



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 PM UTC

PDB ID : 9FOY / pdb_00009foy
Title : Ternary complex of a Mycobacterium tuberculosis DNA gyrase core fusion with DNA and the inhibitor AMK32b
Authors : Kokot, M.; Hrast, M.; Feng, L.; Mitchenall, L.A.; Lawson, D.M.; Maxwell, A.; Minovski, N.; Anderluh, M.
Deposited on : 2024-06-12
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

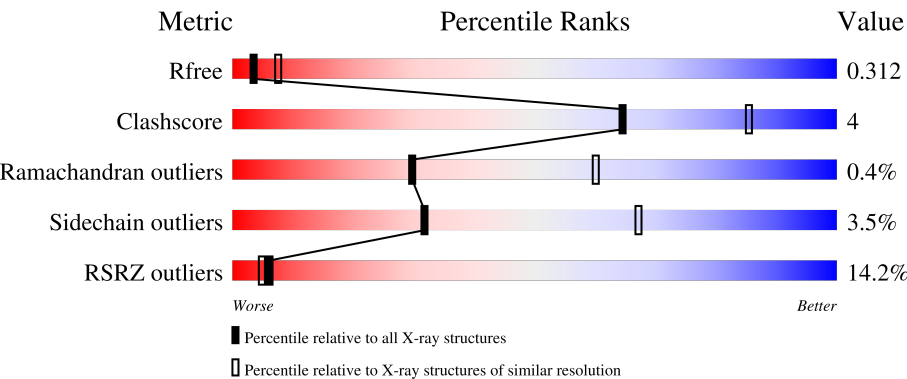
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	756	15% 84% 12% ..
1	B	756	12% 84% 12% ..
2	E	8	12% 88% 12%
2	G	8	25% 25% 62% 12%

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Mol	Chain	Length	Quality of chain
3	F	12	
3	H	12	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5718	3574	1041	1083	20			
1	B	730	Total	C	N	O	S	0	0	0
			5720	3573	1042	1085	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	SER	-	expression tag	UNP P9WG45
A	424	ASN	-	expression tag	UNP P9WG45
A	425	ALA	-	expression tag	UNP P9WG45
A	1501	ILE	-	expression tag	UNP P9WG47
A	1502	GLY	-	expression tag	UNP P9WG47
A	1503	SER	-	expression tag	UNP P9WG47
A	1504	GLY	-	expression tag	UNP P9WG47
B	423	SER	-	expression tag	UNP P9WG45
B	424	ASN	-	expression tag	UNP P9WG45
B	425	ALA	-	expression tag	UNP P9WG45
B	1501	ILE	-	expression tag	UNP P9WG47
B	1502	GLY	-	expression tag	UNP P9WG47
B	1503	SER	-	expression tag	UNP P9WG47
B	1504	GLY	-	expression tag	UNP P9WG47

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3').

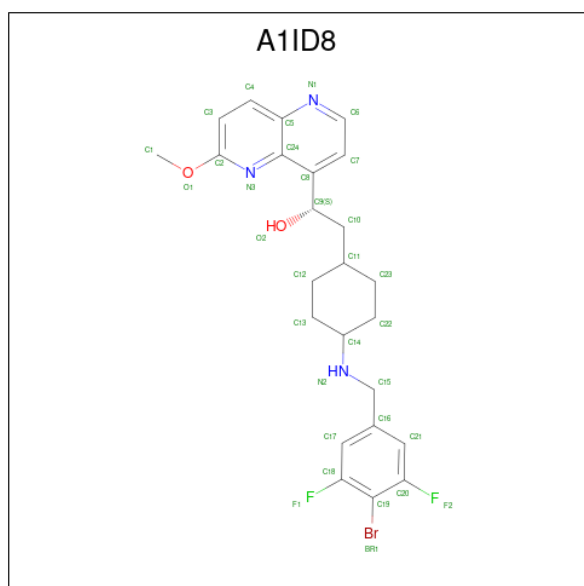
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			
2	G	8	Total	C	N	O	P	0	0	0
			163	78	33	45	7			

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

*CP*T)-3').

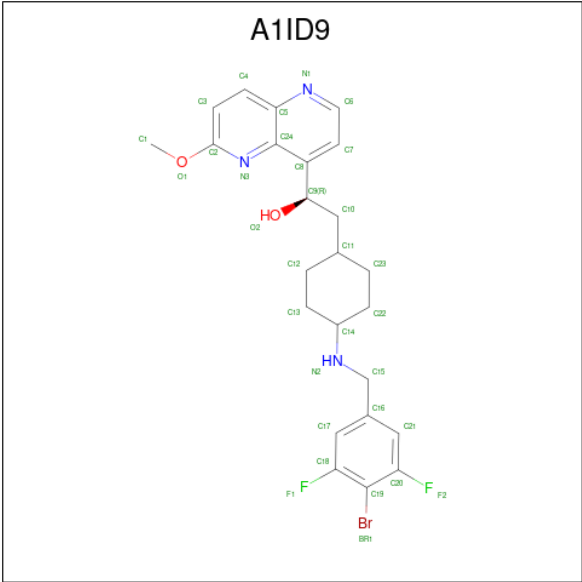
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			244	116	43	73	12			
3	H	12	Total	C	N	O	P	0	0	0
			244	116	43	73	12			

- Molecule 4 is (1 {S})-2-[4-[[4-bromanyl-3,5-bis(fluoranyl)phenyl]methylamino]cyclohexyl]-1-(6-methoxy-1,5-naphthyridin-4-yl)ethanol (CCD ID: A1ID8) (formula: C₂₄H₂₆BrF₂N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	Br	C	F	N	O	0
			32	1	24	2	3	2	

- Molecule 5 is (1 {R})-2-[4-[[4-bromanyl-3,5-bis(fluoranyl)phenyl]methylamino]cyclohexyl]-1-(6-methoxy-1,5-naphthyridin-4-yl)ethanol (CCD ID: A1ID9) (formula: C₂₄H₂₆BrF₂N₃O₂) (labeled as "Ligand of Interest" by depositor).

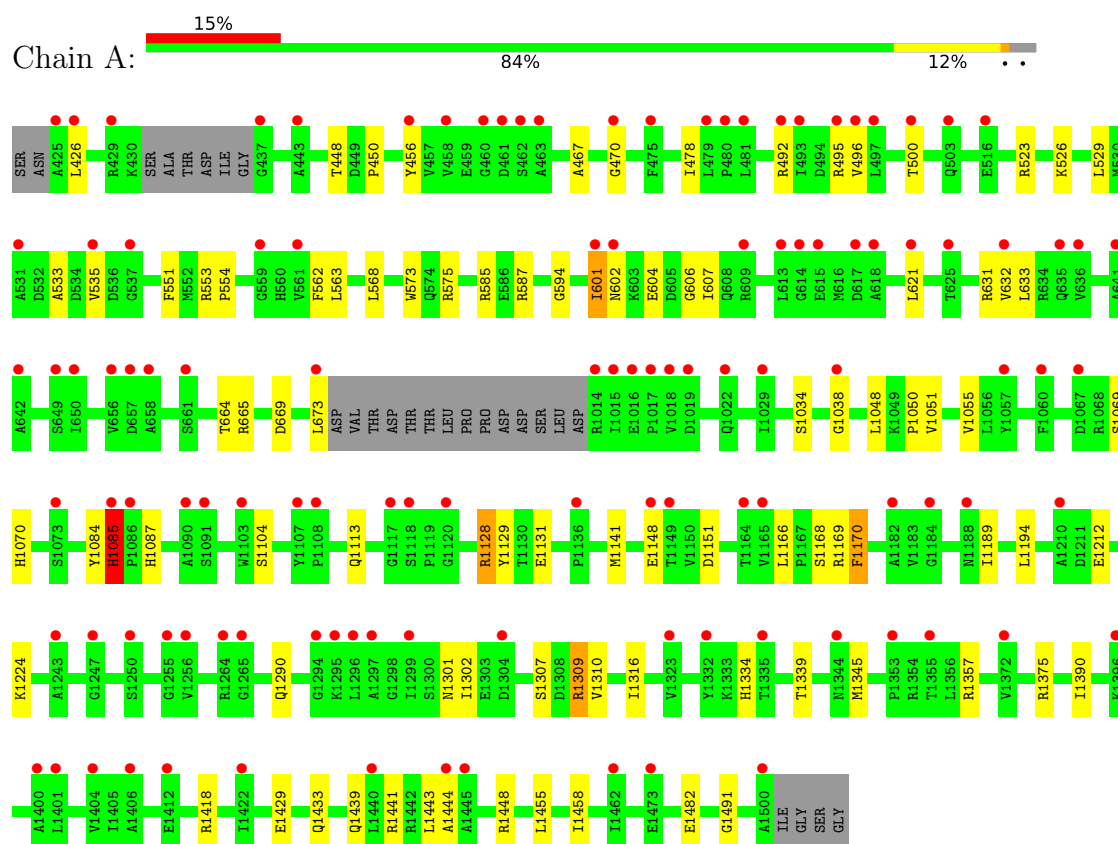


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	F	N	O		
5	H	1	32	1	24	2	3	2	0	0

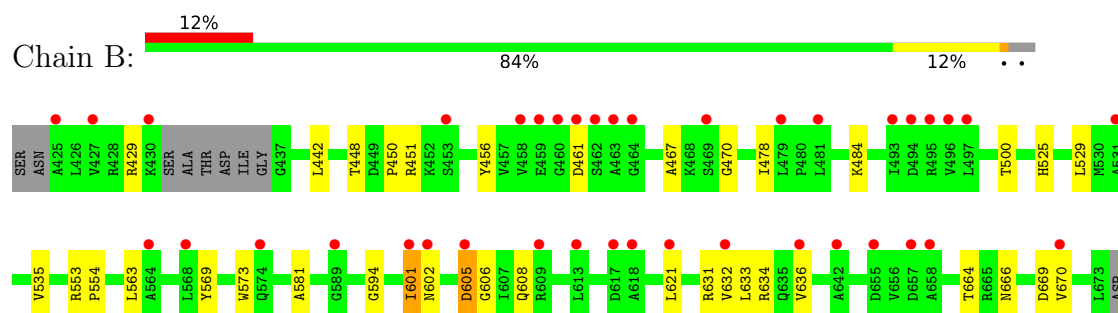
3 Residue-property plots [i](#)

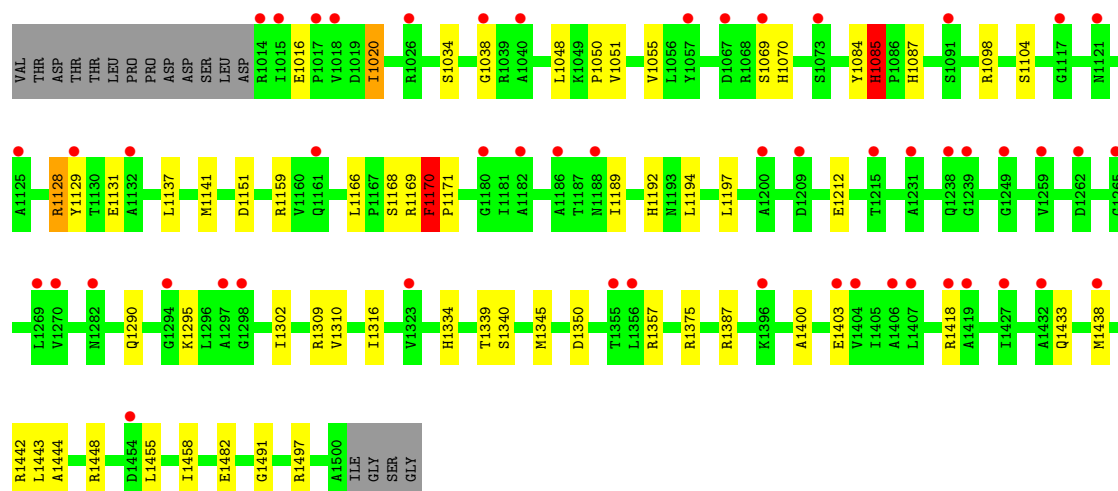
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA gyrase subunit B,DNA gyrase subunit A

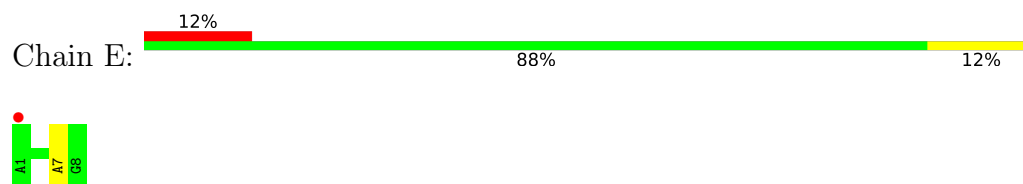


- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit A





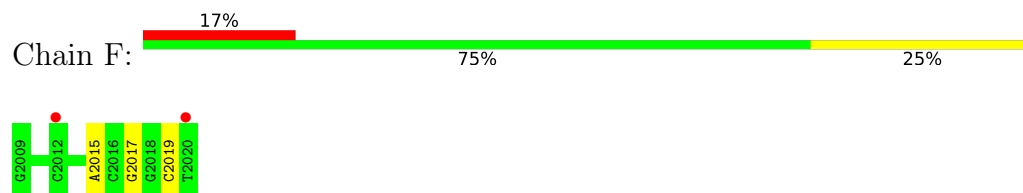
- Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3')



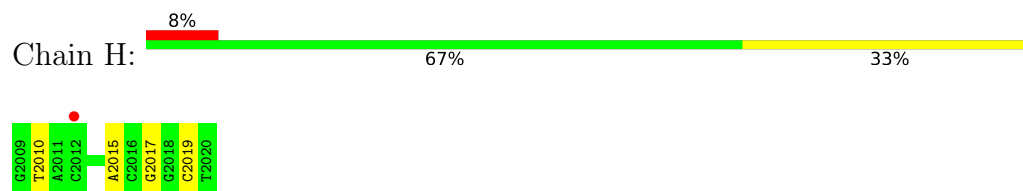
- Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*G)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.04Å 131.70Å 96.28Å 90.00° 97.23° 90.00°	Depositor
Resolution (Å)	69.23 – 2.80 69.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (69.23-2.80) 100.0 (69.23-2.80)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.279 , 0.304 0.284 , 0.312	Depositor DCC
R_{free} test set	2542 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 14.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	12316	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.29% 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: A1ID8, A1ID9

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	0.91	0/5805	1.34	3/7848 (0.0%)
1	B	0.91	0/5807	1.35	3/7849 (0.0%)
2	E	0.67	0/183	1.01	0/281
2	G	0.65	0/183	1.05	2/281 (0.7%)
3	F	0.70	0/272	1.10	3/417 (0.7%)
3	H	0.70	0/272	1.09	3/417 (0.7%)
All	All	0.89	0/12522	1.33	14/17093 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1170	PHE	CB-CA-C	6.86	118.16	108.76
1	A	1170	PHE	CB-CA-C	6.80	118.08	108.76
3	H	2015	DA	P-O3'-C3'	-6.06	111.11	120.20
3	F	2015	DA	P-O3'-C3'	-6.01	111.18	120.20
1	B	1087	HIS	CA-C-N	5.94	125.74	120.10
1	B	1087	HIS	C-N-CA	5.94	125.74	120.10
1	A	1087	HIS	CA-C-N	5.88	125.68	120.10
1	A	1087	HIS	C-N-CA	5.88	125.68	120.10
3	H	2017	DG	P-O3'-C3'	-5.43	112.06	120.20
2	G	3	DC	P-O3'-C3'	-5.36	112.16	120.20
3	H	2019	DC	P-O3'-C3'	-5.26	112.32	120.20
3	F	2017	DG	P-O3'-C3'	-5.25	112.32	120.20
2	G	2	DG	P-O3'-C3'	-5.20	112.41	120.20
3	F	2019	DC	P-O3'-C3'	-5.12	112.52	120.20

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	5718	0	5744	45	0
1	B	5720	0	5741	50	0
2	E	163	0	91	2	0
2	G	163	0	91	4	0
3	F	244	0	136	0	0
3	H	244	0	136	1	0
4	H	32	0	0	0	0
5	H	32	0	0	0	0
All	All	12316	0	11939	94	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 4.

All (94) 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:1085:HIS:HE2	2:E:7:DA:P	2.15	0.70
1:B:1085:HIS:HE2	2:G:7:DA:P	2.18	0.67
1:B:429:ARG:NH1	1:B:442:LEU:O	2.27	0.66
1:A:1169:ARG:NH2	1:A:1482:GLU:OE2	2.28	0.66
1:B:1169:ARG:NH2	1:B:1482:GLU:OE2	2.29	0.66
1:A:1309:ARG:NH1	1:B:470:GLY:O	2.33	0.62
1:B:1128:ARG:HD2	1:B:1129:TYR:CE1	2.38	0.59
1:A:1128:ARG:HD2	1:A:1129:TYR:CE1	2.37	0.59
2:G:1:DA:H2''	2:G:2:DG:OP2	2.02	0.58
1:B:1443:LEU:O	1:B:1448:ARG:NH1	2.37	0.57
1:B:605:ASP:HB2	1:B:1159:ARG:HD2	1.86	0.56
1:A:1128:ARG:HD2	1:A:1129:TYR:CZ	2.40	0.56
1:B:1084:TYR:O	1:B:1085:HIS:C	2.49	0.56
1:A:1084:TYR:O	1:A:1085:HIS:C	2.49	0.55
1:A:1212:GLU:OE2	1:A:1357:ARG:NH2	2.39	0.55
1:A:1307:SER:OG	1:A:1310:VAL:HG22	2.07	0.55
1:A:426:LEU:HD12	1:A:523:ARG:HA	1.89	0.54
1:B:1128:ARG:HD2	1:B:1129:TYR:CZ	2.41	0.54
1:A:1443:LEU:O	1:A:1448:ARG:NH1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:LEU:HD11	1:A:1166:LEU:HD12	1.91	0.53
1:B:1212:GLU:OE2	1:B:1357:ARG:NH2	2.41	0.52
1:B:636:VAL:HG11	1:B:1020:ILE:HD12	1.91	0.52
1:B:1048:LEU:HD11	1:B:1166:LEU:HD12	1.91	0.52
1:A:470:GLY:O	1:B:1309:ARG:NH2	2.43	0.51
1:A:448:THR:O	1:A:450:PRO:HD3	2.10	0.51
1:B:1438:MET:HG2	1:B:1442:ARG:HD3	1.91	0.51
1:B:448:THR:O	1:B:450:PRO:HD3	2.10	0.50
1:A:1455:LEU:O	1:A:1458:ILE:HG22	2.12	0.50
1:B:573:TRP:CH2	1:B:594:GLY:HA3	2.48	0.49
1:A:573:TRP:CH2	1:A:594:GLY:HA3	2.47	0.49
1:B:1400:ALA:O	1:B:1403:GLU:HG2	2.12	0.49
1:B:1455:LEU:O	1:B:1458:ILE:HG22	2.12	0.49
1:A:535:VAL:HG11	1:A:1034:SER:OG	2.13	0.49
1:B:1051:VAL:O	1:B:1055:VAL:HG23	2.13	0.49
1:A:587:ARG:HD2	1:A:607:ILE:HG21	1.94	0.48
1:A:1189:ILE:HG12	1:A:1345:MET:HA	1.96	0.48
1:B:666:ASN:O	1:B:670:VAL:HG13	2.13	0.48
1:A:467:ALA:HA	1:A:621:LEU:HD23	1.96	0.47
1:B:535:VAL:HG11	1:B:1034:SER:OG	2.14	0.47
1:B:1128:ARG:HD2	1:B:1129:TYR:CD1	2.50	0.47
1:A:1051:VAL:O	1:A:1055:VAL:HG23	2.14	0.47
1:B:467:ALA:HA	1:B:621:LEU:HD23	1.96	0.47
1:B:1400:ALA:HB1	1:B:1403:GLU:CG	2.44	0.47
1:A:553:ARG:N	1:A:554:PRO:CD	2.79	0.46
1:B:1098:ARG:NE	2:G:5:DG:H5''	2.31	0.46
1:B:1418:ARG:NH1	1:B:1433:GLN:OE1	2.48	0.46
1:B:1189:ILE:HG12	1:B:1345:MET:HA	1.97	0.46
1:B:553:ARG:N	1:B:554:PRO:CD	2.79	0.46
1:A:1128:ARG:HD2	1:A:1129:TYR:CD1	2.51	0.45
1:B:484:LYS:HG2	2:G:8:DG:H1'	1.98	0.45
1:A:496:VAL:HG11	1:A:551:PHE:CZ	2.51	0.45
1:A:1194:LEU:HD23	1:A:1491:GLY:HA2	1.99	0.45
1:B:1137:LEU:HD23	1:B:1137:LEU:HA	1.87	0.45
1:B:451:ARG:HG2	1:B:525:HIS:CE1	2.52	0.45
1:A:1085:HIS:NE2	2:E:7:DA:OP1	2.49	0.45
1:B:1070:HIS:HB3	1:B:1131:GLU:HB3	1.99	0.45
1:A:1444:ALA:O	1:A:1448:ARG:HG3	2.17	0.44
1:B:1194:LEU:HD23	1:B:1491:GLY:HA2	1.99	0.44
1:A:1439:GLN:OE1	1:A:1441:ARG:NH2	2.51	0.44
1:A:602:ASN:O	1:A:606:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASP:HB2	3:H:2010:DT:OP1	2.18	0.44
1:A:526:LYS:HG2	1:A:562:PHE:CE2	2.53	0.43
1:B:1444:ALA:O	1:B:1448:ARG:HG3	2.17	0.43
1:B:602:ASN:O	1:B:606:GLY:N	2.51	0.43
1:A:575:ARG:CZ	1:A:575:ARG:HB3	2.48	0.43
1:A:1038:GLY:C	1:A:1050:PRO:HG2	2.44	0.43
1:B:631:ARG:CZ	1:B:633:LEU:HD11	2.49	0.43
1:A:533:ALA:HB1	1:A:568:LEU:CD2	2.48	0.43
1:A:631:ARG:CZ	1:A:633:LEU:HD11	2.48	0.43
1:B:1038:GLY:C	1:B:1050:PRO:HG2	2.44	0.43
1:A:533:ALA:HB1	1:A:568:LEU:HD22	2.01	0.42
1:B:456:TYR:HB2	1:B:478:ILE:HD13	2.01	0.42
1:B:569:TYR:HB2	1:B:581:ALA:HB3	2.01	0.42
1:B:1128:ARG:HD2	1:B:1129:TYR:CE2	2.55	0.42
1:A:1128:ARG:HD2	1:A:1129:TYR:CE2	2.54	0.42
1:A:1070:HIS:HB3	1:A:1131:GLU:HB3	2.00	0.42
1:B:1151:ASP:OD1	1:B:1375:ARG:NH2	2.53	0.41
1:B:1170:PHE:HA	1:B:1171:PRO:HD3	1.84	0.41
1:B:1048:LEU:CD1	1:B:1166:LEU:HD12	2.50	0.41
1:B:1295:LYS:HE3	1:B:1334:HIS:CE1	2.55	0.41
1:B:529:LEU:HB2	1:B:563:LEU:HD23	2.02	0.41
1:B:1290:GLN:NE2	1:B:1334:HIS:O	2.54	0.41
1:A:492:ARG:HH21	1:A:495:ARG:HD3	1.84	0.41
1:A:1418:ARG:NH1	1:A:1433:GLN:OE1	2.52	0.41
1:B:634:ARG:HA	1:B:1016:GLU:O	2.21	0.41
1:A:456:TYR:HB2	1:A:478:ILE:HD13	2.02	0.41
1:A:1290:GLN:NE2	1:A:1334:HIS:O	2.54	0.41
1:B:1192:HIS:HB2	1:B:1197:LEU:HD11	2.02	0.41
1:A:529:LEU:HB2	1:A:563:LEU:HD23	2.02	0.41
1:A:1141:MET:HA	1:A:1168:SER:HA	2.04	0.40
1:A:1151:ASP:OD1	1:A:1375:ARG:NH2	2.54	0.40
1:A:1148:GLU:O	1:A:1375:ARG:NH1	2.54	0.40
1:A:1048:LEU:CD1	1:A:1166:LEU:HD12	2.51	0.40
1:B:1141:MET:HA	1:B:1168:SER:HA	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	724/756 (96%)	698 (96%)	23 (3%)	3 (0%)	30	60
1	B	724/756 (96%)	697 (96%)	24 (3%)	3 (0%)	30	60
All	All	1448/1512 (96%)	1395 (96%)	47 (3%)	6 (0%)	30	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	GLU
1	B	605	ASP
1	A	1085	HIS
1	B	1085	HIS
1	A	601	ILE
1	B	601	ILE

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	604/632 (96%)	582 (96%)	22 (4%)	31	66
1	B	604/632 (96%)	584 (97%)	20 (3%)	33	69
All	All	1208/1264 (96%)	1166 (96%)	42 (4%)	32	67

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	THR
1	A	585	ARG
1	A	601	ILE
1	A	632	VAL
1	A	664	THR
1	A	665	ARG
1	A	669	ASP
1	A	673	LEU
1	A	1069	SER
1	A	1085	HIS
1	A	1104	SER
1	A	1113	GLN
1	A	1128	ARG
1	A	1170	PHE
1	A	1224	LYS
1	A	1301	ASN
1	A	1302	ILE
1	A	1309	ARG
1	A	1316	ILE
1	A	1339	THR
1	A	1390	ILE
1	A	1429	GLU
1	B	500	THR
1	B	601	ILE
1	B	608	GLN
1	B	632	VAL
1	B	664	THR
1	B	669	ASP
1	B	1020	ILE
1	B	1069	SER
1	B	1085	HIS
1	B	1104	SER
1	B	1128	ARG
1	B	1170	PHE
1	B	1302	ILE
1	B	1310	VAL
1	B	1316	ILE
1	B	1339	THR
1	B	1340	SER
1	B	1350	ASP
1	B	1387	ARG
1	B	1497	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	GLN
1	A	574	GLN
1	A	1113	GLN
1	A	1161	GLN
1	A	1301	ASN
1	A	1490	HIS
1	B	476	GLN
1	B	574	GLN
1	B	602	ASN
1	B	608	GLN
1	B	1161	GLN
1	B	1290	GLN
1	B	1334	HIS
1	B	1490	HIS

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](#)

2 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
4	A1ID8	H	2101	5	35,35,35	0.43	0	43,49,49	0.52	0
5	A1ID9	H	2102	4	35,35,35	0.41	0	43,49,49	0.52	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
4	A1ID8	H	2101	5	-	5/15/25/25	0/4/4/4
5	A1ID9	H	2102	4	-	8/15/25/25	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

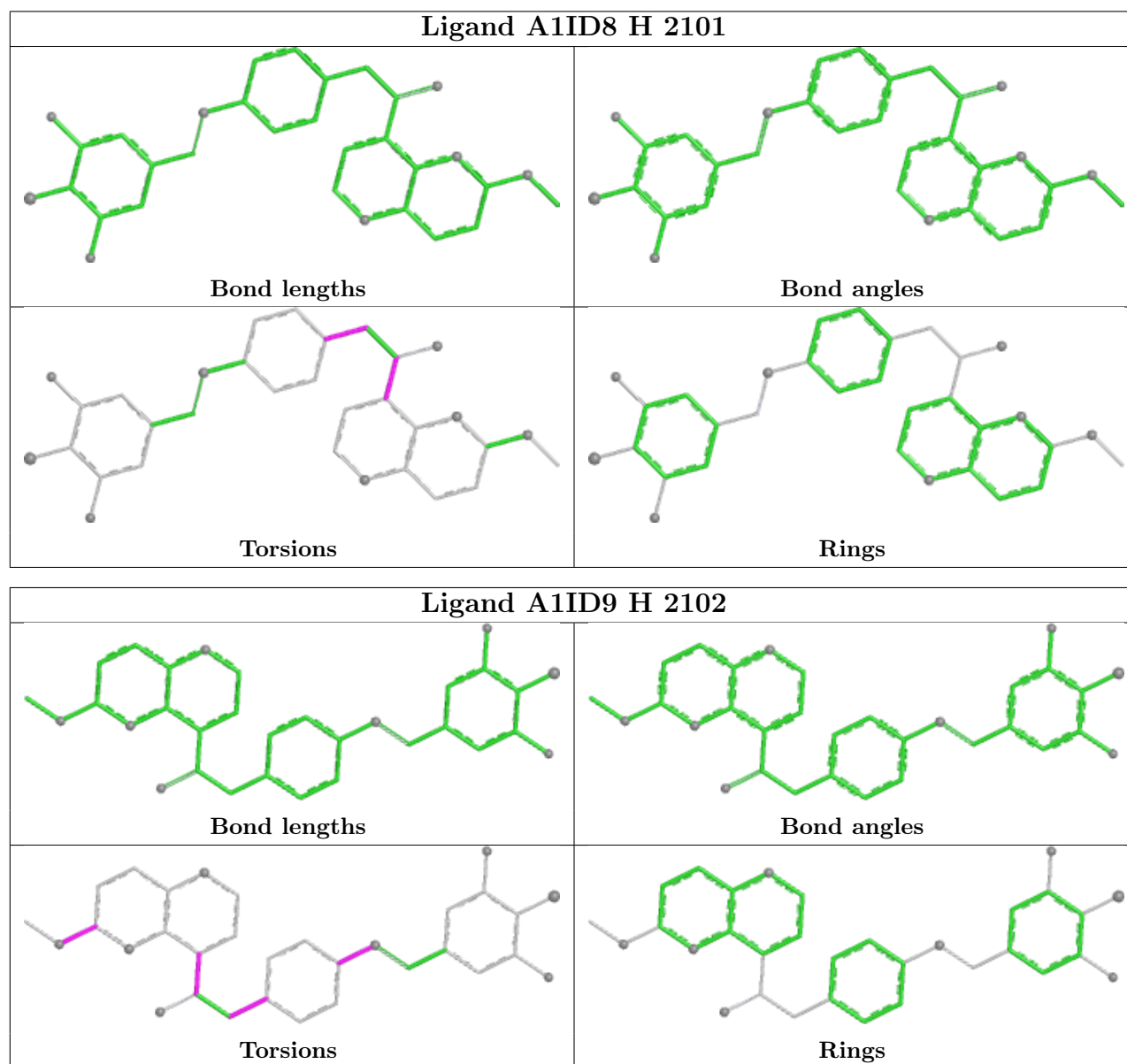
Mol	Chain	Res	Type	Atoms
4	H	2101	A1ID8	C7-C8-C9-C10
4	H	2101	A1ID8	C24-C8-C9-C10
5	H	2102	A1ID9	C7-C8-C9-C10
5	H	2102	A1ID9	C24-C8-C9-C10
5	H	2102	A1ID9	C13-C14-N2-C15
5	H	2102	A1ID9	C22-C14-N2-C15
5	H	2102	A1ID9	N3-C2-O1-C1
5	H	2102	A1ID9	C3-C2-O1-C1
4	H	2101	A1ID8	C7-C8-C9-O2
5	H	2102	A1ID9	C9-C10-C11-C12
5	H	2102	A1ID9	C9-C10-C11-C23
4	H	2101	A1ID8	C9-C10-C11-C12
4	H	2101	A1ID8	C24-C8-C9-O2

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.



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	730/756 (96%)	1.23	116 (15%) 5 4	32, 44, 59, 66	0
1	B	730/756 (96%)	1.14	91 (12%) 8 6	32, 41, 57, 68	0
2	E	8/8 (100%)	1.14	1 (12%) 8 6	27, 36, 65, 72	0
2	G	8/8 (100%)	0.91	2 (25%) 2 1	27, 35, 54, 57	0
3	F	12/12 (100%)	1.12	2 (16%) 4 3	34, 39, 52, 59	0
3	H	12/12 (100%)	1.13	1 (8%) 17 12	35, 38, 55, 60	0
All	All	1500/1552 (96%)	1.18	213 (14%) 6 5	27, 42, 58, 72	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	613	LEU	5.2
1	B	1121	ASN	4.4
1	B	469	SER	4.2
1	B	458	VAL	4.0
1	A	1255	GLY	4.0
1	B	1117	GLY	3.9
1	B	1239	GLY	3.8
1	A	462	SER	3.8
1	B	493	ILE	3.7
1	B	1297	ALA	3.7
1	A	618	ALA	3.7
1	B	1014	ARG	3.6
1	A	497	LEU	3.6
1	B	1294	GLY	3.6
1	A	437	GLY	3.5
1	A	458	VAL	3.5
1	B	605	ASP	3.5
1	A	1149	THR	3.4
1	B	1182	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1186	ALA	3.4
1	A	1182	ALA	3.4
1	B	495	ARG	3.4
1	A	425	ALA	3.3
1	A	1297	ALA	3.3
1	B	1432	ALA	3.2
1	A	495	ARG	3.2
1	A	493	ILE	3.2
1	A	492	ARG	3.2
1	A	429	ARG	3.1
1	B	1038	GLY	3.1
1	A	1073	SER	3.1
1	A	496	VAL	3.1
1	A	1086	PRO	3.1
2	E	1	DA	3.1
1	A	657	ASP	3.1
1	A	1136	PRO	3.1
1	A	460	GLY	3.0
1	A	613	LEU	3.0
1	B	481	LEU	3.0
1	A	531	ALA	3.0
1	A	1243	ALA	3.0
1	A	632	VAL	3.0
1	A	1412	GLU	2.9
1	A	601	ILE	2.9
1	A	1294	GLY	2.9
1	A	1016	GLU	2.9
1	B	1406	ALA	2.9
1	B	621	LEU	2.9
1	A	1038	GLY	2.9
1	A	1022	GLN	2.9
1	B	496	VAL	2.9
1	B	618	ALA	2.9
1	B	1180	GLY	2.9
1	A	617	ASP	2.9
1	A	656	VAL	2.9
1	B	1209	ASP	2.9
1	A	1148	GLU	2.8
1	B	601	ILE	2.8
1	A	1355	THR	2.8
1	A	480	PRO	2.8
1	B	1161	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	463	ALA	2.8
1	A	1085	HIS	2.8
1	A	635	GLN	2.8
1	A	641	ALA	2.8
1	A	658	ALA	2.8
1	A	621	LEU	2.8
1	B	497	LEU	2.8
1	A	625	THR	2.7
1	B	464	GLY	2.7
1	B	1073	SER	2.7
1	A	1165	VAL	2.7
1	A	1323	VAL	2.7
1	A	426	LEU	2.7
1	B	658	ALA	2.7
1	B	1404	VAL	2.7
1	B	1057	TYR	2.7
1	B	1215	THR	2.7
1	A	1372	VAL	2.7
1	A	479	LEU	2.7
1	B	479	LEU	2.7
1	A	1017	PRO	2.7
1	B	1282	ASN	2.7
1	B	1403	GLU	2.7
1	A	661	SER	2.7
1	B	568	LEU	2.7
1	A	602	ASN	2.6
1	A	1188	ASN	2.6
1	B	655	ASP	2.6
1	B	1091	SER	2.6
1	B	1026	ARG	2.6
1	B	1259	VAL	2.6
1	A	1029	ILE	2.6
1	A	650	ILE	2.6
1	B	1265	GLY	2.6
1	A	1164	THR	2.6
1	B	1018	VAL	2.6
1	A	642	ALA	2.6
3	F	2020	DT	2.5
1	A	481	LEU	2.5
1	A	559	GLY	2.5
1	A	1265	GLY	2.5
1	B	1298	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1067	ASP	2.5
1	B	460	GLY	2.5
1	A	1335	THR	2.5
1	B	602	ASN	2.5
1	A	1184	GLY	2.5
1	A	1296	LEU	2.5
1	B	636	VAL	2.5
1	A	1210	ALA	2.5
1	A	1344	ASN	2.5
1	B	463	ALA	2.4
1	A	1019	ASP	2.4
1	B	1015	ILE	2.4
1	A	1404	VAL	2.4
1	B	589	GLY	2.4
1	A	1014	ARG	2.4
1	B	1238	GLN	2.4
1	A	1440	LEU	2.4
1	A	649	SER	2.4
1	B	462	SER	2.4
1	B	1419	ALA	2.4
1	A	1400	ALA	2.4
1	B	564	ALA	2.4
1	A	1015	ILE	2.4
1	B	1396	LYS	2.3
1	A	1406	ALA	2.3
1	A	1256	VAL	2.3
1	A	1091	SER	2.3
1	B	1356	LEU	2.3
1	A	500	THR	2.3
1	B	670	VAL	2.3
1	A	475	PHE	2.3
1	B	531	ALA	2.3
1	B	1200	ALA	2.3
1	B	461	ASP	2.3
1	B	494	ASP	2.3
1	B	1067	ASP	2.3
1	B	1262	ASP	2.3
1	A	1103	TRP	2.3
1	A	1299	ILE	2.3
1	A	1018	VAL	2.3
1	B	1249	GLY	2.3
1	B	617	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1264	ARG	2.3
1	A	1117	GLY	2.3
1	A	1473	GLU	2.2
1	B	642	ALA	2.2
1	B	1438	MET	2.2
1	B	430	LYS	2.2
1	A	443	ALA	2.2
1	A	1090	ALA	2.2
1	B	1407	LEU	2.2
1	A	1304	ASP	2.2
1	B	632	VAL	2.2
1	A	470	GLY	2.2
1	A	1120	GLY	2.2
1	B	1069	SER	2.2
1	B	1269	LEU	2.2
1	B	1231	ALA	2.2
1	A	503	GLN	2.2
1	A	1353	PRO	2.2
1	A	615	GLU	2.2
1	A	1445	ALA	2.2
1	B	609	ARG	2.1
1	A	1108	PRO	2.1
1	B	427	VAL	2.1
1	B	657	ASP	2.1
1	A	1295	LYS	2.1
1	A	673	LEU	2.1
1	B	425	ALA	2.1
1	A	1422	ILE	2.1
1	A	636	VAL	2.1
1	A	1057	TYR	2.1
1	B	1132	ALA	2.1
1	A	516	GLU	2.1
1	A	1396	LYS	2.1
2	G	2	DG	2.1
1	A	537	GLY	2.1
1	A	1401	LEU	2.1
1	B	1125	ALA	2.1
1	A	456	TYR	2.1
1	B	1427	ILE	2.1
1	B	574	GLN	2.1
1	A	1060	PHE	2.1
1	A	461	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	609	ARG	2.1
1	B	1355	THR	2.1
1	B	1418	ARG	2.1
1	A	1462	ILE	2.1
1	B	459	GLU	2.1
1	B	1129	TYR	2.1
1	B	453	SER	2.0
1	A	561	VAL	2.0
1	B	1270	VAL	2.0
1	B	1017	PRO	2.0
1	A	1247	GLY	2.0
3	F	2012	DC	2.0
3	H	2012	DC	2.0
1	A	1444	ALA	2.0
1	B	1040	ALA	2.0
1	B	1454	ASP	2.0
1	A	1118	SER	2.0
1	A	1250	SER	2.0
1	B	1323	VAL	2.0
1	B	1188	ASN	2.0
1	A	614	GLY	2.0
2	G	1	DA	2.0
1	A	1500	ALA	2.0
1	A	1107	TYR	2.0
1	A	1332	TYR	2.0
1	A	535	VAL	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](#)

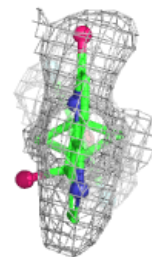
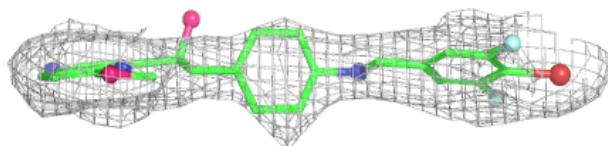
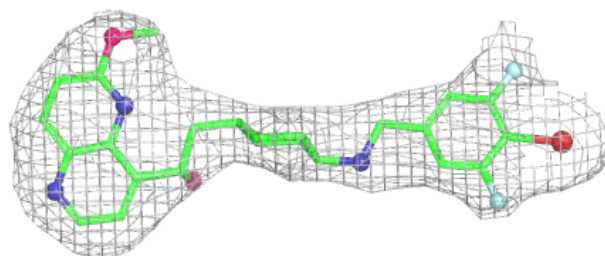
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1ID8	H	2101	32/32	0.92	0.14	38,38,39,39	32
5	A1ID9	H	2102	32/32	0.93	0.13	37,37,38,38	32

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.

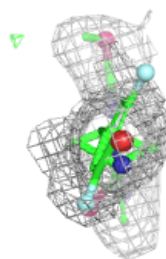
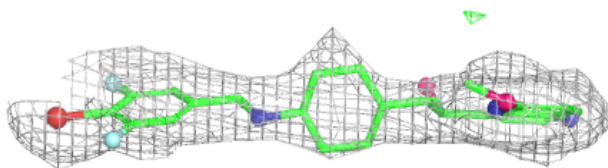
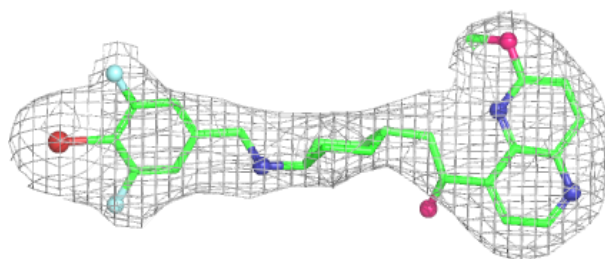
Electron density around A1ID8 H 2101:

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 A1ID9 H 2102:

$2mF_o - DF_c$ (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.