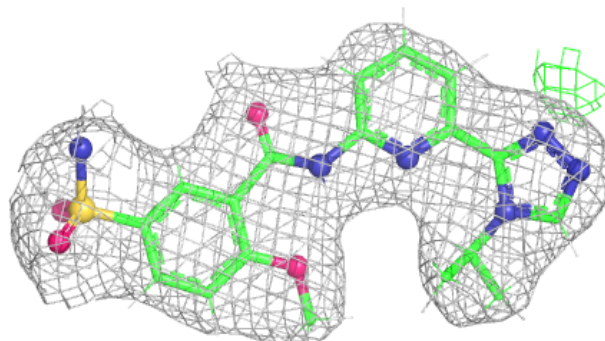


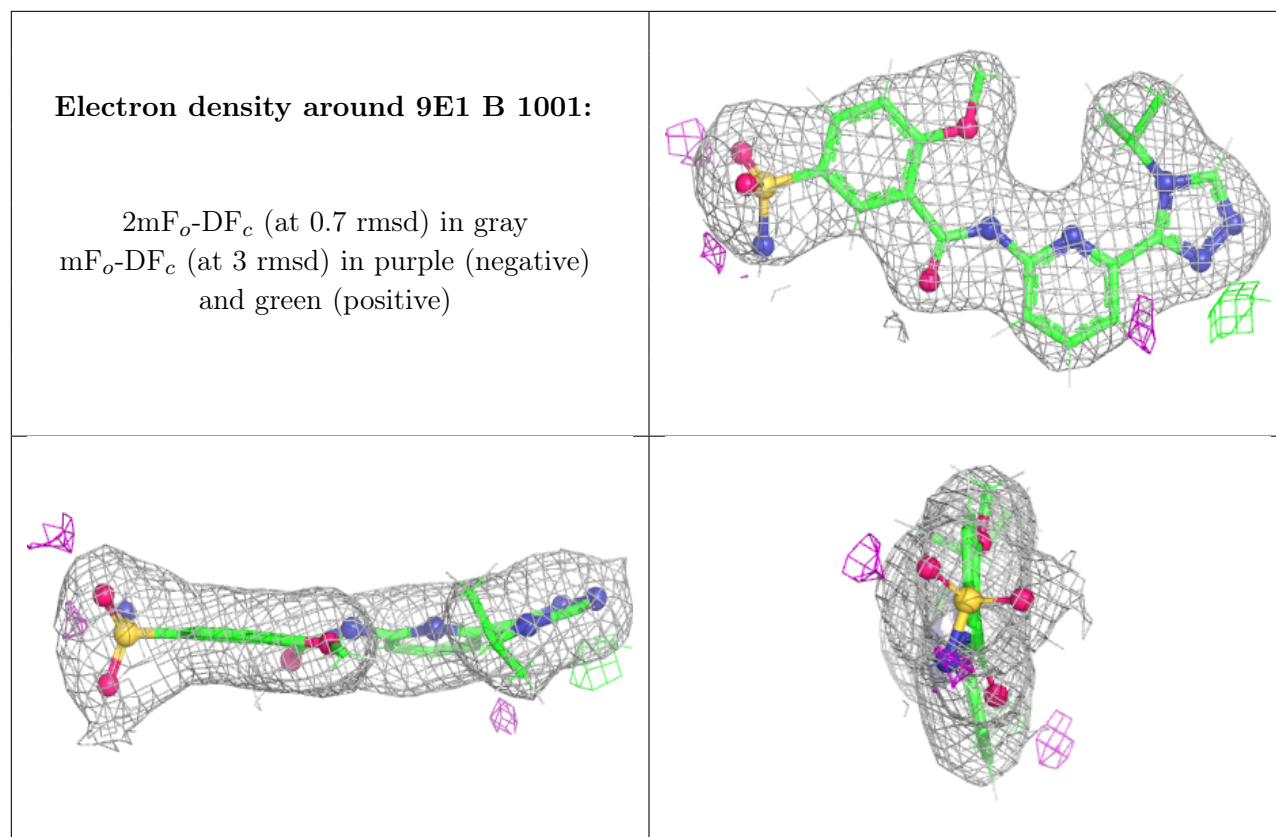
Electron density around 9E1 D 4000:

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

**Electron density around 9E1 A 1001:**

$2mF_o-DF_c$ (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.