



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 11:46 am BST

PDB ID : 5VIL
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

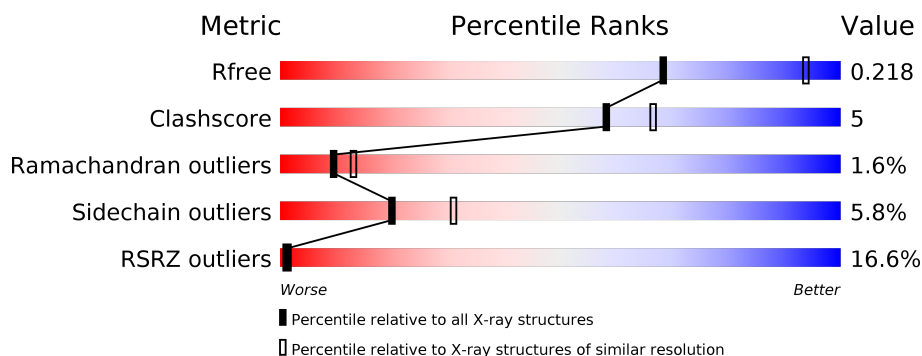
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	293	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	293	<div> <div>29%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	293	<div> <div>23%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition [i](#)

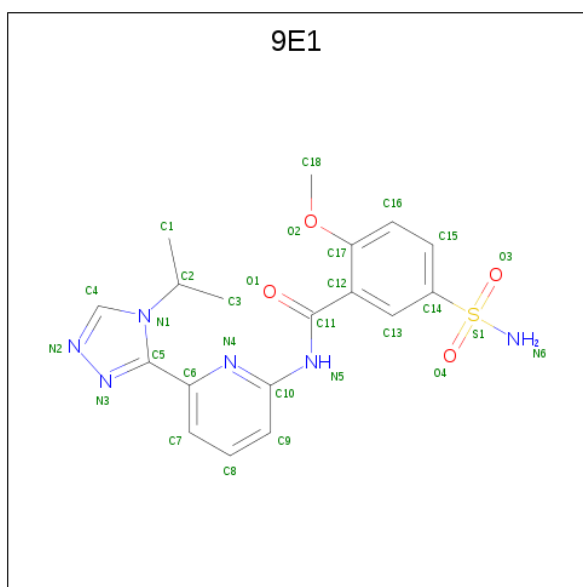
There are 4 unique types of molecules in this entry. The entry contains 8958 atoms, of which 104 are hydrogens and 0 are deuteriums.

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 (three-letter code: 9E1) (formula: C₁₈H₂₀N₆O₄S).



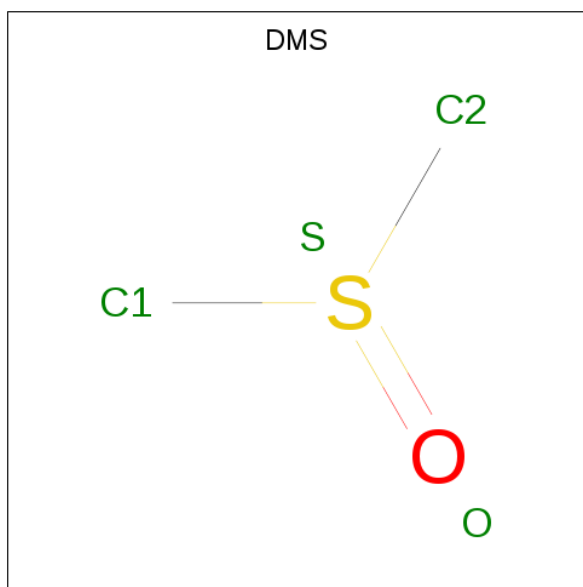
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	20	0
			49	18	20	6	4		
2	B	1	Total	C	H	N	O	20	0
			49	18	20	6	4		

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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 (three-letter code: DMS) (formula: C₂H₆OS).



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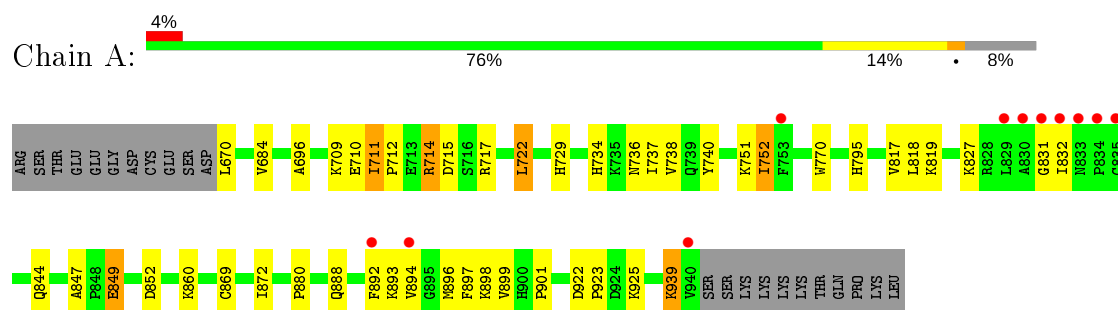
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	14	Total	O	0	0
			14	14		

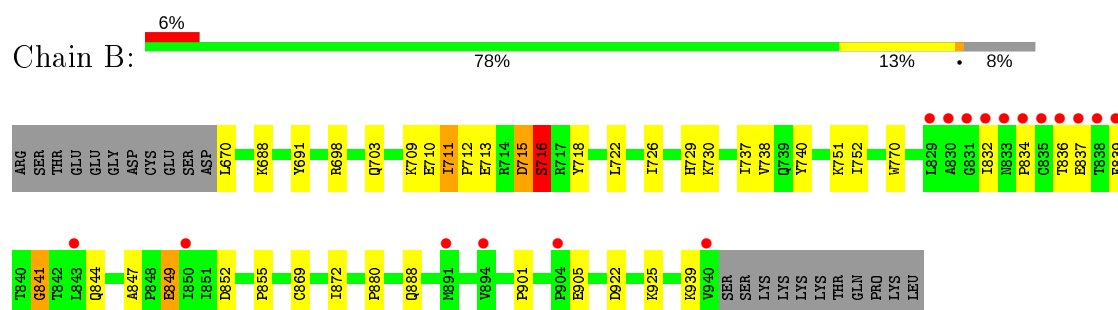
3 Residue-property plots [i](#)

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

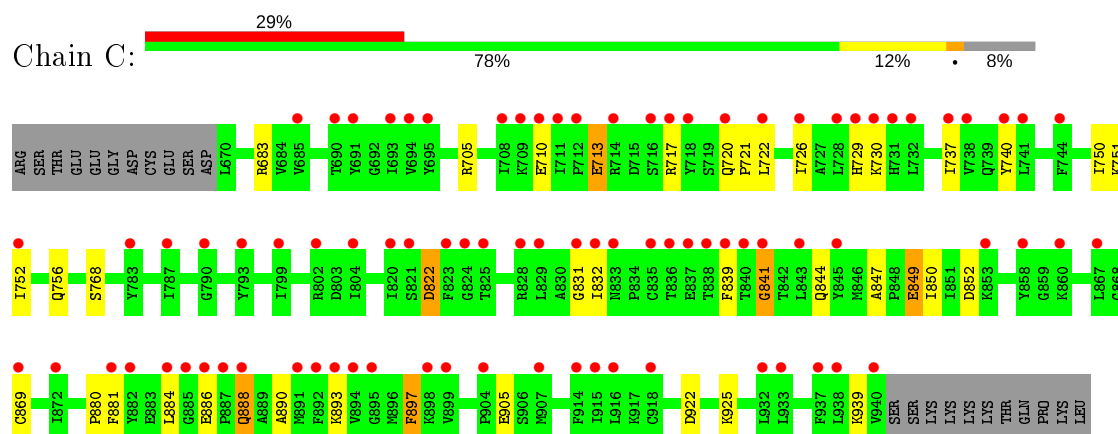
- Molecule 1: Mitogen-activated protein kinase kinase kinase 5



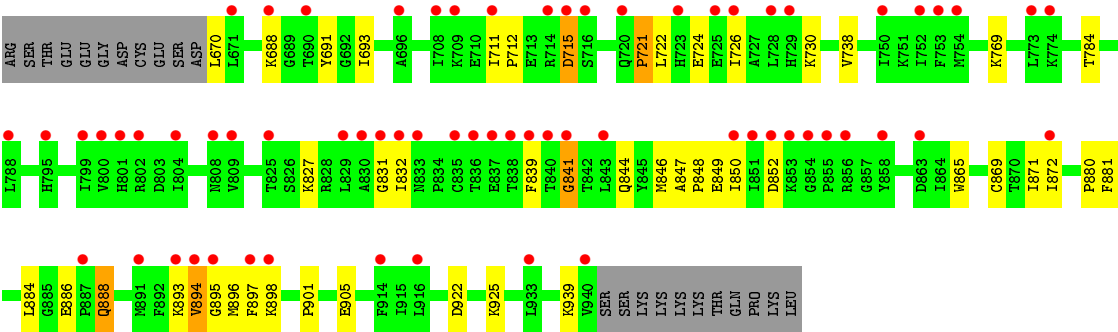
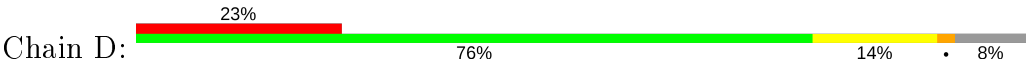
- Molecule 1: Mitogen-activated protein kinase kinase kinase 5



- 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 – 2.64 135.06 – 2.64	Depositor EDS
% Data completeness (in resolution range)	82.7 (135.00-2.64) 82.6 (135.06-2.64)	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 (5.13%)	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)	0.31 , 88.6	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	0.57	0/2195	0.74	0/2963
1	B	0.57	0/2195	0.72	0/2963
1	C	0.44	0/2195	0.69	0/2963
1	D	0.44	0/2195	0.68	0/2963
All	All	0.51	0/8780	0.71	0/11852

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	22	0
1	B	2146	0	2136	21	0
1	C	2146	0	2136	18	0
1	D	2146	0	2136	24	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	18	18	4	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	83	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 (83) 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: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:B:770:TRP:HE1	3:B:1002:DMS:H12	1.56	0.68
1:B:770:TRP:HE1	3:B:1002:DMS:C1	2.09	0.65
1:D:896:MET:C	1:D:898:LYS:H	2.01	0.64
1:B:836:THR:O	1:B:839:PHE:HB3	1.98	0.63
1:C:705:ARG:HH22	1:D:769:LYS:HZ3	1.48	0.62
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:D:691:TYR:C	1:D:711:ILE:HD12	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:886:GLU:C	1:C:888:GLN:H	2.22	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: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: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 [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	269/293 (92%)	249 (93%)	18 (7%)	2 (1%)	22	32
1	B	269/293 (92%)	254 (94%)	11 (4%)	4 (2%)	10	14
1	C	269/293 (92%)	237 (88%)	27 (10%)	5 (2%)	8	10
1	D	269/293 (92%)	241 (90%)	22 (8%)	6 (2%)	6	9
All	All	1076/1172 (92%)	981 (91%)	78 (7%)	17 (2%)	9	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	939	LYS

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Mol	Chain	Res	Type
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 ⓘ

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%)	217 (94%)	14 (6%)	18	29
1	B	231/252 (92%)	216 (94%)	15 (6%)	17	26
1	C	231/252 (92%)	217 (94%)	14 (6%)	18	29
1	D	231/252 (92%)	220 (95%)	11 (5%)	25	39
All	All	924/1008 (92%)	870 (94%)	54 (6%)	20	31

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	670	LEU
1	A	711	ILE
1	A	714	ARG
1	A	717	ARG
1	A	722	LEU

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Mol	Chain	Res	Type
1	A	738	VAL
1	A	752	ILE
1	A	827	LYS
1	A	832	ILE
1	A	844	GLN
1	A	849	GLU
1	A	852	ASP
1	A	896	MET
1	A	939	LYS
1	B	670	LEU
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	737	ILE
1	B	738	VAL
1	B	832	ILE
1	B	844	GLN
1	B	849	GLU
1	B	852	ASP
1	B	888	GLN
1	B	905	GLU
1	C	683	ARG
1	C	717	ARG
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	888	GLN
1	C	897	PHE
1	C	905	GLU
1	D	670	LEU
1	D	722	LEU
1	D	738	VAL
1	D	827	LYS

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Mol	Chain	Res	Type
1	D	832	ILE
1	D	844	GLN
1	D	849	GLU
1	D	852	ASP
1	D	888	GLN
1	D	897	PHE
1	D	905	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	888	GLN
1	C	720	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 carbohydrates 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
2	9E1	A	1001	-	28,31,31	1.53	1 (3%)	39,45,45	1.23	6 (15%)
2	9E1	C	4000	-	28,31,31	1.52	1 (3%)	39,45,45	1.20	5 (12%)
3	DMS	B	1004	-	3,3,3	0.28	0	3,3,3	0.76	0
2	9E1	D	4000	-	28,31,31	1.54	1 (3%)	39,45,45	1.26	6 (15%)
3	DMS	B	1003	-	3,3,3	0.90	0	3,3,3	1.45	1 (33%)
2	9E1	B	1001	-	28,31,31	1.50	1 (3%)	39,45,45	1.28	6 (15%)
3	DMS	A	1002	-	3,3,3	0.30	0	3,3,3	0.69	0
3	DMS	B	1002	-	3,3,3	0.23	0	3,3,3	0.59	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
2	9E1	A	1001	-	-	4/24/24/24	0/3/3/3
2	9E1	D	4000	-	-	6/24/24/24	0/3/3/3
2	9E1	C	4000	-	-	4/24/24/24	0/3/3/3
2	9E1	B	1001	-	-	4/24/24/24	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	9E1	C14-S1	-6.74	1.66	1.77
2	B	1001	9E1	C14-S1	-6.65	1.66	1.77
2	D	4000	9E1	C14-S1	-6.63	1.66	1.77
2	C	4000	9E1	C14-S1	-6.60	1.66	1.77

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	9E1	C14-S1-N6	-3.40	103.57	108.38
2	A	1001	9E1	C14-S1-N6	-3.00	104.14	108.38
2	C	4000	9E1	C14-S1-N6	-2.98	104.17	108.38
2	D	4000	9E1	C4-N1-C5	-2.93	105.28	108.66
2	B	1001	9E1	C4-N1-C5	-2.91	105.30	108.66
2	C	4000	9E1	C4-N1-C5	-2.91	105.30	108.66
2	A	1001	9E1	C4-N1-C5	-2.88	105.32	108.66
2	D	4000	9E1	C14-S1-N6	-2.88	104.31	108.38
2	D	4000	9E1	C13-C14-S1	2.71	124.71	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	9E1	C16-C15-C14	2.68	122.23	119.45
2	A	1001	9E1	C16-C15-C14	2.61	122.15	119.45
2	B	1001	9E1	C15-C14-C13	-2.60	117.42	120.62
2	C	4000	9E1	C15-C14-C13	-2.51	117.53	120.62
2	A	1001	9E1	C15-C14-C13	-2.48	117.58	120.62
2	D	4000	9E1	C15-C14-C13	-2.47	117.59	120.62
2	C	4000	9E1	C16-C15-C14	2.47	122.00	119.45
2	D	4000	9E1	C16-C15-C14	2.46	121.99	119.45
2	C	4000	9E1	C13-C14-S1	2.44	124.16	119.31
2	B	1001	9E1	C13-C14-S1	2.37	124.03	119.31
2	A	1001	9E1	C13-C14-S1	2.36	124.01	119.31
3	B	1003	DMS	O-S-C1	2.33	118.44	106.54
2	D	4000	9E1	C6-N4-C10	-2.19	116.41	118.06
2	B	1001	9E1	O3-S1-C14	2.02	109.60	107.35
2	A	1001	9E1	C6-N4-C10	-2.00	116.56	118.06

There are no chirality outliers.

All (18) torsion outliers are listed below:

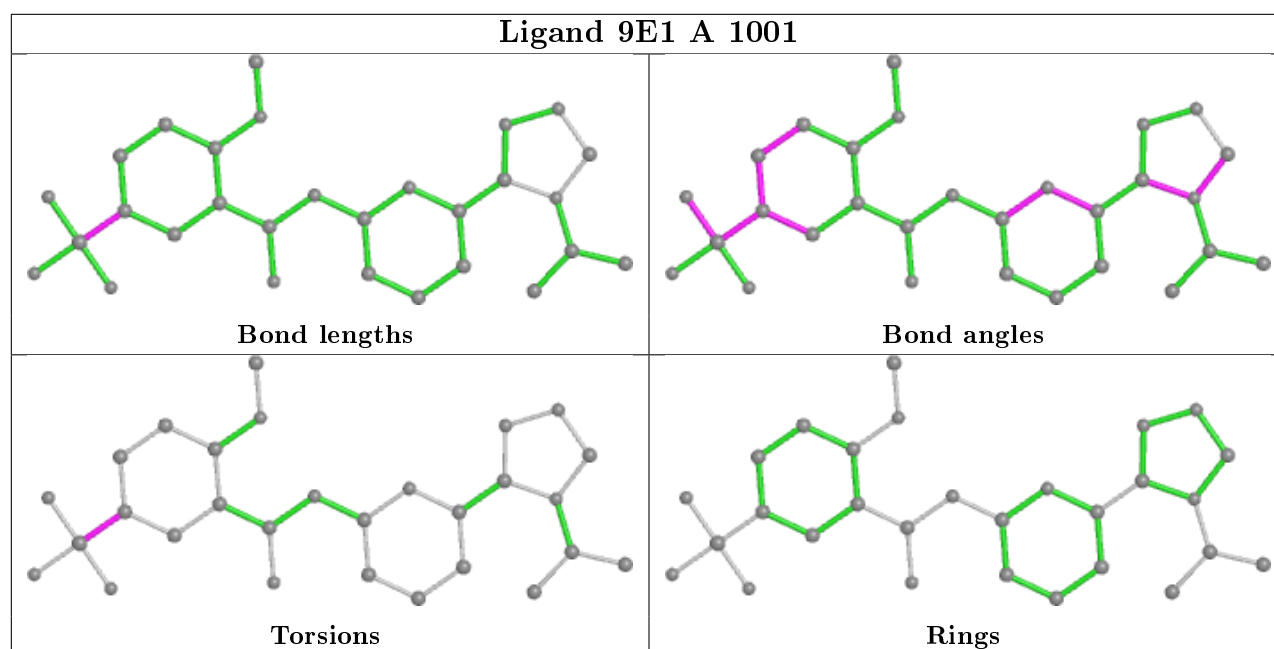
Mol	Chain	Res	Type	Atoms
2	B	1001	9E1	C15-C14-S1-O3
2	C	4000	9E1	C15-C14-S1-O3
2	C	4000	9E1	C13-C14-S1-O3
2	A	1001	9E1	C13-C14-S1-O3
2	A	1001	9E1	C15-C14-S1-O3
2	B	1001	9E1	C13-C14-S1-O3
2	A	1001	9E1	C13-C14-S1-N6
2	B	1001	9E1	C13-C14-S1-N6
2	B	1001	9E1	C15-C14-S1-N6
2	A	1001	9E1	C15-C14-S1-N6
2	C	4000	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
2	D	4000	9E1	N5-C11-C12-C17

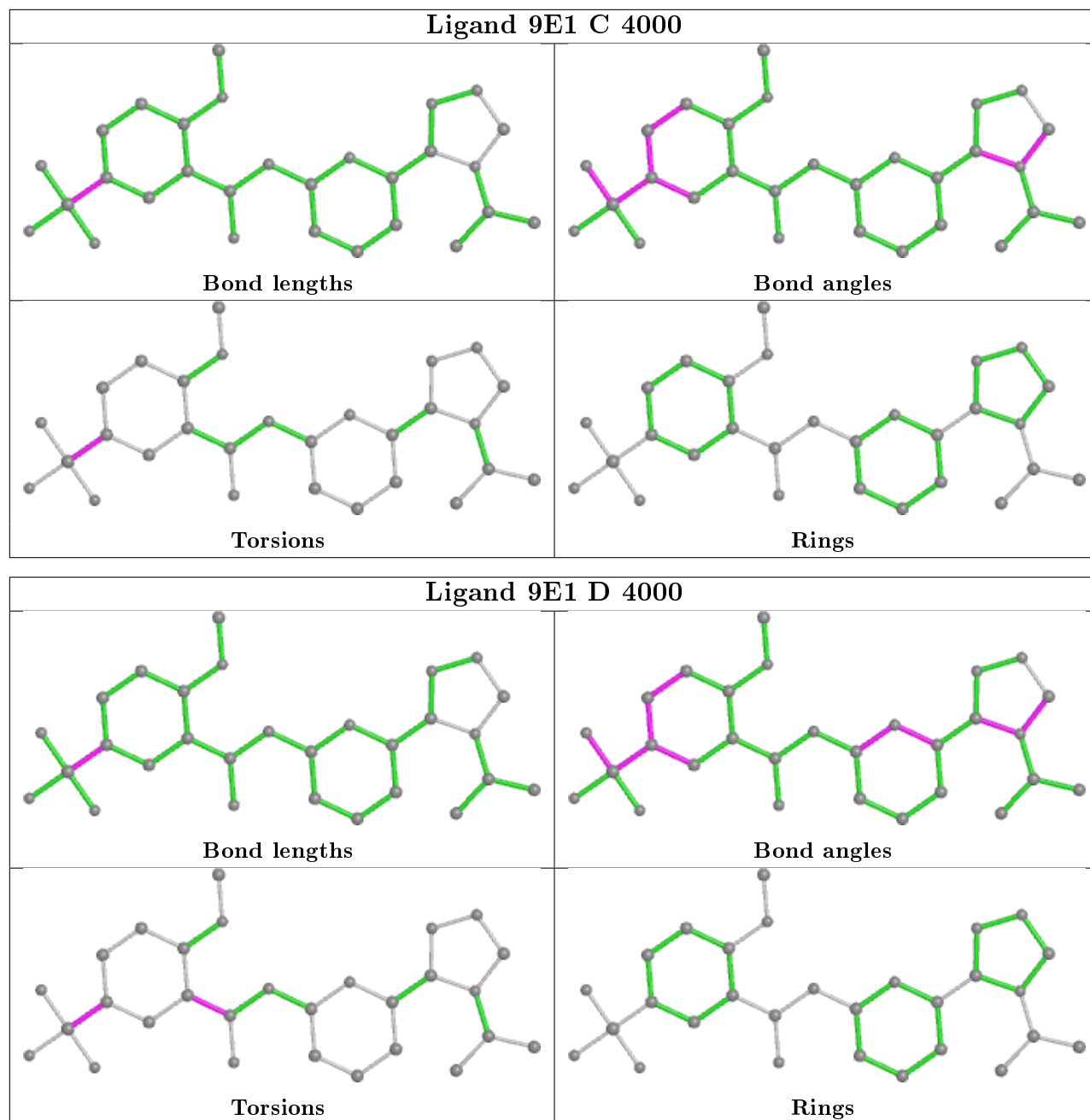
There are no ring outliers.

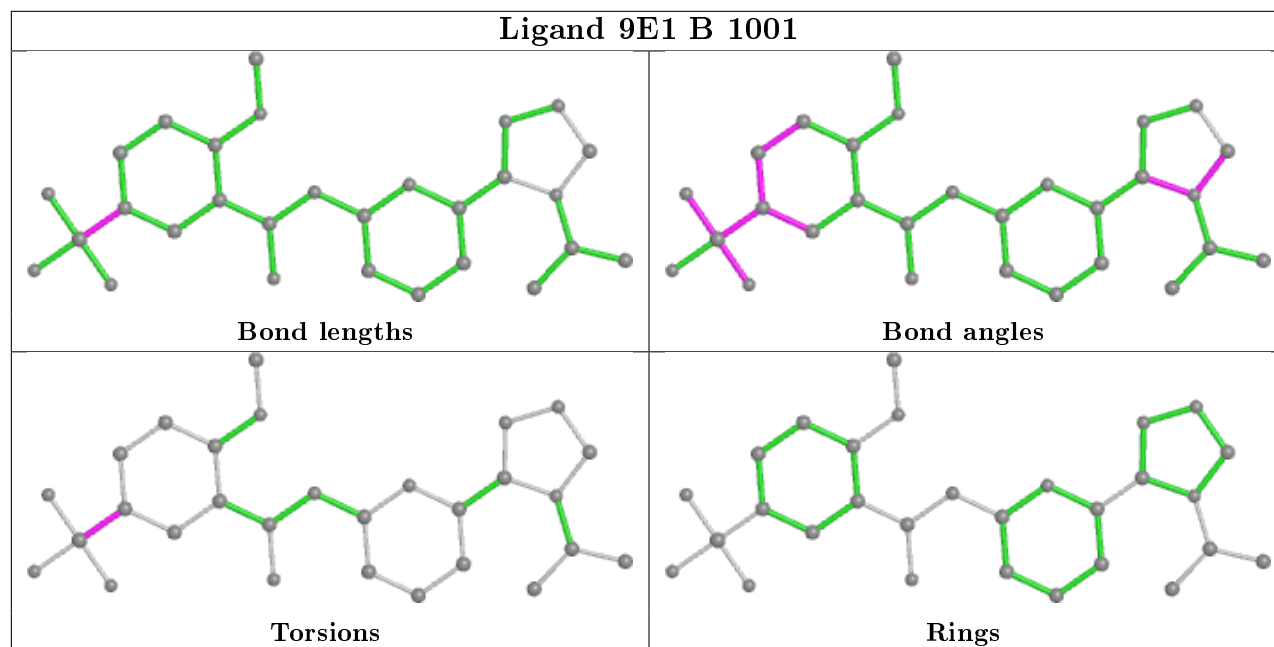
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4000	9E1	1	0
3	B	1003	DMS	2	0
3	B	1002	DMS	2	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%)	0.43	11 (4%) 37 33	46, 84, 143, 197	0
1	B	271/293 (92%)	0.56	17 (6%) 20 16	46, 78, 136, 173	0
1	C	271/293 (92%)	1.76	86 (31%) 0 0	93, 165, 230, 243	0
1	D	271/293 (92%)	1.40	66 (24%) 0 0	96, 161, 208, 229	0
All	All	1084/1172 (92%)	1.04	180 (16%) 1 1	46, 117, 207, 243	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	892	PHE	14.0
1	D	894	VAL	14.0
1	D	854	GLY	13.4
1	C	891	MET	13.2
1	D	832	ILE	12.6
1	C	833	ASN	12.4
1	C	887	PRO	12.4
1	C	832	ILE	12.1
1	C	835	CYS	11.0
1	C	886	GLU	10.8
1	A	831	GLY	10.6
1	C	839	PHE	10.5
1	D	838	THR	10.0
1	C	717	ARG	9.8
1	B	835	CYS	9.2
1	D	940	VAL	8.9
1	A	833	ASN	8.5
1	C	888	GLN	8.5
1	D	850	ILE	8.4
1	A	832	ILE	8.3
1	D	853	LYS	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	834	PRO	8.1
1	B	837	GLU	8.0
1	C	894	VAL	7.8
1	B	836	THR	7.7
1	D	839	PHE	7.4
1	C	711	ILE	7.4
1	D	897	PHE	7.3
1	B	834	PRO	6.9
1	B	832	ILE	6.7
1	D	895	GLY	6.6
1	C	695	TYR	6.4
1	C	716	SER	6.3
1	D	801	HIS	6.3
1	C	712	PRO	6.2
1	B	833	ASN	6.1
1	C	885	GLY	6.0
1	D	891	MET	6.0
1	D	836	THR	6.0
1	D	728	LEU	5.9
1	D	887	PRO	5.9
1	D	716	SER	5.8
1	C	718	TYR	5.7
1	D	898	LYS	5.7
1	D	858	TYR	5.5
1	C	824	GLY	5.4
1	C	898	LYS	5.4
1	B	831	GLY	5.3
1	D	833	ASN	5.3
1	D	831	GLY	5.1
1	C	694	VAL	5.0
1	D	893	LYS	5.0
1	C	710	GLU	5.0
1	A	835	CYS	4.9
1	B	940	VAL	4.9
1	C	714	ARG	4.9
1	D	800	VAL	4.8
1	C	933	LEU	4.8
1	C	884	LEU	4.8
1	C	691	TYR	4.7
1	D	830	ALA	4.7
1	C	729	HIS	4.6
1	D	752	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	802	ARG	4.6
1	D	856	ARG	4.6
1	D	726	ILE	4.4
1	D	750	ILE	4.4
1	C	709	LYS	4.4
1	C	840	THR	4.4
1	C	881	PHE	4.3
1	C	829	LEU	4.3
1	C	858	TYR	4.3
1	C	752	ILE	4.2
1	C	837	GLU	4.2
1	D	804	ILE	4.1
1	C	732	LEU	4.0
1	D	774	LYS	4.0
1	D	729	HIS	4.0
1	C	726	ILE	4.0
1	C	938	LEU	4.0
1	D	840	THR	3.8
1	C	831	GLY	3.8
1	D	829	LEU	3.8
1	C	690	THR	3.8
1	C	932	LEU	3.8
1	C	907	MET	3.6
1	C	799	ILE	3.6
1	C	838	THR	3.6
1	C	744	PHE	3.5
1	C	914	PHE	3.5
1	D	725	GLU	3.5
1	B	839	PHE	3.5
1	C	722	LEU	3.4
1	C	872	ILE	3.4
1	D	825	THR	3.3
1	C	820	ILE	3.3
1	D	711	ILE	3.3
1	C	899	VAL	3.2
1	C	895	GLY	3.2
1	D	841	GLY	3.1
1	D	916	LEU	3.1
1	C	793	TYR	3.1
1	C	893	LYS	3.1
1	D	720	GLN	3.1
1	A	894	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	904	PRO	3.1
1	C	882	TYR	3.1
1	A	892	PHE	3.1
1	A	830	ALA	3.1
1	D	835	CYS	3.1
1	C	685	VAL	3.0
1	D	671	LEU	3.0
1	C	693	ILE	3.0
1	B	838	THR	2.9
1	C	730	LYS	2.9
1	C	853	LYS	2.9
1	D	799	ILE	2.9
1	C	867	LEU	2.9
1	A	829	LEU	2.8
1	C	731	HIS	2.8
1	C	741	LEU	2.8
1	D	773	LEU	2.8
1	D	933	LEU	2.8
1	D	837	GLU	2.8
1	C	740	TYR	2.8
1	C	937	PHE	2.7
1	B	829	LEU	2.7
1	D	688	LYS	2.7
1	A	753	PHE	2.7
1	C	728	LEU	2.7
1	B	891	MET	2.6
1	D	788	LEU	2.6
1	D	802	ARG	2.6
1	D	855	PRO	2.6
1	D	852	ASP	2.6
1	C	860	LYS	2.6
1	C	836	THR	2.6
1	C	918	CYS	2.6
1	C	843	LEU	2.6
1	B	830	ALA	2.5
1	B	904	PRO	2.5
1	C	828	ARG	2.5
1	C	823	PHE	2.5
1	D	863	ASP	2.5
1	D	872	ILE	2.5
1	C	708	ILE	2.5
1	B	894	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	869	CYS	2.4
1	D	708	ILE	2.4
1	C	804	ILE	2.4
1	D	753	PHE	2.4
1	D	795	HIS	2.4
1	C	787	ILE	2.4
1	C	783	TYR	2.3
1	D	843	LEU	2.3
1	D	809	VAL	2.3
1	C	825	THR	2.3
1	B	850	ILE	2.3
1	D	714	ARG	2.2
1	C	720	GLN	2.2
1	D	808	ASN	2.2
1	C	790	GLY	2.2
1	A	940	VAL	2.2
1	D	723	HIS	2.2
1	C	841	GLY	2.1
1	D	715	ASP	2.1
1	D	696	ALA	2.1
1	C	845	TYR	2.1
1	C	940	VAL	2.1
1	D	690	THR	2.1
1	C	821	SER	2.1
1	C	738	VAL	2.1
1	C	915	ILE	2.1
1	C	916	LEU	2.1
1	B	843	LEU	2.1
1	D	851	ILE	2.1
1	C	737	ILE	2.0
1	D	709	LYS	2.0
1	D	754	MET	2.0
1	D	914	PHE	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 ⓘ

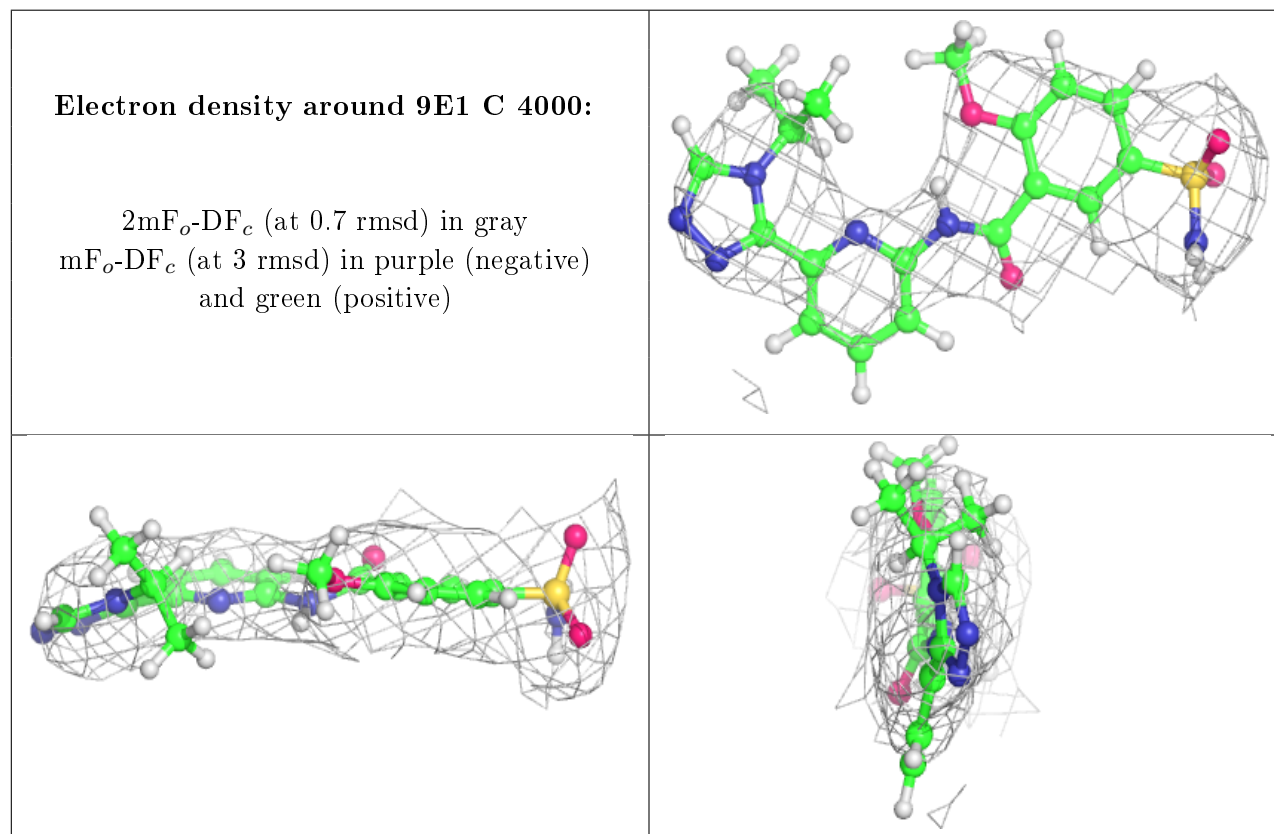
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

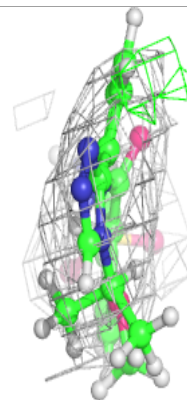
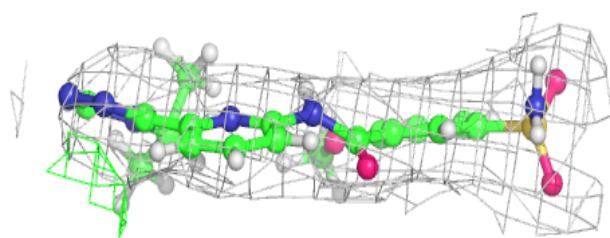
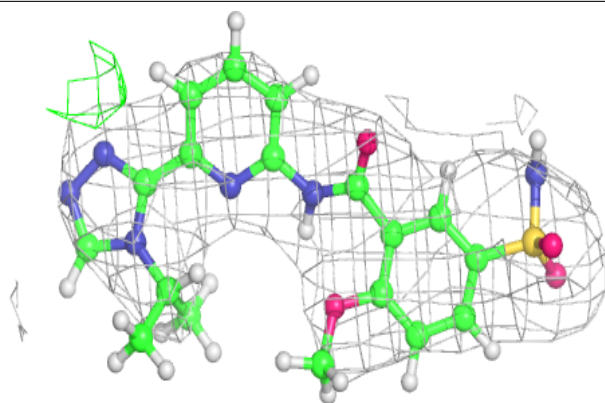
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	DMS	B	1003	4/4	0.90	0.20	63,75,77,84	0
3	DMS	B	1002	4/4	0.93	0.19	98,100,103,104	0
2	9E1	C	4000	29/29	0.96	0.21	102,123,139,143	20
2	9E1	D	4000	29/29	0.97	0.22	104,114,131,135	20
3	DMS	A	1002	4/4	0.98	0.24	78,86,88,90	0
3	DMS	B	1004	4/4	0.98	0.25	80,86,89,90	0
2	9E1	A	1001	29/29	0.99	0.19	50,58,63,66	20
2	9E1	B	1001	29/29	0.99	0.22	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.

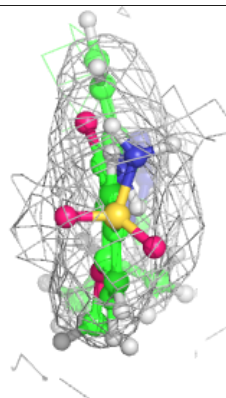
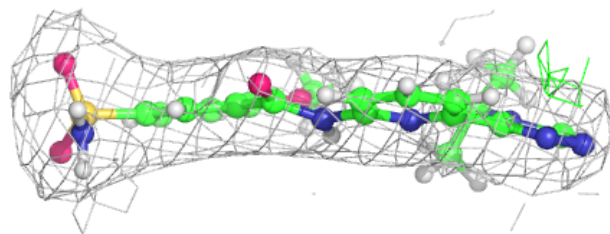
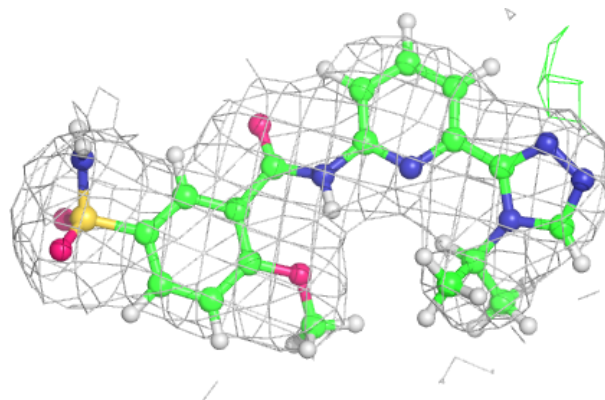


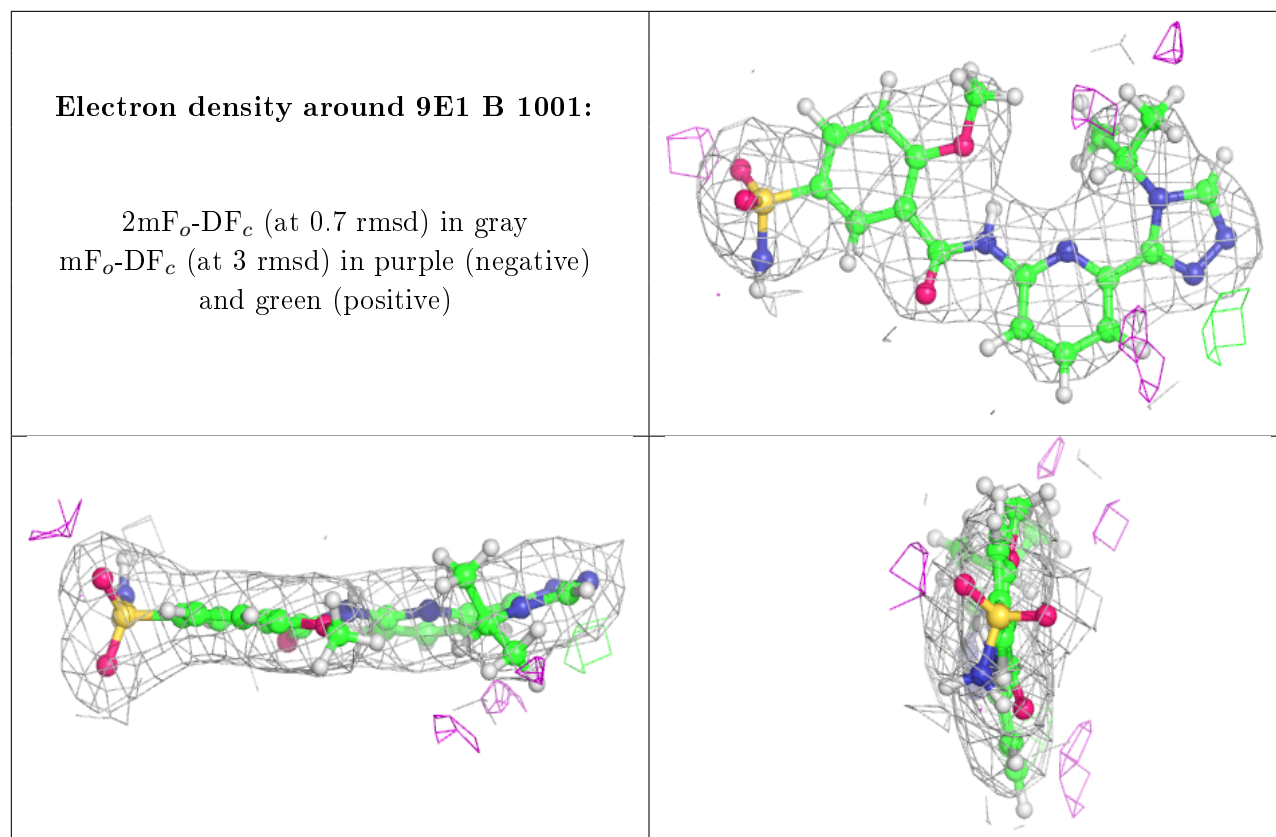
Electron density around 9E1 D 4000:

$2mF_o-DF_c$ (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.