



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:48 PM UTC

PDB ID : 9CZU / pdb_00009czu
Title : HPK1 kinase domain T165E,S171E phosphomimetic mutant in complex with compound 9
Authors : Johnson, E.; Mc Tigue, M.
Deposited on : 2024-08-05
Resolution : 1.85 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

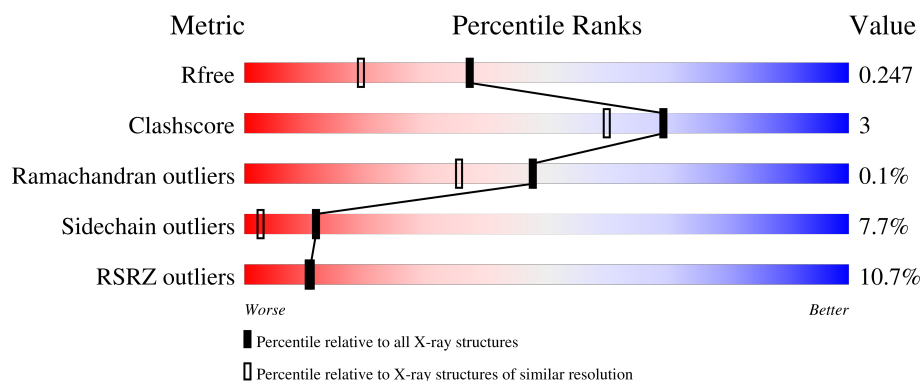
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	309	8% 74% 16% • • 6%
1	B	309	8% 77% 13% • 9%
1	C	309	14% 78% 13% • 7%
1	D	309	10% 76% 13% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9919 atoms, of which 92 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 kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	1	0
			2292	1476	395	410	11			
1	B	281	Total	C	N	O	S	0	1	0
			2220	1432	384	393	11			
1	C	287	Total	C	N	O	S	0	1	0
			2270	1463	393	403	11			
1	D	282	Total	C	N	O	S	0	1	0
			2237	1445	388	393	11			

There are 16 discrepancies between the modelled and reference sequences:

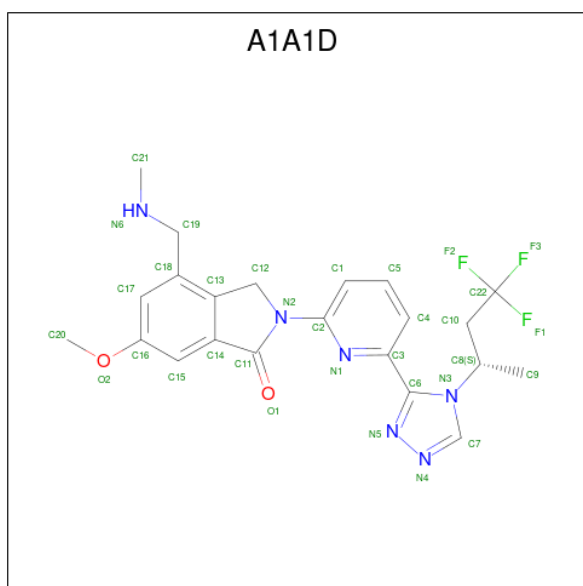
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q92918
A	0	SER	-	expression tag	UNP Q92918
A	165	GLU	THR	engineered mutation	UNP Q92918
A	171	GLU	SER	engineered mutation	UNP Q92918
B	-1	GLY	-	expression tag	UNP Q92918
B	0	SER	-	expression tag	UNP Q92918
B	165	GLU	THR	engineered mutation	UNP Q92918
B	171	GLU	SER	engineered mutation	UNP Q92918
C	-1	GLY	-	expression tag	UNP Q92918
C	0	SER	-	expression tag	UNP Q92918
C	165	GLU	THR	engineered mutation	UNP Q92918
C	171	GLU	SER	engineered mutation	UNP Q92918
D	-1	GLY	-	expression tag	UNP Q92918
D	0	SER	-	expression tag	UNP Q92918
D	165	GLU	THR	engineered mutation	UNP Q92918
D	171	GLU	SER	engineered mutation	UNP Q92918

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 6-methoxy-4-[(methylamino)methyl]-2-(6-{4-[(2S)-4,4,4-trifluorobutan-2-yl]-4H-1,2,4-triazol-3-yl}pyridin-2-yl)-2,3-dihydro-1H-isoindol-1-one (CCD ID: A1A1D) (formula: C₂₂H₂₃F₃N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	23	0
			56	22	3	23	6	2		
3	B	1	Total	C	F	H	N	O	23	0
			56	22	3	23	6	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	F	H	N	O	23	0
			56	22	3	23	6	2		
3	D	1	Total	C	F	H	N	O	23	0
			56	22	3	23	6	2		

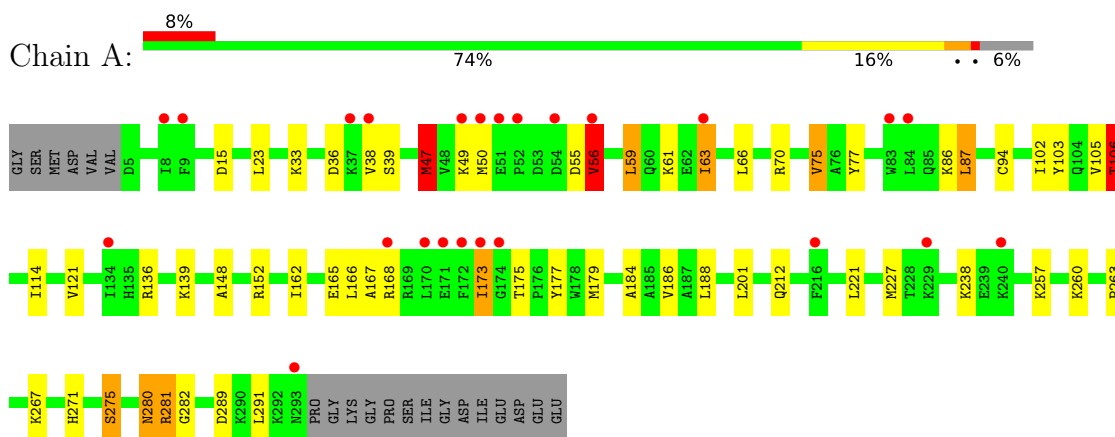
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		
4	B	179	Total	O	0	0
			179	179		
4	C	148	Total	O	0	0
			148	148		
4	D	145	Total	O	0	0
			145	145		

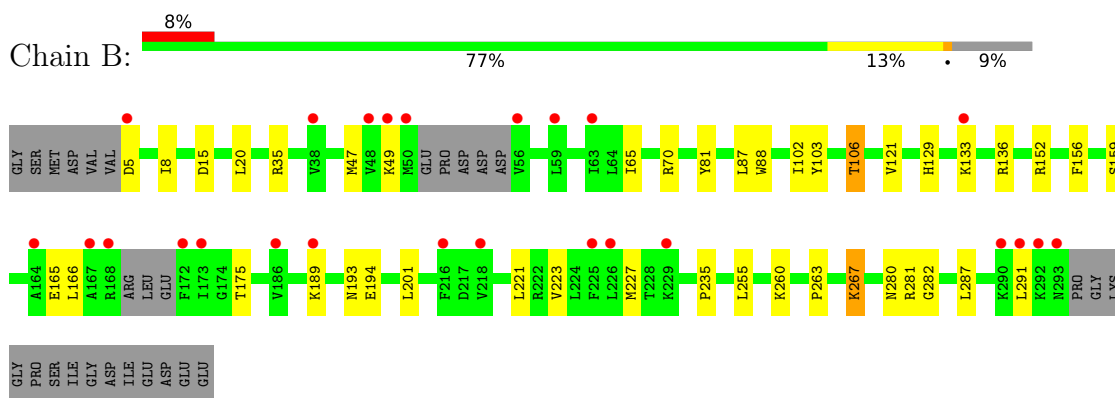
3 Residue-property plots [i](#)

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.

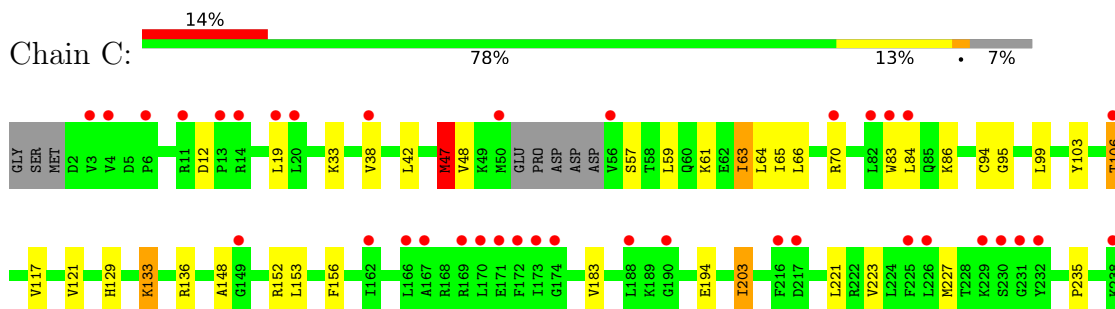
- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1

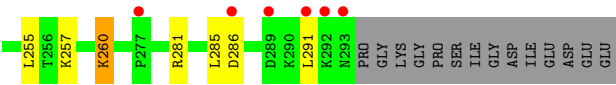


- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1

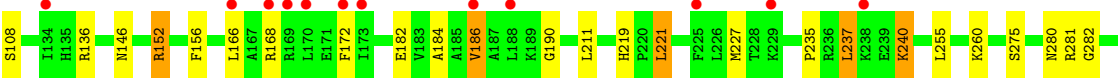
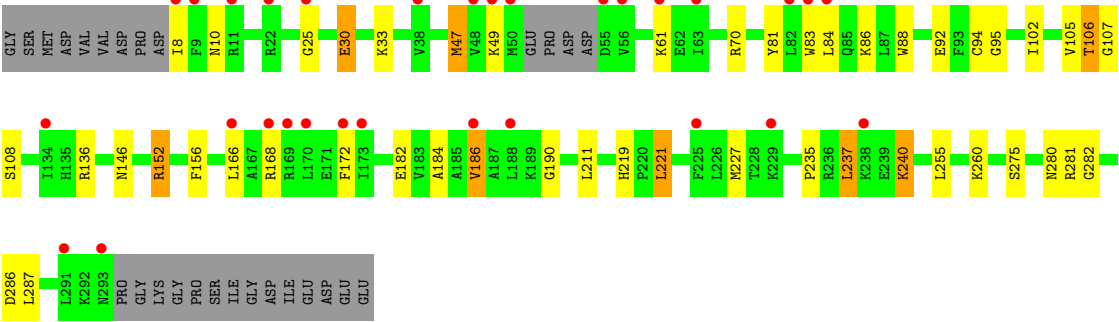


- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.19Å 84.26Å 87.32Å 67.33° 73.51° 76.15°	Depositor
Resolution (Å)	78.71 – 1.85 78.71 – 1.85	Depositor EDS
% Data completeness (in resolution range)	54.1 (78.71-1.85) 54.4 (78.71-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.195 , 0.248 0.196 , 0.247	Depositor DCC
R_{free} test set	3427 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9919	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, A1A1D

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	0.90	1/2345 (0.0%)	1.32	19/3170 (0.6%)
1	B	0.93	0/2269	1.33	11/3064 (0.4%)
1	C	0.90	2/2320 (0.1%)	1.33	9/3135 (0.3%)
1	D	0.85	1/2287 (0.0%)	1.31	16/3087 (0.5%)
All	All	0.89	4/9221 (0.0%)	1.32	55/12456 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	203	ILE	CG1-CD1	-6.94	1.24	1.51
1	A	47	MET	SD-CE	-6.01	1.64	1.79
1	D	227	MET	SD-CE	-5.52	1.65	1.79
1	C	47	MET	SD-CE	-5.17	1.66	1.79

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	105	VAL	CA-C-N	7.96	130.95	120.28
1	D	105	VAL	C-N-CA	7.96	130.95	120.28
1	B	156	PHE	CA-C-N	7.34	128.09	119.94
1	B	156	PHE	C-N-CA	7.34	128.09	119.94
1	C	94	CYS	CA-C-N	6.80	127.64	120.03
1	C	94	CYS	C-N-CA	6.80	127.64	120.03
1	C	286	ASP	CA-C-N	6.55	128.96	120.44
1	C	286	ASP	C-N-CA	6.55	128.96	120.44
1	D	94	CYS	CA-C-N	6.42	127.22	120.03
1	D	94	CYS	C-N-CA	6.42	127.22	120.03
1	D	190	GLY	N-CA-C	6.41	123.61	114.64
1	B	189	LYS	N-CA-C	-6.22	102.50	110.53
1	D	172	PHE	CA-CB-CG	6.03	119.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	THR	CB-CA-C	5.89	116.93	110.15
1	A	106	THR	N-CA-CB	-5.81	101.61	110.33
1	A	94	CYS	CA-C-N	5.80	127.44	120.13
1	A	94	CYS	C-N-CA	5.80	127.44	120.13
1	D	95	GLY	N-CA-C	5.71	119.79	112.83
1	D	146	ASN	CA-CB-CG	5.64	118.25	112.60
1	B	15	ASP	N-CA-C	-5.62	104.63	112.45
1	A	167	ALA	CA-C-N	5.57	127.68	120.44
1	A	167	ALA	C-N-CA	5.57	127.68	120.44
1	C	156	PHE	CA-C-N	5.57	126.12	119.94
1	C	156	PHE	C-N-CA	5.57	126.12	119.94
1	B	15	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	184	ALA	CA-C-N	5.48	127.62	120.28
1	A	184	ALA	C-N-CA	5.48	127.62	120.28
1	A	15	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	183	VAL	N-CA-C	-5.44	105.42	110.53
1	C	95	GLY	N-CA-C	5.43	119.46	112.83
1	B	193	ASN	CA-C-N	5.43	128.10	120.28
1	B	193	ASN	C-N-CA	5.43	128.10	120.28
1	C	12	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	66	LEU	CA-C-N	5.35	127.45	120.28
1	A	66	LEU	C-N-CA	5.35	127.45	120.28
1	A	105	VAL	CA-C-N	5.33	131.32	121.52
1	A	105	VAL	C-N-CA	5.33	131.32	121.52
1	A	75	VAL	N-CA-CB	5.30	117.05	110.05
1	D	156	PHE	CA-C-N	5.26	125.78	119.94
1	D	156	PHE	C-N-CA	5.26	125.78	119.94
1	B	5	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	33	LYS	N-CA-C	-5.19	101.50	109.76
1	B	159	SER	CA-C-N	5.18	127.18	120.44
1	B	159	SER	C-N-CA	5.18	127.18	120.44
1	D	237	LEU	CA-C-N	5.17	127.67	120.63
1	D	237	LEU	C-N-CA	5.17	127.67	120.63
1	D	184	ALA	CA-C-N	5.14	127.12	120.44
1	D	184	ALA	C-N-CA	5.14	127.12	120.44
1	A	114	ILE	CA-C-N	5.08	127.09	120.28
1	A	114	ILE	C-N-CA	5.08	127.09	120.28
1	A	36	ASP	CA-C-N	5.04	127.28	120.38
1	A	36	ASP	C-N-CA	5.04	127.28	120.38
1	D	286	ASP	CA-CB-CG	5.03	117.62	112.60
1	A	289	ASP	CA-C-N	5.02	127.41	120.29
1	A	289	ASP	C-N-CA	5.02	127.41	120.29

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	2292	0	2345	20	0
1	B	2220	0	2286	15	0
1	C	2270	0	2339	16	0
1	D	2237	0	2308	16	0
2	A	5	0	0	0	0
3	A	33	23	0	0	0
3	B	33	23	0	0	0
3	C	33	23	0	0	0
3	D	33	23	0	0	0
4	A	199	0	0	1	0
4	B	179	0	0	2	0
4	C	148	0	0	1	0
4	D	145	0	0	0	0
All	All	9827	92	9278	64	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 3.

All (64) 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:47:MET:HE3	1:A:86:LYS:HG2	1.69	0.74
1:B:280:ASN:HD22	1:B:282:GLY:H	1.36	0.73
1:D:106:THR:HG21	1:D:287:LEU:HD11	1.76	0.67
1:A:173:ILE:HG12	1:A:179:MET:HE1	1.77	0.66
1:D:280:ASN:HD22	1:D:282:GLY:H	1.44	0.65
1:A:280:ASN:HD22	1:A:282:GLY:H	1.46	0.63
1:D:83:TRP:CD1	1:D:84:LEU:HG	2.34	0.62
1:A:103:TYR:HA	1:A:106:THR:HG22	1.83	0.61
1:B:263:PRO:HB3	1:B:267:LYS:HD2	1.83	0.61
1:B:223:VAL:O	1:B:227:MET:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:HG12	1:B:133:LYS:HD2	1.88	0.55
1:A:23:LEU:HD21	1:A:33:LYS:HB2	1.89	0.55
1:D:106:THR:HG22	1:D:107:GLY:O	2.07	0.55
1:C:65:ILE:HG12	1:C:133:LYS:HD2	1.90	0.54
1:A:148:ALA:HB1	1:A:281:ARG:HH21	1.73	0.54
1:A:175:THR:HG21	4:A:664:HOH:O	2.07	0.53
1:A:55:ASP:O	1:A:56:VAL:HB	2.10	0.51
1:B:281:ARG:HG2	4:B:593:HOH:O	2.11	0.51
1:C:83:TRP:CD1	1:C:84:LEU:HG	2.46	0.51
1:A:271:HIS:O	1:A:275:SER:HB2	2.11	0.50
1:C:148:ALA:HB1	1:C:281:ARG:HH21	1.75	0.50
1:A:59:LEU:HG	1:A:87:LEU:HD22	1.94	0.50
1:A:263:PRO:HB3	1:A:267:LYS:HD3	1.94	0.49
1:B:103:TYR:HA	1:B:106:THR:HG22	1.94	0.48
1:C:103:TYR:HA	1:C:106:THR:HG22	1.95	0.48
1:B:106:THR:HG21	1:B:287:LEU:HD11	1.97	0.47
1:C:260:LYS:HE2	1:C:260:LYS:H	1.79	0.47
1:A:63:ILE:HD13	1:A:77:TYR:OH	2.14	0.47
1:B:129:HIS:CD2	1:B:194:GLU:HB2	2.50	0.46
1:D:92:GLU:OE2	1:D:152:ARG:HD2	2.15	0.46
1:D:237:LEU:O	1:D:240:LYS:HE2	2.15	0.46
1:D:47:MET:HG3	1:D:88:TRP:CE2	2.51	0.46
1:A:177:TYR:HE1	1:B:223:VAL:HG21	1.81	0.46
1:B:20:LEU:HD11	1:B:35:ARG:HB2	1.98	0.45
1:D:25:GLY:HA2	1:D:30:GLU:HG2	1.97	0.45
1:B:81:TYR:HB2	1:B:88:TRP:HB2	1.98	0.44
1:C:33:LYS:HE2	1:C:42:LEU:HD22	1.99	0.44
1:C:129:HIS:CD2	1:C:194:GLU:HB2	2.52	0.44
1:D:81:TYR:HB2	1:D:88:TRP:HB2	2.00	0.44
1:C:99:LEU:HD11	1:C:117:VAL:HG11	2.00	0.44
1:C:223:VAL:O	1:C:227:MET:HG3	2.18	0.43
1:B:102:ILE:HG23	1:B:291:LEU:HD12	2.00	0.43
1:C:133:LYS:HG3	4:C:579:HOH:O	2.19	0.42
1:D:235:PRO:HD2	1:D:255:LEU:HD13	2.00	0.42
1:C:48:VAL:HG11	1:C:59:LEU:HD21	2.01	0.42
1:D:102:ILE:O	1:D:106:THR:HB	2.19	0.42
1:C:285:LEU:HD13	1:D:281:ARG:HG3	2.02	0.42
1:A:38:VAL:HG23	1:A:39:SER:H	1.85	0.42
1:A:179:MET:O	1:B:227:MET:HE1	2.20	0.42
1:B:235:PRO:HD2	1:B:255:LEU:HD13	2.01	0.41
1:A:165:GLU:HA	1:A:168:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:MET:HE3	1:D:86:LYS:HG2	2.01	0.41
1:C:47:MET:HE3	1:C:86:LYS:HG2	2.02	0.41
1:C:121:VAL:HG13	1:C:153:LEU:HD21	2.03	0.41
1:D:219:HIS:CE1	1:D:221:LEU:HB2	2.56	0.41
1:C:235:PRO:HD2	1:C:255:LEU:HD13	2.03	0.41
1:D:182:GLU:O	1:D:186:VAL:HG13	2.21	0.41
1:A:102:ILE:O	1:A:106:THR:HB	2.22	0.40
1:A:227:MET:HE1	4:B:504:HOH:O	2.20	0.40
1:B:121:VAL:HG11	1:B:201:LEU:HD13	2.02	0.40
1:C:59:LEU:O	1:C:63:ILE:HG23	2.20	0.40
1:D:108:SER:N	1:D:211:LEU:HD21	2.36	0.40
1:A:121:VAL:HG11	1:A:201:LEU:HD13	2.03	0.40
1:A:162:ILE:O	1:A:166:LEU:HB2	2.21	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	288/309 (93%)	281 (98%)	6 (2%)	1 (0%)	36	25
1	B	276/309 (89%)	264 (96%)	12 (4%)	0	100	100
1	C	284/309 (92%)	271 (95%)	13 (5%)	0	100	100
1	D	279/309 (90%)	269 (96%)	10 (4%)	0	100	100
All	All	1127/1236 (91%)	1085 (96%)	41 (4%)	1 (0%)	48	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	VAL

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	247/262 (94%)	221 (90%)	26 (10%)	6	1
1	B	239/262 (91%)	226 (95%)	13 (5%)	20	7
1	C	245/262 (94%)	227 (93%)	18 (7%)	13	3
1	D	240/262 (92%)	223 (93%)	17 (7%)	13	3
All	All	971/1048 (93%)	897 (92%)	74 (8%)	12	3

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	MET
1	A	49	LYS
1	A	50	MET
1	A	56	VAL
1	A	59	LEU
1	A	61	LYS
1	A	63	ILE
1	A	70	ARG
1	A	75	VAL
1	A	87	LEU
1	A	106	THR
1	A	136	ARG
1	A	139	LYS
1	A	152	ARG
1	A	173	ILE
1	A	186	VAL
1	A	188	LEU
1	A	212	GLN
1	A	221	LEU
1	A	238	LYS
1	A	257	LYS
1	A	260	LYS
1	A	275	SER
1	A	280	ASN

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Mol	Chain	Res	Type
1	A	281	ARG
1	A	291	LEU
1	B	8	ILE
1	B	47	MET
1	B	49	LYS
1	B	70	ARG
1	B	87	LEU
1	B	106	THR
1	B	136	ARG
1	B	152	ARG
1	B	165	GLU
1	B	166	LEU
1	B	221	LEU
1	B	260	LYS
1	B	267	LYS
1	C	19	LEU
1	C	38	VAL
1	C	47	MET
1	C	57	SER
1	C	61	LYS
1	C	63	ILE
1	C	64	LEU
1	C	66	LEU
1	C	70	ARG
1	C	106	THR
1	C	133	LYS
1	C	136	ARG
1	C	152	ARG
1	C	203	ILE
1	C	221	LEU
1	C	257	LYS
1	C	260	LYS
1	C	291	LEU
1	D	8	ILE
1	D	10	ASN
1	D	30	GLU
1	D	47	MET
1	D	49	LYS
1	D	61	LYS
1	D	70	ARG
1	D	106	THR
1	D	136	ARG

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Mol	Chain	Res	Type
1	D	152	ARG
1	D	166	LEU
1	D	168	ARG
1	D	186	VAL
1	D	221	LEU
1	D	240	LYS
1	D	260	LYS
1	D	275	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	78	HIS
1	A	104	GLN
1	A	123	GLN
1	A	142	ASN
1	A	280	ASN
1	B	60	GLN
1	B	104	GLN
1	B	142	ASN
1	B	212	GLN
1	B	280	ASN
1	C	100	GLN
1	C	104	GLN
1	C	142	ASN
1	C	233	GLN
1	D	123	GLN
1	D	131	GLN
1	D	142	ASN
1	D	280	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	A1A1D	A	402	-	35,36,36	0.48	0	45,53,53	0.78	1 (2%)
3	A1A1D	B	401	-	35,36,36	0.47	0	45,53,53	0.86	3 (6%)
3	A1A1D	C	401	-	35,36,36	0.48	1 (2%)	45,53,53	0.72	2 (4%)
3	A1A1D	D	401	-	35,36,36	0.49	0	45,53,53	0.79	2 (4%)
2	SO4	A	401	-	4,4,4	0.34	0	6,6,6	0.12	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
3	A1A1D	A	402	-	-	2/22/34/34	0/4/4/4
3	A1A1D	C	401	-	-	1/22/34/34	0/4/4/4
3	A1A1D	D	401	-	-	2/22/34/34	0/4/4/4
3	A1A1D	B	401	-	-	1/22/34/34	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	A1A1D	C19-N6	2.02	1.49	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	A1A1D	C19-C18-C13	-3.22	116.68	122.71
3	A	402	A1A1D	C19-C18-C13	-2.97	117.15	122.71
3	D	401	A1A1D	C19-C18-C13	-2.94	117.21	122.71
3	C	401	A1A1D	C19-C18-C13	-2.54	117.97	122.71
3	B	401	A1A1D	C15-C14-C13	-2.29	121.13	123.27
3	D	401	A1A1D	C15-C14-C13	-2.22	121.19	123.27
3	B	401	A1A1D	C19-C18-C17	2.15	124.47	120.34
3	C	401	A1A1D	C15-C14-C13	-2.02	121.38	123.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

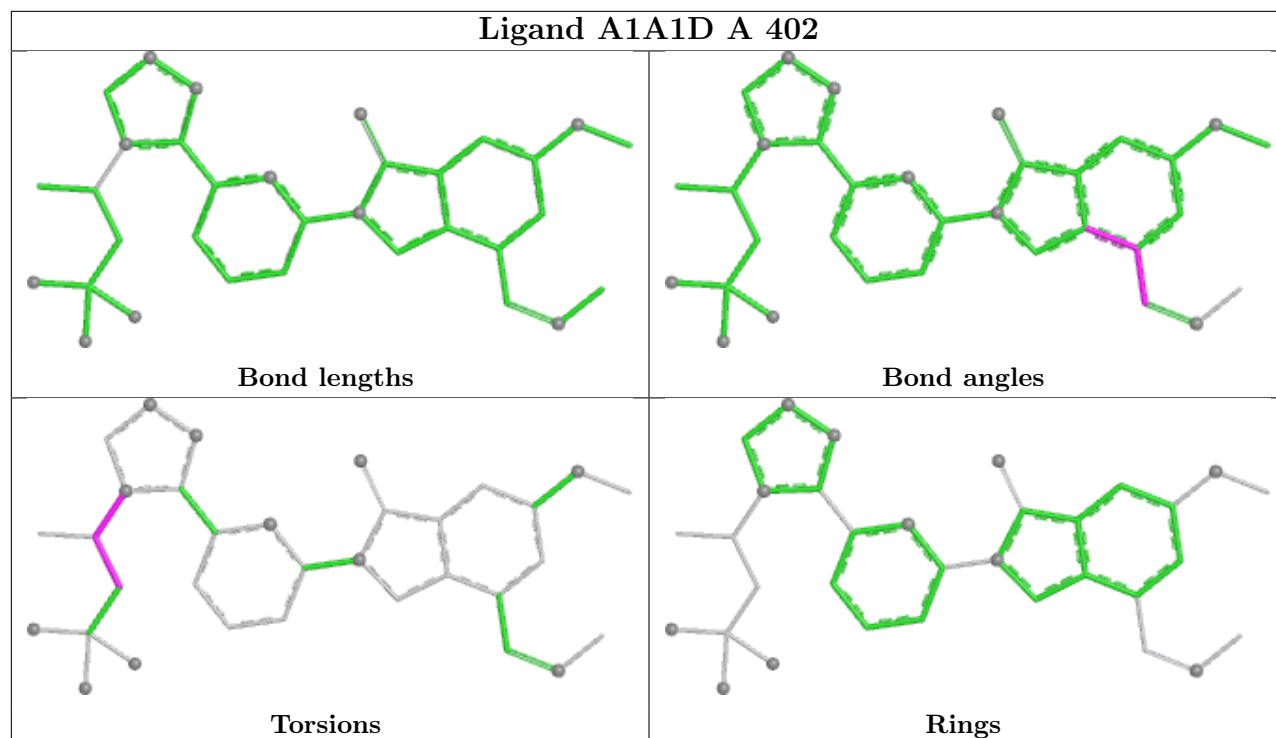
Mol	Chain	Res	Type	Atoms
3	D	401	A1A1D	C10-C8-N3-C6
3	A	402	A1A1D	C22-C10-C8-N3
3	A	402	A1A1D	C10-C8-N3-C6
3	B	401	A1A1D	C10-C8-N3-C6
3	C	401	A1A1D	C10-C8-N3-C6
3	D	401	A1A1D	C10-C8-N3-C7

There are no ring outliers.

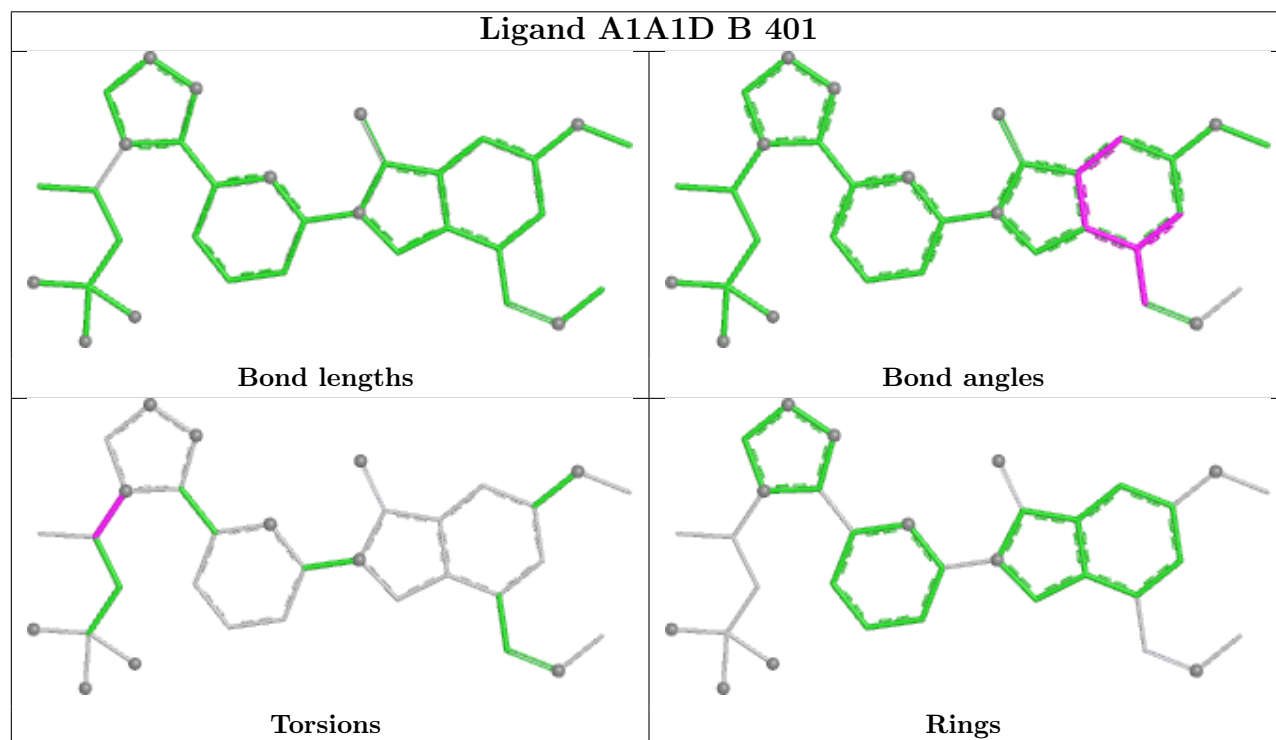
No monomer is involved in short contacts.

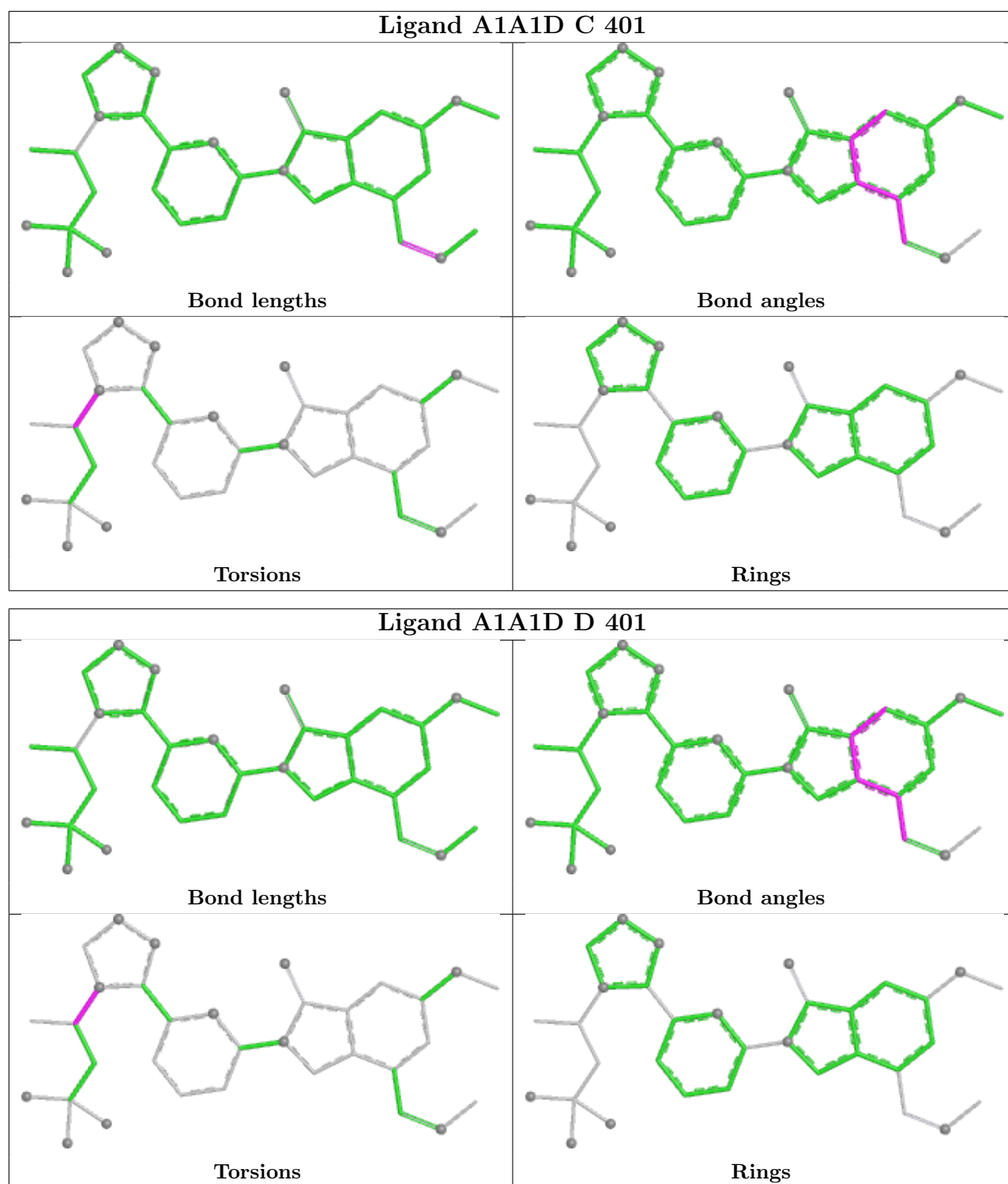
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand A1A1D A 402



Ligand A1A1D B 401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	289/309 (93%)	0.50	24 (8%)	17 18	23, 38, 70, 98	1 (0%)
1	B	281/309 (90%)	0.55	25 (8%)	15 15	22, 38, 64, 116	1 (0%)
1	C	287/309 (92%)	0.87	43 (14%)	5 5	22, 44, 83, 122	1 (0%)
1	D	282/309 (91%)	0.73	30 (10%)	11 11	22, 42, 73, 106	1 (0%)
All	All	1139/1236 (92%)	0.66	122 (10%)	11 10	22, 40, 74, 122	4 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216[A]	PHE	5.2
1	D	8	ILE	5.1
1	A	173	ILE	5.0
1	C	170	LEU	4.9
1	A	52	PRO	4.8
1	C	225	PHE	4.7
1	D	50	MET	4.5
1	D	63	ILE	4.4
1	A	84	LEU	4.3
1	C	173	ILE	4.1
1	B	291	LEU	4.1
1	B	50	MET	3.9
1	C	167	ALA	3.9
1	D	49	LYS	3.7
1	D	38	VAL	3.7
1	B	63	ILE	3.7
1	B	173	ILE	3.7
1	C	166	LEU	3.6
1	D	169	ARG	3.5
1	A	38	VAL	3.5
1	C	172	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	168	ARG	3.4
1	A	56	VAL	3.4
1	C	3	VAL	3.3
1	B	292	LYS	3.3
1	C	229	LYS	3.3
1	D	225[A]	PHE	3.3
1	A	50	MET	3.2
1	B	293	ASN	3.2
1	C	232	TYR	3.2
1	B	56	VAL	3.1
1	C	291	LEU	3.1
1	D	173	ILE	3.1
1	C	83	TRP	3.1
1	D	56	VAL	3.1
1	D	172	PHE	3.1
1	B	5	ASP	3.1
1	D	293	ASN	3.1
1	D	55	ASP	3.0
1	B	229	LYS	3.0
1	A	37	LYS	2.9
1	C	190	GLY	2.9
1	C	82	LEU	2.9
1	D	84	LEU	2.9
1	B	226	LEU	2.8
1	A	168	ARG	2.8
1	A	49	LYS	2.8
1	C	70	ARG	2.7
1	A	83	TRP	2.7
1	A	51	GLU	2.7
1	C	56	VAL	2.7
1	C	84	LEU	2.7
1	D	82	LEU	2.7
1	B	290	LYS	2.7
1	A	293	ASN	2.6
1	C	293	ASN	2.6
1	A	174	GLY	2.6
1	A	229	LYS	2.6
1	C	169	ARG	2.5
1	A	172	PHE	2.5
1	D	170	LEU	2.5
1	A	8	ILE	2.5
1	B	133	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	59	LEU	2.5
1	C	238	LYS	2.5
1	B	225	PHE	2.4
1	C	226	LEU	2.4
1	D	166	LEU	2.4
1	D	83	TRP	2.4
1	C	4	VAL	2.4
1	C	149	GLY	2.4
1	C	231	GLY	2.4
1	B	49	LYS	2.4
1	C	6	PRO	2.4
1	C	50	MET	2.4
1	A	170	LEU	2.4
1	B	216	PHE	2.4
1	D	9	PHE	2.4
1	B	186	VAL	2.4
1	C	292	LYS	2.4
1	D	61	LYS	2.3
1	D	48	VAL	2.3
1	A	63	ILE	2.3
1	C	162	ILE	2.3
1	C	19	LEU	2.3
1	D	25	GLY	2.3
1	C	38	VAL	2.3
1	D	186	VAL	2.3
1	D	11	ARG	2.2
1	B	164	ALA	2.2
1	B	172	PHE	2.2
1	B	48	VAL	2.2
1	D	168	ARG	2.2
1	D	188	LEU	2.2
1	C	277	PRO	2.2
1	B	189	LYS	2.2
1	C	106	THR	2.2
1	B	167	ALA	2.2
1	C	230	SER	2.2
1	C	20	LEU	2.2
1	A	171	GLU	2.1
1	A	54	ASP	2.1
1	C	11	ARG	2.1
1	C	13	PRO	2.1
1	C	188	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	38	VAL	2.1
1	B	218	VAL	2.1
1	C	174	GLY	2.1
1	D	22	ARG	2.1
1	A	9	PHE	2.1
1	D	134	ILE	2.1
1	C	14	ARG	2.1
1	A	240	LYS	2.1
1	C	171	GLU	2.1
1	C	286	ASP	2.1
1	A	134	ILE	2.0
1	D	229	LYS	2.0
1	D	291	LEU	2.0
1	C	217	ASP	2.0
1	C	289	ASP	2.0
1	D	238	LYS	2.0
1	C	216	PHE	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 [i](#)

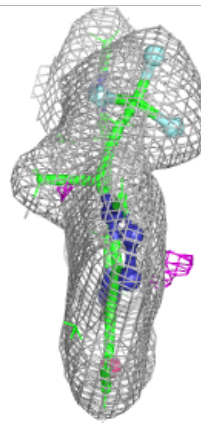
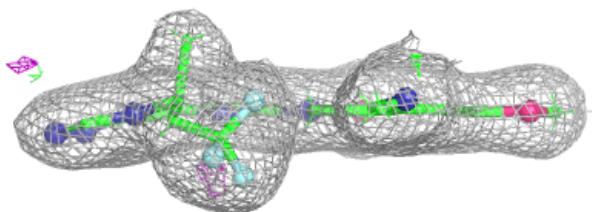
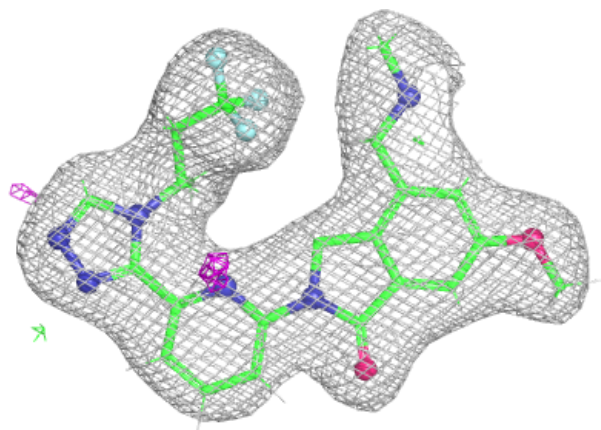
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	401	5/5	0.94	0.07	66,66,69,70	0
3	A1A1D	D	401	33/33	0.94	0.07	27,29,41,48	23
3	A1A1D	C	401	33/33	0.95	0.07	25,28,38,44	23
3	A1A1D	A	402	33/33	0.95	0.06	23,28,33,37	23
3	A1A1D	B	401	33/33	0.96	0.06	27,28,37,42	23

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.

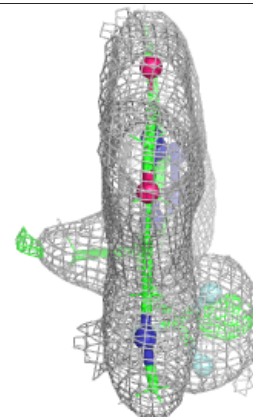
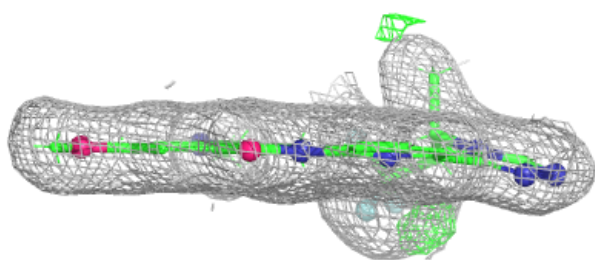
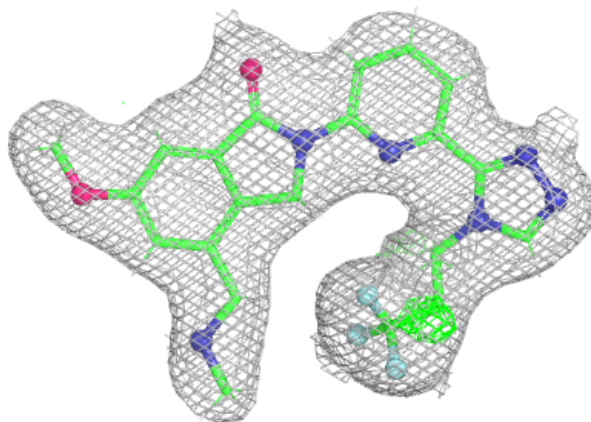
Electron density around A1A1D D 401:

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



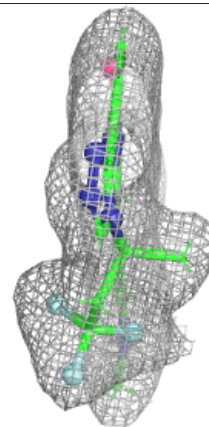
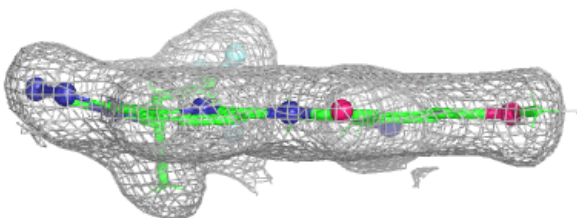
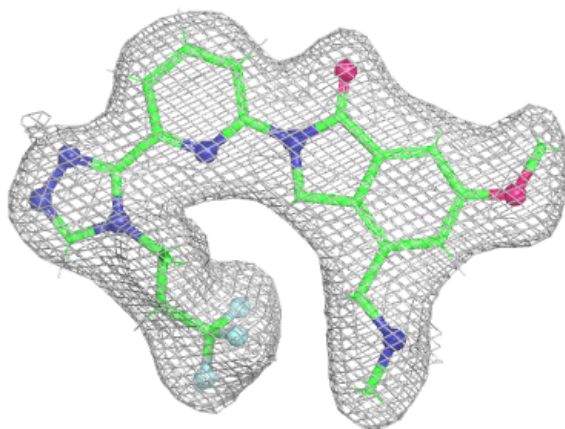
Electron density around A1A1D C 401:

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



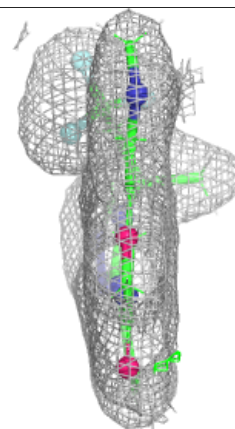
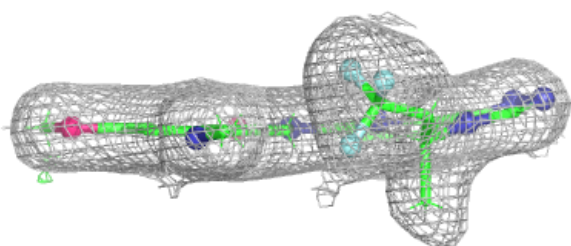
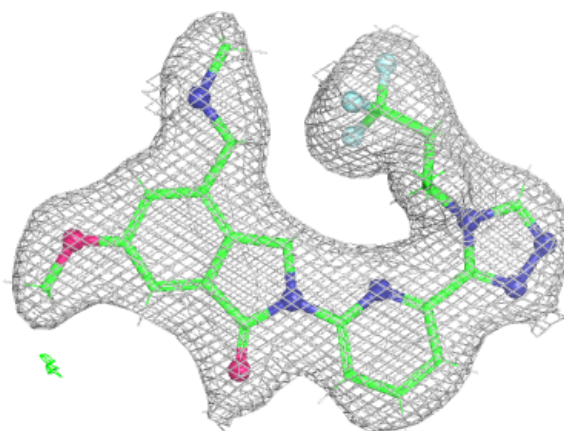
Electron density around A1A1D A 402:

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



Electron density around A1A1D B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.