



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:37 AM UTC

PDB ID : 1NX9 / pdb_00001nx9
Title : Acetobacter turbidans alpha-amino acid ester hydrolase S205A mutant complexed with ampicillin
Authors : Barends, T.R.M.; Polderman-Tijmes, J.J.; Jekel, P.A.; Janssen, D.B.; Dijkstra, B.W.
Deposited on : 2003-02-10
Resolution : 2.20 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

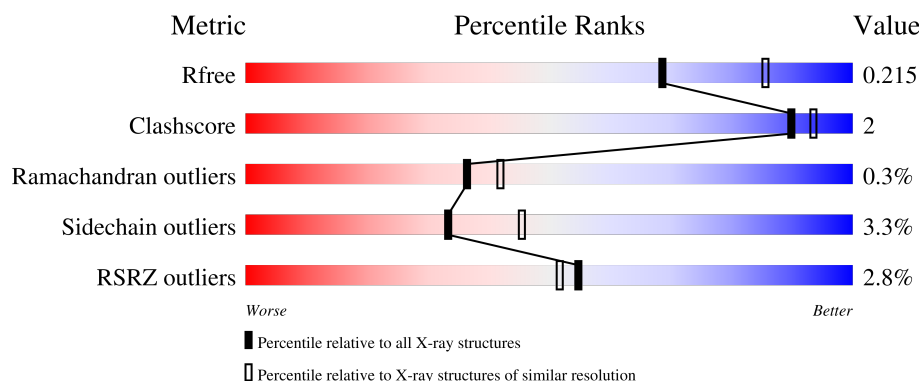
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	652	2% 87% 7% 5%
1	B	652	3% 86% 8% 5%
1	C	652	3% 88% 6% 5%
1	D	652	3% 86% 8% 5%

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
2	AIC	A	5001	X	-	-	-
2	AIC	B	5002	X	-	-	-
2	AIC	C	5003	X	-	-	-
2	AIC	D	5004	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21877 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 alpha-amino acid ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	617	Total	C	N	O	S	0	0	0
			4882	3111	845	906	20			
1	B	617	Total	C	N	O	S	0	0	0
			4882	3111	845	906	20			
1	C	617	Total	C	N	O	S	0	0	0
			4882	3111	845	906	20			
1	D	617	Total	C	N	O	S	0	0	0
			4882	3111	845	906	20			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	SER	engineered mutation	UNP Q8VRK8
A	668	LYS	-	expression tag	UNP Q8VRK8
A	669	LEU	-	expression tag	UNP Q8VRK8
A	670	GLY	-	expression tag	UNP Q8VRK8
A	671	PRO	-	expression tag	UNP Q8VRK8
A	672	GLU	-	expression tag	UNP Q8VRK8
A	673	GLN	-	expression tag	UNP Q8VRK8
A	674	LYS	-	expression tag	UNP Q8VRK8
A	675	LEU	-	expression tag	UNP Q8VRK8
A	676	ILE	-	expression tag	UNP Q8VRK8
A	677	SER	-	expression tag	UNP Q8VRK8
A	678	GLU	-	expression tag	UNP Q8VRK8
A	679	GLU	-	expression tag	UNP Q8VRK8
A	680	ASP	-	expression tag	UNP Q8VRK8
A	681	LEU	-	expression tag	UNP Q8VRK8
A	682	ASN	-	expression tag	UNP Q8VRK8
A	683	SER	-	expression tag	UNP Q8VRK8
A	684	ALA	-	expression tag	UNP Q8VRK8
A	685	VAL	-	expression tag	UNP Q8VRK8
A	686	ASP	-	expression tag	UNP Q8VRK8
A	687	HIS	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	688	HIS	-	expression tag	UNP Q8VRK8
A	689	HIS	-	expression tag	UNP Q8VRK8
A	690	HIS	-	expression tag	UNP Q8VRK8
A	691	HIS	-	expression tag	UNP Q8VRK8
A	692	HIS	-	expression tag	UNP Q8VRK8
B	205	ALA	SER	engineered mutation	UNP Q8VRK8
B	668	LYS	-	expression tag	UNP Q8VRK8
B	669	LEU	-	expression tag	UNP Q8VRK8
B	670	GLY	-	expression tag	UNP Q8VRK8
B	671	PRO	-	expression tag	UNP Q8VRK8
B	672	GLU	-	expression tag	UNP Q8VRK8
B	673	GLN	-	expression tag	UNP Q8VRK8
B	674	LYS	-	expression tag	UNP Q8VRK8
B	675	LEU	-	expression tag	UNP Q8VRK8
B	676	ILE	-	expression tag	UNP Q8VRK8
B	677	SER	-	expression tag	UNP Q8VRK8
B	678	GLU	-	expression tag	UNP Q8VRK8
B	679	GLU	-	expression tag	UNP Q8VRK8
B	680	ASP	-	expression tag	UNP Q8VRK8
B	681	LEU	-	expression tag	UNP Q8VRK8
B	682	ASN	-	expression tag	UNP Q8VRK8
B	683	SER	-	expression tag	UNP Q8VRK8
B	684	ALA	-	expression tag	UNP Q8VRK8
B	685	VAL	-	expression tag	UNP Q8VRK8
B	686	ASP	-	expression tag	UNP Q8VRK8
B	687	HIS	-	expression tag	UNP Q8VRK8
B	688	HIS	-	expression tag	UNP Q8VRK8
B	689	HIS	-	expression tag	UNP Q8VRK8
B	690	HIS	-	expression tag	UNP Q8VRK8
B	691	HIS	-	expression tag	UNP Q8VRK8
B	692	HIS	-	expression tag	UNP Q8VRK8
C	205	ALA	SER	engineered mutation	UNP Q8VRK8
C	668	LYS	-	expression tag	UNP Q8VRK8
C	669	LEU	-	expression tag	UNP Q8VRK8
C	670	GLY	-	expression tag	UNP Q8VRK8
C	671	PRO	-	expression tag	UNP Q8VRK8
C	672	GLU	-	expression tag	UNP Q8VRK8
C	673	GLN	-	expression tag	UNP Q8VRK8
C	674	LYS	-	expression tag	UNP Q8VRK8
C	675	LEU	-	expression tag	UNP Q8VRK8
C	676	ILE	-	expression tag	UNP Q8VRK8
C	677	SER	-	expression tag	UNP Q8VRK8

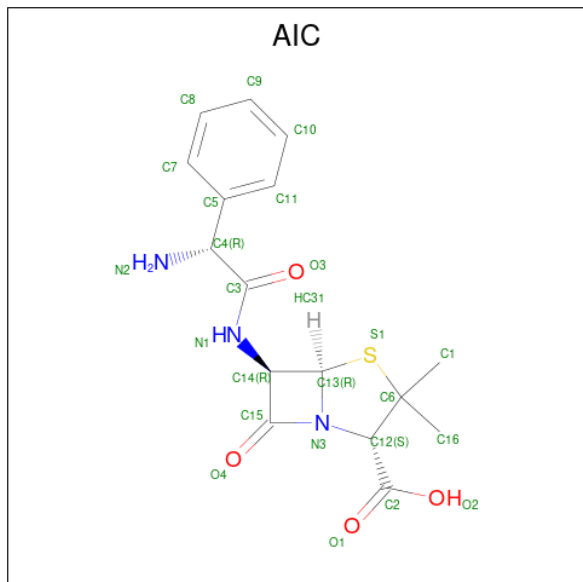
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Chain	Residue	Modelled	Actual	Comment	Reference
C	678	GLU	-	expression tag	UNP Q8VRK8
C	679	GLU	-	expression tag	UNP Q8VRK8
C	680	ASP	-	expression tag	UNP Q8VRK8
C	681	LEU	-	expression tag	UNP Q8VRK8
C	682	ASN	-	expression tag	UNP Q8VRK8
C	683	SER	-	expression tag	UNP Q8VRK8
C	684	ALA	-	expression tag	UNP Q8VRK8
C	685	VAL	-	expression tag	UNP Q8VRK8
C	686	ASP	-	expression tag	UNP Q8VRK8
C	687	HIS	-	expression tag	UNP Q8VRK8
C	688	HIS	-	expression tag	UNP Q8VRK8
C	689	HIS	-	expression tag	UNP Q8VRK8
C	690	HIS	-	expression tag	UNP Q8VRK8
C	691	HIS	-	expression tag	UNP Q8VRK8
C	692	HIS	-	expression tag	UNP Q8VRK8
D	205	ALA	SER	engineered mutation	UNP Q8VRK8
D	668	LYS	-	expression tag	UNP Q8VRK8
D	669	LEU	-	expression tag	UNP Q8VRK8
D	670	GLY	-	expression tag	UNP Q8VRK8
D	671	PRO	-	expression tag	UNP Q8VRK8
D	672	GLU	-	expression tag	UNP Q8VRK8
D	673	GLN	-	expression tag	UNP Q8VRK8
D	674	LYS	-	expression tag	UNP Q8VRK8
D	675	LEU	-	expression tag	UNP Q8VRK8
D	676	ILE	-	expression tag	UNP Q8VRK8
D	677	SER	-	expression tag	UNP Q8VRK8
D	678	GLU	-	expression tag	UNP Q8VRK8
D	679	GLU	-	expression tag	UNP Q8VRK8
D	680	ASP	-	expression tag	UNP Q8VRK8
D	681	LEU	-	expression tag	UNP Q8VRK8
D	682	ASN	-	expression tag	UNP Q8VRK8
D	683	SER	-	expression tag	UNP Q8VRK8
D	684	ALA	-	expression tag	UNP Q8VRK8
D	685	VAL	-	expression tag	UNP Q8VRK8
D	686	ASP	-	expression tag	UNP Q8VRK8
D	687	HIS	-	expression tag	UNP Q8VRK8
D	688	HIS	-	expression tag	UNP Q8VRK8
D	689	HIS	-	expression tag	UNP Q8VRK8
D	690	HIS	-	expression tag	UNP Q8VRK8
D	691	HIS	-	expression tag	UNP Q8VRK8
D	692	HIS	-	expression tag	UNP Q8VRK8

- Molecule 2 is (2S,5R,6R)-6-([(2R)-2-AMINO-2-PHENYLETHANOYL]AMINO)-3,3-DIME

THYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID (CCD ID: AIC) (formula: $C_{16}H_{19}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
2	B	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
2	C	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
2	D	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

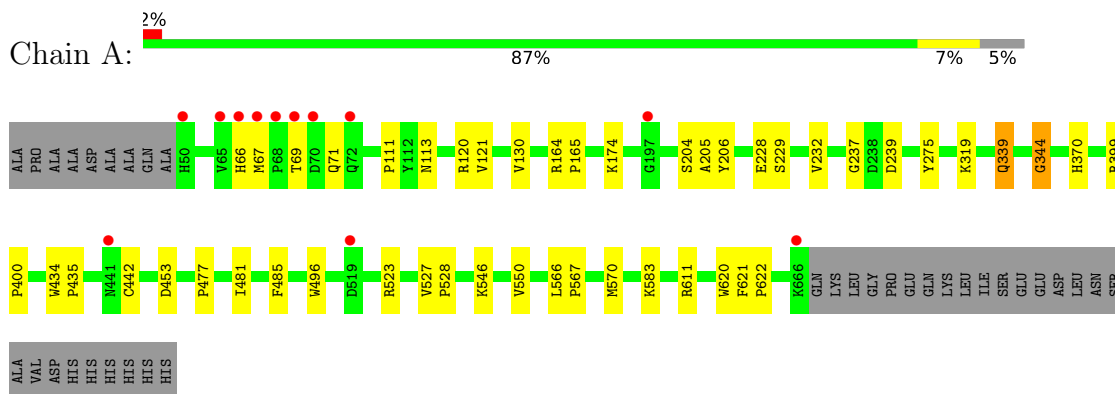
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	571	Total	O	0	0
			571	571		
4	B	573	Total	O	0	0
			573	573		
4	C	589	Total	O	0	0
			589	589		
4	D	496	Total	O	0	0
			496	496		

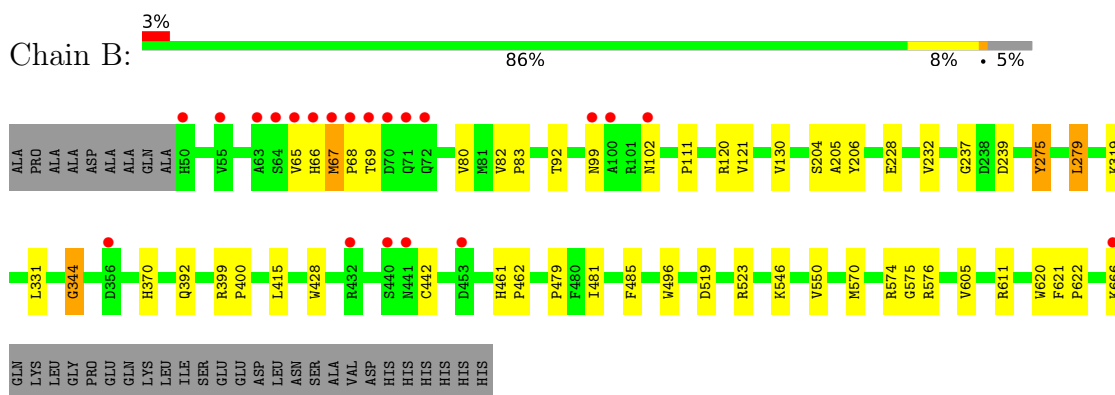
3 Residue-property plots

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

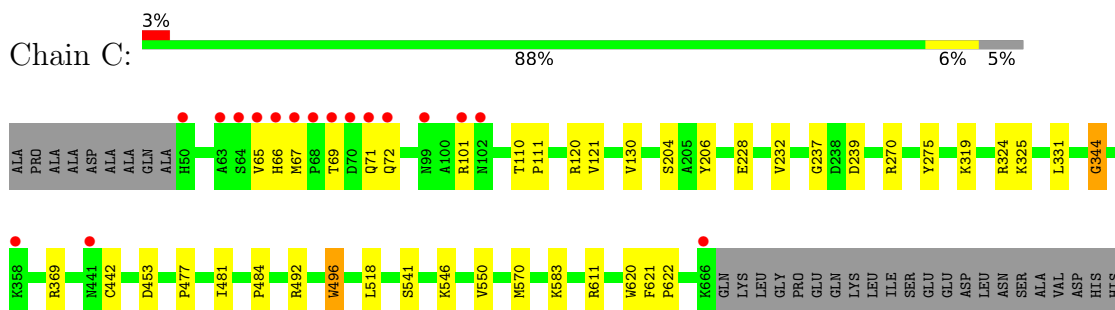
- Molecule 1: alpha-amino acid ester hydrolase



- Molecule 1: alpha-amino acid ester hydrolase

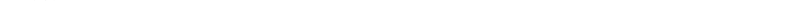


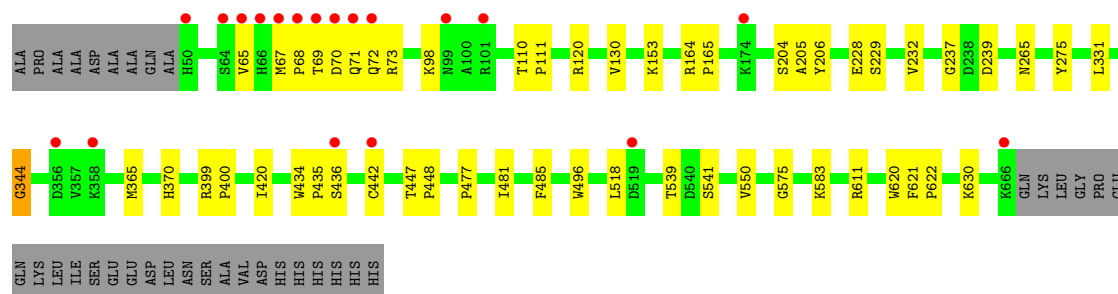
- Molecule 1: alpha-amino acid ester hydrolase



HIS
HIS
HIS
HIS

- Molecule 1: alpha-amino acid ester hydrolase

Chain D:  3% 86% 8% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	341.83Å 341.83Å 341.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (15.00-2.20) 96.5 (15.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.166 , 0.184 0.204 , 0.215	Depositor DCC
R_{free} test set	16105 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21877	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: AIC, GOL

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	0.44	0/5041	0.86	3/6886 (0.0%)
1	B	0.45	0/5041	0.86	4/6886 (0.1%)
1	C	0.44	0/5041	0.86	4/6886 (0.1%)
1	D	0.43	0/5041	0.86	4/6886 (0.1%)
All	All	0.44	0/20164	0.86	15/27544 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	ASP	N-CA-C	6.95	120.24	111.69
1	B	239	ASP	N-CA-C	6.84	120.10	111.69
1	A	239	ASP	N-CA-C	6.75	120.00	111.69
1	D	239	ASP	N-CA-C	6.61	119.82	111.69
1	D	575	GLY	N-CA-C	6.40	120.64	112.83
1	C	275	TYR	N-CA-C	-6.34	104.37	111.28
1	B	121	VAL	N-CA-C	-6.14	102.07	108.15
1	C	121	VAL	N-CA-C	-5.75	101.45	107.60
1	B	275	TYR	N-CA-C	-5.65	105.12	111.28
1	A	121	VAL	N-CA-C	-5.64	101.56	107.60
1	A	275	TYR	N-CA-C	-5.63	105.15	111.28
1	D	275	TYR	N-CA-C	-5.59	105.19	111.28
1	B	575	GLY	N-CA-C	5.46	120.53	113.27
1	D	110	THR	N-CA-C	5.27	117.72	108.82
1	C	110	THR	N-CA-C	5.19	117.58	108.82

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	4882	0	4648	21	0
1	B	4882	0	4648	19	0
1	C	4882	0	4648	10	0
1	D	4882	0	4648	18	0
2	A	24	0	17	1	0
2	B	24	0	17	1	0
2	C	24	0	17	0	0
2	D	24	0	17	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	571	0	0	2	0
4	B	573	0	0	1	0
4	C	589	0	0	0	0
4	D	496	0	0	0	0
All	All	21877	0	18692	70	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 2.

All (70) 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:339:GLN:HE22	1:A:370:HIS:H	1.43	0.64
1:B:550:VAL:HB	1:B:611:ARG:HB2	1.80	0.63
1:A:232:VAL:HB	1:A:344:GLY:HA2	1.83	0.60
1:A:550:VAL:HB	1:A:611:ARG:HB2	1.84	0.59
1:D:550:VAL:HB	1:D:611:ARG:HB2	1.84	0.58
1:B:232:VAL:HB	1:B:344:GLY:HA2	1.85	0.58
1:D:232:VAL:HB	1:D:344:GLY:HA2	1.86	0.57
2:A:5001:AIC:N2	4:A:6359:HOH:O	2.32	0.57
1:C:550:VAL:HB	1:C:611:ARG:HB2	1.90	0.54
1:C:204:SER:HA	1:C:228:GLU:O	2.09	0.52
1:C:232:VAL:HB	1:C:344:GLY:HA2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:621:PHE:CG	1:D:622:PRO:HA	2.46	0.51
1:A:339:GLN:NE2	1:A:370:HIS:H	2.08	0.51
1:A:204:SER:HA	1:A:228:GLU:O	2.11	0.50
1:D:399:ARG:HB3	1:D:400:PRO:HD3	1.94	0.50
1:B:621:PHE:CG	1:B:622:PRO:HA	2.47	0.50
1:A:621:PHE:CG	1:A:622:PRO:HA	2.47	0.49
1:C:621:PHE:CG	1:C:622:PRO:HA	2.47	0.49
1:A:339:GLN:NE2	1:A:339:GLN:H	2.11	0.49
1:B:204:SER:HA	1:B:228:GLU:O	2.13	0.49
1:B:523:ARG:HG3	1:B:605:VAL:HG22	1.95	0.48
1:B:392:GLN:HE21	1:B:428:TRP:HE1	1.62	0.47
1:A:399:ARG:HB3	1:A:400:PRO:HD3	1.97	0.47
1:A:546:LYS:HA	1:A:570:MET:HB3	1.97	0.46
1:D:204:SER:HA	1:D:228:GLU:O	2.15	0.46
1:D:153:LYS:HA	1:D:153:LYS:HD2	1.83	0.45
1:A:481:ILE:HD11	1:A:485:PHE:CD1	2.51	0.45
1:B:546:LYS:HA	1:B:570:MET:HB3	1.98	0.45
2:B:5002:AIC:N2	4:B:6304:HOH:O	2.36	0.45
1:A:111:PRO:HG3	1:A:206:TYR:CG	2.52	0.45
1:D:70:ASP:HA	1:D:73:ARG:HD2	1.97	0.44
1:D:164:ARG:HA	1:D:165:PRO:HD3	1.87	0.44
1:A:164:ARG:HA	1:A:165:PRO:HD3	1.87	0.44
1:C:481:ILE:HG21	1:C:496:TRP:HB2	1.98	0.44
1:A:205:ALA:HB2	1:A:370:HIS:CE1	2.52	0.44
1:A:339:GLN:H	1:A:339:GLN:HE21	1.64	0.43
1:B:574:ARG:HG2	1:B:576:ARG:HG2	2.00	0.43
1:B:111:PRO:HG3	1:B:206:TYR:CG	2.53	0.43
1:B:80:VAL:HG23	1:B:92:THR:HB	2.01	0.43
1:B:205:ALA:HB2	1:B:370:HIS:CE1	2.53	0.43
1:B:399:ARG:HB3	1:B:400:PRO:HD3	2.00	0.43
1:D:111:PRO:HG3	1:D:206:TYR:CG	2.53	0.43
1:B:479:PRO:HA	1:B:621:PHE:O	2.18	0.43
1:B:67:MET:HA	1:B:68:PRO:HD3	1.76	0.43
1:A:113:ASN:ND2	4:A:6047:HOH:O	2.52	0.42
1:C:111:PRO:HG3	1:C:206:TYR:CG	2.55	0.42
1:C:484:PRO:O	1:C:492:ARG:NH1	2.48	0.42
1:B:481:ILE:HG21	1:B:496:TRP:HB2	2.01	0.42
1:A:228:GLU:O	1:A:229:SER:C	2.62	0.42
1:D:481:ILE:HD11	1:D:485:PHE:CD1	2.54	0.42
1:B:82:VAL:HA	1:B:83:PRO:HD3	1.82	0.42
1:D:67:MET:HA	1:D:68:PRO:HD3	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TRP:CG	1:A:435:PRO:HA	2.55	0.42
1:C:369:ARG:H	1:C:369:ARG:HG3	1.65	0.42
1:B:275:TYR:O	1:B:279:LEU:HB2	2.19	0.41
1:A:477:PRO:HB2	1:A:621:PHE:HB2	2.01	0.41
1:A:566:LEU:HA	1:A:567:PRO:HD3	1.89	0.41
1:D:365:MET:HB2	1:D:420:ILE:HG23	2.03	0.41
1:D:477:PRO:HB2	1:D:621:PHE:HB2	2.03	0.41
1:A:481:ILE:HG21	1:A:496:TRP:HB2	2.02	0.41
1:A:527:VAL:HA	1:A:528:PRO:HD3	1.91	0.41
1:B:481:ILE:HD11	1:B:485:PHE:CD1	2.55	0.41
1:D:481:ILE:HG21	1:D:496:TRP:HB2	2.03	0.41
1:C:477:PRO:HB2	1:C:621:PHE:HB2	2.01	0.41
1:C:546:LYS:HA	1:C:570:MET:HB3	2.03	0.41
1:D:434:TRP:CG	1:D:435:PRO:HA	2.55	0.40
1:D:447:THR:HA	1:D:448:PRO:HD3	1.85	0.40
1:D:228:GLU:O	1:D:229:SER:C	2.64	0.40
1:D:205:ALA:HB2	1:D:370:HIS:CE1	2.56	0.40
1:B:461:HIS:HA	1:B:462:PRO:HD3	1.90	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	615/652 (94%)	586 (95%)	27 (4%)	2 (0%)	36	42
1	B	615/652 (94%)	591 (96%)	22 (4%)	2 (0%)	36	42
1	C	615/652 (94%)	585 (95%)	28 (5%)	2 (0%)	36	42
1	D	615/652 (94%)	584 (95%)	29 (5%)	2 (0%)	36	42
All	All	2460/2608 (94%)	2346 (95%)	106 (4%)	8 (0%)	36	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	GLY
1	B	344	GLY
1	C	344	GLY
1	D	344	GLY
1	B	237	GLY
1	C	237	GLY
1	A	237	GLY
1	D	237	GLY

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	516/543 (95%)	502 (97%)	14 (3%)	39	53
1	B	516/543 (95%)	500 (97%)	16 (3%)	35	48
1	C	516/543 (95%)	495 (96%)	21 (4%)	27	37
1	D	516/543 (95%)	499 (97%)	17 (3%)	33	45
All	All	2064/2172 (95%)	1996 (97%)	68 (3%)	33	45

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	67	MET
1	A	69	THR
1	A	71	GLN
1	A	120	ARG
1	A	130	VAL
1	A	174	LYS
1	A	319	LYS
1	A	339	GLN
1	A	442	CYS
1	A	453	ASP
1	A	523	ARG
1	A	583	LYS
1	A	620	TRP

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Mol	Chain	Res	Type
1	B	65	VAL
1	B	66	HIS
1	B	67	MET
1	B	69	THR
1	B	99	ASN
1	B	102	ASN
1	B	120	ARG
1	B	130	VAL
1	B	279	LEU
1	B	319	LYS
1	B	331	LEU
1	B	415	LEU
1	B	442	CYS
1	B	519	ASP
1	B	620	TRP
1	B	666	LYS
1	C	65	VAL
1	C	66	HIS
1	C	67	MET
1	C	69	THR
1	C	71	GLN
1	C	72	GLN
1	C	101	ARG
1	C	120	ARG
1	C	130	VAL
1	C	270	ARG
1	C	319	LYS
1	C	324	ARG
1	C	325	LYS
1	C	331	LEU
1	C	442	CYS
1	C	453	ASP
1	C	496	TRP
1	C	518	LEU
1	C	541	SER
1	C	583	LYS
1	C	620	TRP
1	D	65	VAL
1	D	69	THR
1	D	71	GLN
1	D	72	GLN
1	D	98	LYS

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Mol	Chain	Res	Type
1	D	120	ARG
1	D	130	VAL
1	D	265	ASN
1	D	331	LEU
1	D	436	SER
1	D	442	CYS
1	D	518	LEU
1	D	539	THR
1	D	541	SER
1	D	583	LYS
1	D	620	TRP
1	D	630	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	113	ASN
1	A	133	GLN
1	A	191	ASN
1	A	248	GLN
1	A	295	GLN
1	A	339	GLN
1	A	455	HIS
1	A	648	GLN
1	B	71	GLN
1	B	72	GLN
1	B	133	GLN
1	B	167	HIS
1	B	248	GLN
1	B	391	HIS
1	B	392	GLN
1	B	551	GLN
1	B	648	GLN
1	C	102	ASN
1	C	248	GLN
1	C	648	GLN
1	D	113	ASN
1	D	133	GLN
1	D	391	HIS
1	D	648	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	GOL	C	6006	-	5,5,5	0.36	0	5,5,5	0.26	0
2	AIC	A	5001	-	24,26,26	2.53	6 (25%)	36,40,40	2.45	8 (22%)
2	AIC	B	5002	-	24,26,26	2.53	6 (25%)	36,40,40	2.46	9 (25%)
3	GOL	A	6002	-	5,5,5	0.36	0	5,5,5	0.23	0
3	GOL	B	6004	-	5,5,5	0.37	0	5,5,5	0.25	0
2	AIC	D	5004	-	24,26,26	2.55	6 (25%)	36,40,40	2.46	9 (25%)
2	AIC	C	5003	-	24,26,26	2.56	6 (25%)	36,40,40	2.48	10 (27%)
3	GOL	D	6008	-	5,5,5	0.34	0	5,5,5	0.25	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	GOL	C	6006	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AIC	A	5001	-	1/1/9/10	2/16/47/47	0/3/3/3
2	AIC	B	5002	-	1/1/9/10	0/16/47/47	0/3/3/3
3	GOL	A	6002	-	-	2/4/4/4	-
3	GOL	B	6004	-	-	2/4/4/4	-
2	AIC	D	5004	-	1/1/9/10	1/16/47/47	0/3/3/3
2	AIC	C	5003	-	1/1/9/10	0/16/47/47	0/3/3/3
3	GOL	D	6008	-	-	0/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5003	AIC	C14-C15	-6.74	1.39	1.54
2	D	5004	AIC	C14-C15	-6.71	1.39	1.54
2	B	5002	AIC	C14-C15	-6.69	1.39	1.54
2	A	5001	AIC	C14-C15	-6.69	1.39	1.54
2	D	5004	AIC	C14-N1	-6.05	1.33	1.45
2	C	5003	AIC	C14-N1	-6.03	1.33	1.45
2	B	5002	AIC	C14-N1	-6.02	1.33	1.45
2	A	5001	AIC	C14-N1	-5.98	1.33	1.45
2	C	5003	AIC	C6-S1	-4.54	1.76	1.85
2	D	5004	AIC	C6-S1	-4.49	1.76	1.85
2	B	5002	AIC	C6-S1	-4.47	1.76	1.85
2	C	5003	AIC	C13-C14	-4.44	1.48	1.56
2	A	5001	AIC	C6-S1	-4.41	1.76	1.85
2	D	5004	AIC	C13-C14	-4.41	1.48	1.56
2	A	5001	AIC	C13-C14	-4.35	1.48	1.56
2	B	5002	AIC	C13-C14	-4.35	1.48	1.56
2	A	5001	AIC	C13-S1	-3.40	1.76	1.81
2	D	5004	AIC	C13-S1	-3.37	1.76	1.81
2	C	5003	AIC	C13-S1	-3.36	1.76	1.81
2	B	5002	AIC	C13-S1	-3.22	1.76	1.81
2	B	5002	AIC	C15-N3	3.01	1.44	1.37
2	C	5003	AIC	C15-N3	3.00	1.44	1.37
2	A	5001	AIC	C15-N3	2.99	1.44	1.37
2	D	5004	AIC	C15-N3	2.95	1.44	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5004	AIC	C15-C14-N1	7.51	136.53	115.29
2	C	5003	AIC	C15-C14-N1	7.50	136.51	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	AIC	C15-C14-N1	7.40	136.22	115.29
2	B	5002	AIC	C15-C14-N1	7.39	136.20	115.29
2	A	5001	AIC	C13-C14-N1	6.46	131.88	118.49
2	B	5002	AIC	C13-C14-N1	6.44	131.82	118.49
2	D	5004	AIC	C13-C14-N1	6.29	131.53	118.49
2	C	5003	AIC	C13-C14-N1	6.28	131.51	118.49
2	C	5003	AIC	C14-C13-S1	-5.65	110.36	119.22
2	D	5004	AIC	C14-C13-S1	-5.54	110.53	119.22
2	A	5001	AIC	C14-C13-S1	-5.49	110.61	119.22
2	B	5002	AIC	C14-C13-S1	-5.34	110.85	119.22
2	C	5003	AIC	C13-C14-C15	4.48	91.94	85.15
2	B	5002	AIC	C13-C14-C15	4.47	91.93	85.15
2	D	5004	AIC	C13-C14-C15	4.46	91.92	85.15
2	A	5001	AIC	C13-C14-C15	4.42	91.87	85.15
2	C	5003	AIC	C13-N3-C15	-4.07	88.93	93.92
2	B	5002	AIC	C13-N3-C15	-4.05	88.95	93.92
2	A	5001	AIC	C13-N3-C15	-4.04	88.97	93.92
2	D	5004	AIC	C13-N3-C15	-3.98	89.03	93.92
2	C	5003	AIC	C12-N3-C15	-3.41	116.92	126.38
2	B	5002	AIC	C12-N3-C15	-3.37	117.05	126.38
2	D	5004	AIC	C12-N3-C15	-3.35	117.08	126.38
2	A	5001	AIC	C12-N3-C15	-3.19	117.54	126.38
2	D	5004	AIC	O2-C2-C12	2.39	119.33	112.47
2	C	5003	AIC	O2-C2-C12	2.37	119.29	112.47
2	B	5002	AIC	O2-C2-C12	2.37	119.28	112.47
2	A	5001	AIC	O2-C2-C12	2.33	119.15	112.47
2	A	5001	AIC	O4-C15-N3	2.33	134.95	131.75
2	B	5002	AIC	O4-C15-N3	2.27	134.88	131.75
2	B	5002	AIC	C13-N3-C12	-2.26	114.64	117.30
2	D	5004	AIC	O4-C15-N3	2.25	134.85	131.75
2	C	5003	AIC	O4-C15-N3	2.23	134.82	131.75
2	C	5003	AIC	C13-N3-C12	-2.14	114.78	117.30
2	D	5004	AIC	C13-N3-C12	-2.07	114.87	117.30
2	C	5003	AIC	C6-C12-N3	2.06	109.41	106.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	5001	AIC	C14
2	B	5002	AIC	C14
2	C	5003	AIC	C14
2	D	5004	AIC	C14

All (11) torsion outliers are listed below:

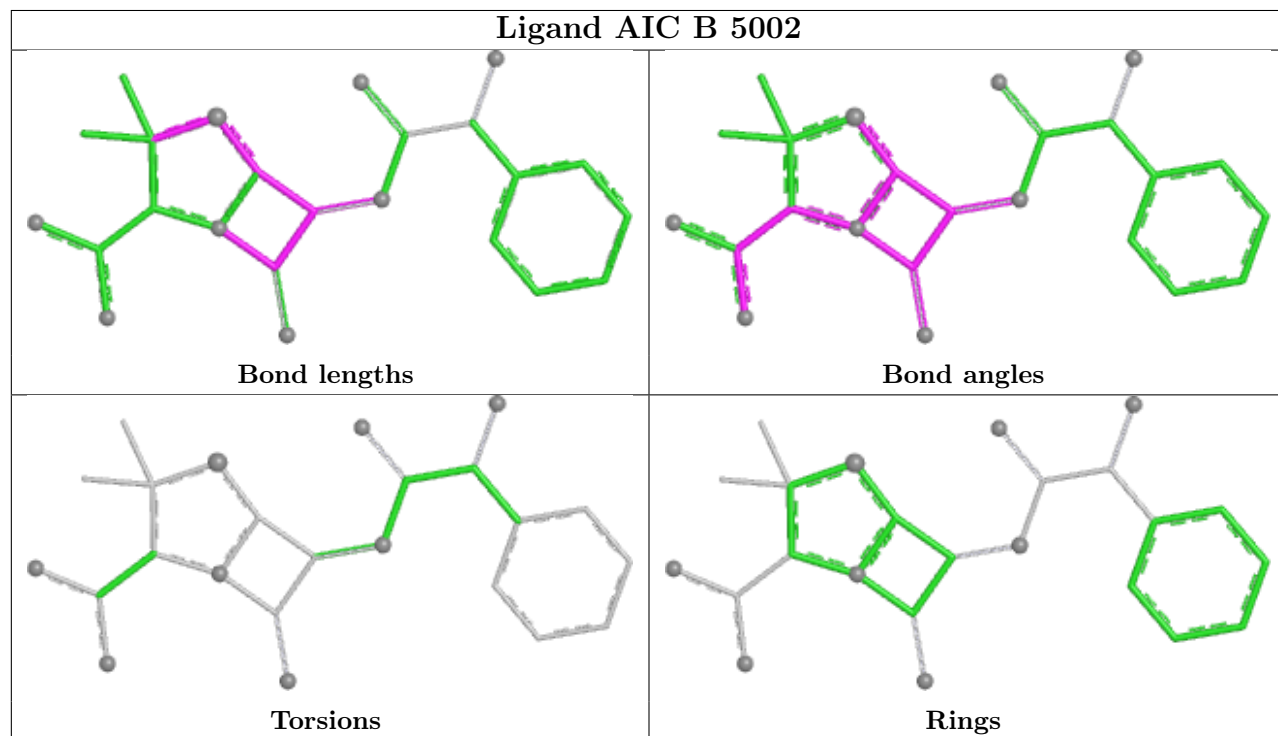
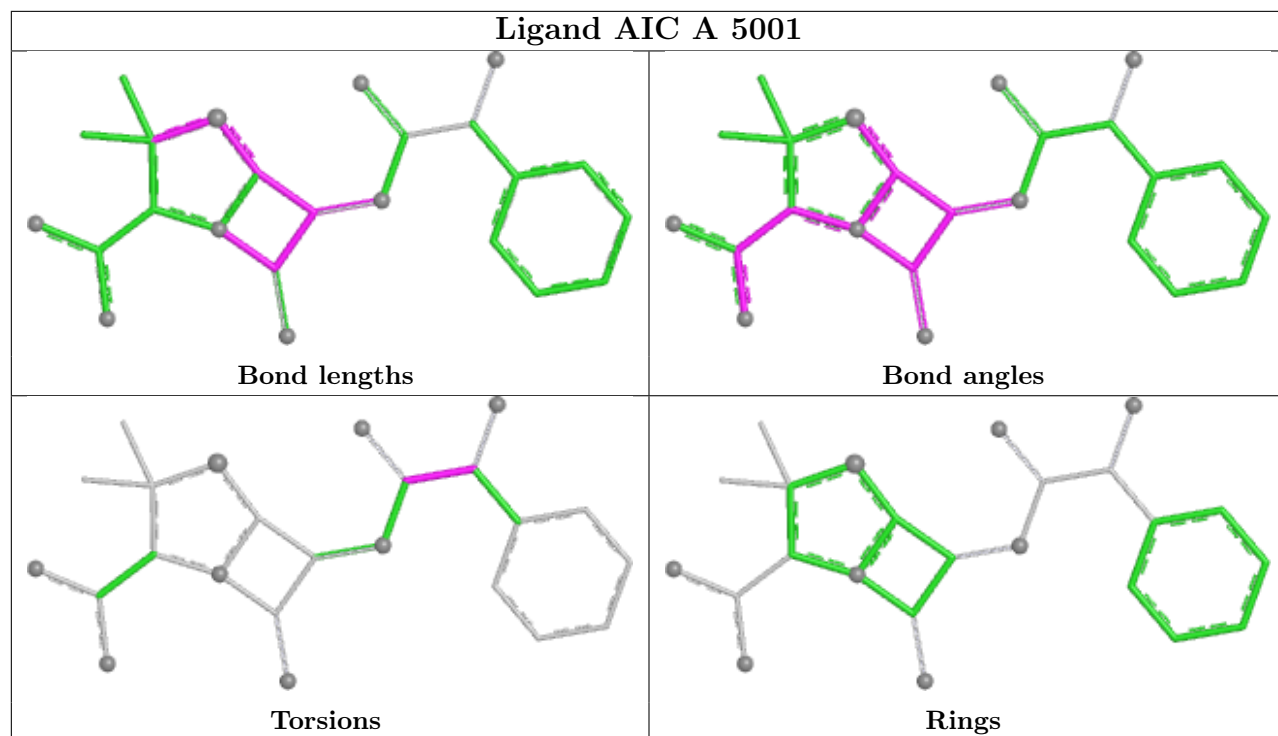
Mol	Chain	Res	Type	Atoms
3	B	6004	GOL	O1-C1-C2-C3
3	C	6006	GOL	O1-C1-C2-C3
3	A	6002	GOL	O1-C1-C2-C3
3	C	6006	GOL	C1-C2-C3-O3
3	B	6004	GOL	O1-C1-C2-O2
3	C	6006	GOL	O2-C2-C3-O3
3	C	6006	GOL	O1-C1-C2-O2
3	A	6002	GOL	O1-C1-C2-O2
2	A	5001	AIC	N1-C3-C4-N2
2	A	5001	AIC	O3-C3-C4-N2
2	D	5004	AIC	N1-C3-C4-N2

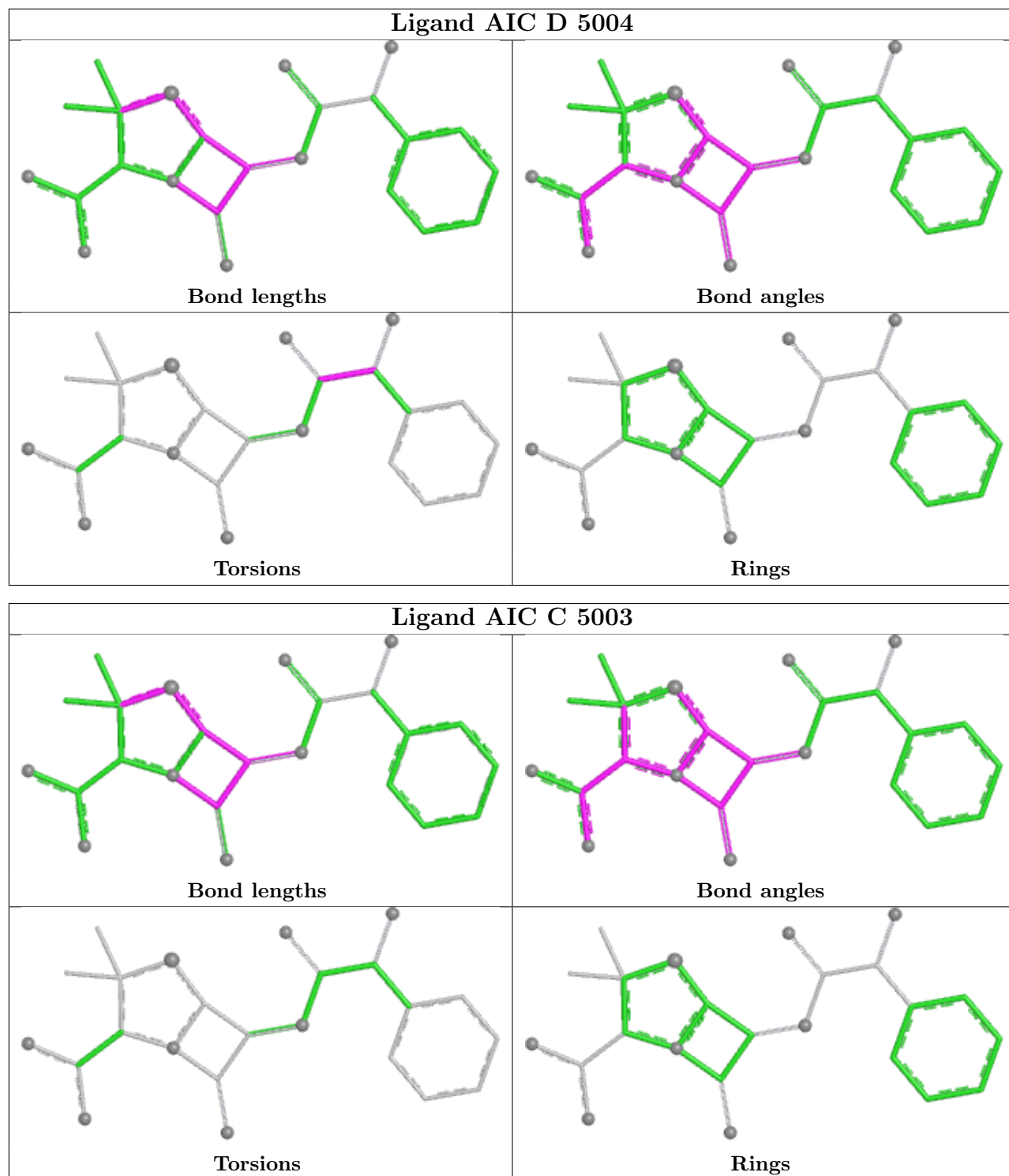
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	AIC	1	0
2	B	5002	AIC	1	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 ⓘ

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	617/652 (94%)	-0.11	12 (1%) 66 63	13, 18, 32, 77	0
1	B	617/652 (94%)	-0.13	21 (3%) 48 45	14, 18, 33, 86	0
1	C	617/652 (94%)	-0.11	17 (2%) 55 52	14, 18, 32, 79	0
1	D	617/652 (94%)	0.05	19 (3%) 51 48	13, 18, 32, 82	0
All	All	2468/2608 (94%)	-0.07	69 (2%) 55 52	13, 18, 32, 86	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	ASN	8.5
1	B	69	THR	7.3
1	C	66	HIS	5.9
1	B	67	MET	5.8
1	B	71	GLN	5.7
1	D	69	THR	5.4
1	A	69	THR	5.3
1	B	50	HIS	5.2
1	C	69	THR	5.2
1	B	70	ASP	5.1
1	B	66	HIS	5.1
1	A	67	MET	4.9
1	A	50	HIS	4.8
1	D	68	PRO	4.6
1	C	67	MET	4.5
1	A	70	ASP	4.3
1	D	70	ASP	4.1
1	A	66	HIS	3.9
1	C	65	VAL	3.8
1	B	441	ASN	3.7
1	C	72	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	70	ASP	3.6
1	D	65	VAL	3.6
1	D	666	LYS	3.6
1	A	666	LYS	3.5
1	C	99	ASN	3.5
1	C	50	HIS	3.4
1	D	50	HIS	3.4
1	D	71	GLN	3.4
1	D	64	SER	3.4
1	A	72	GLN	3.3
1	C	101	ARG	3.3
1	D	66	HIS	3.3
1	D	67	MET	3.3
1	B	72	GLN	3.2
1	A	68	PRO	3.1
1	B	68	PRO	3.1
1	C	441	ASN	3.0
1	A	65	VAL	2.9
1	D	99	ASN	2.8
1	B	65	VAL	2.8
1	B	64	SER	2.8
1	C	64	SER	2.8
1	D	72	GLN	2.7
1	B	453	ASP	2.7
1	D	358	LYS	2.6
1	B	102	ASN	2.6
1	C	68	PRO	2.6
1	D	436	SER	2.5
1	B	63	ALA	2.4
1	C	63	ALA	2.4
1	B	440	SER	2.4
1	D	174	LYS	2.4
1	C	358	LYS	2.4
1	D	442	CYS	2.4
1	C	102	ASN	2.3
1	B	55	VAL	2.3
1	D	101	ARG	2.3
1	B	100	ALA	2.3
1	A	197	GLY	2.3
1	A	519	ASP	2.2
1	A	441	ASN	2.2
1	B	356	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	432	ARG	2.1
1	C	666	LYS	2.1
1	D	356	ASP	2.1
1	B	666	LYS	2.0
1	C	71	GLN	2.0
1	D	519	ASP	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](#)

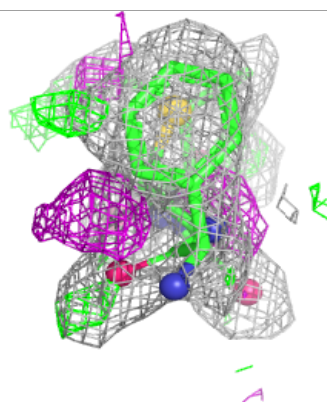
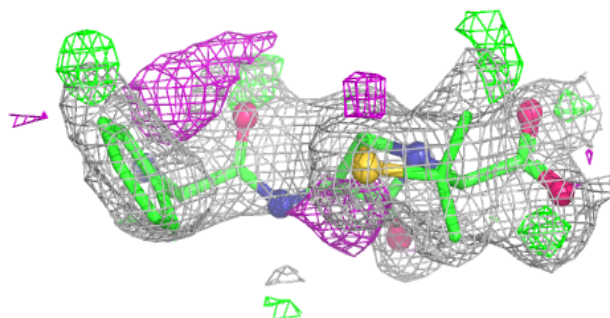
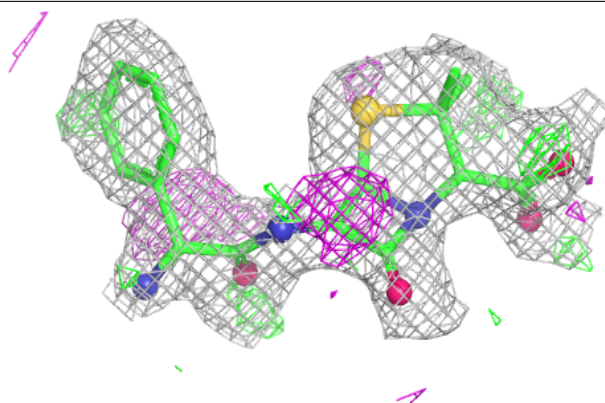
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	AIC	D	5004	24/24	0.76	0.19	53,62,67,68	0
2	AIC	B	5002	24/24	0.78	0.21	47,63,66,68	0
2	AIC	A	5001	24/24	0.80	0.18	49,63,71,73	0
2	AIC	C	5003	24/24	0.81	0.20	48,60,66,68	0
3	GOL	A	6002	6/6	0.82	0.20	35,57,59,59	0
3	GOL	B	6004	6/6	0.83	0.18	33,53,59,67	0
3	GOL	D	6008	6/6	0.83	0.20	36,59,63,63	0
3	GOL	C	6006	6/6	0.90	0.16	30,50,50,53	0

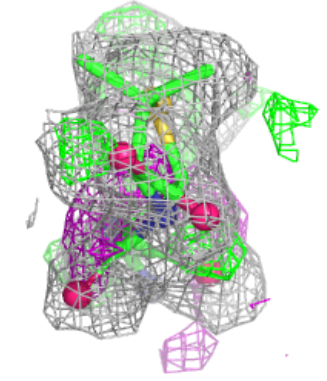
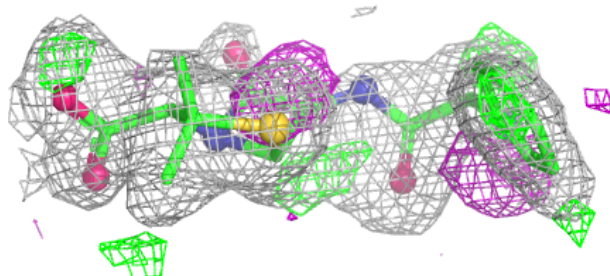
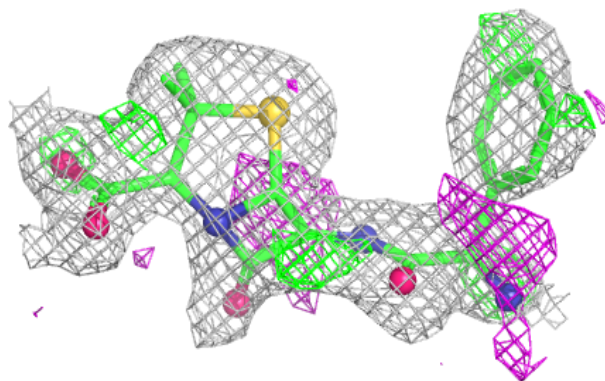
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AIC D 5004:

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

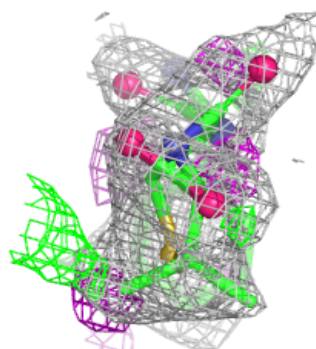
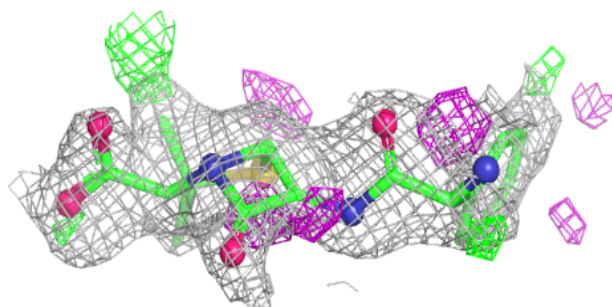
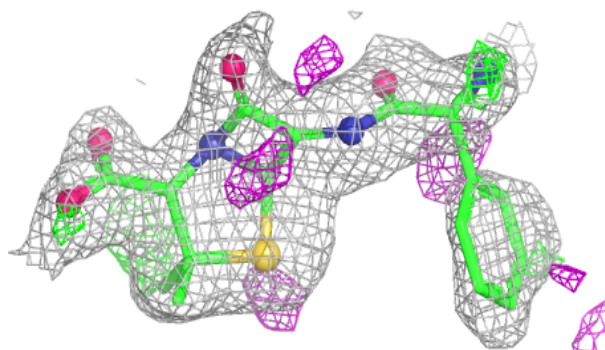
**Electron density around AIC B 5002:**

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

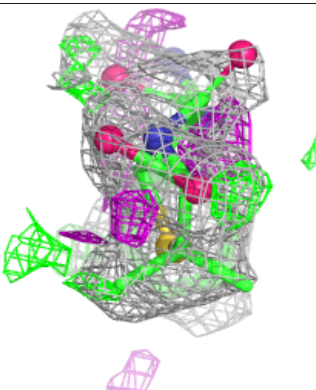
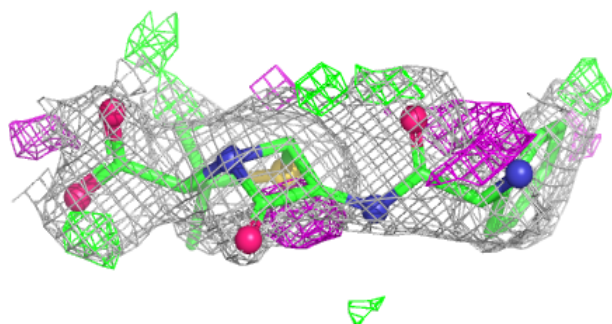
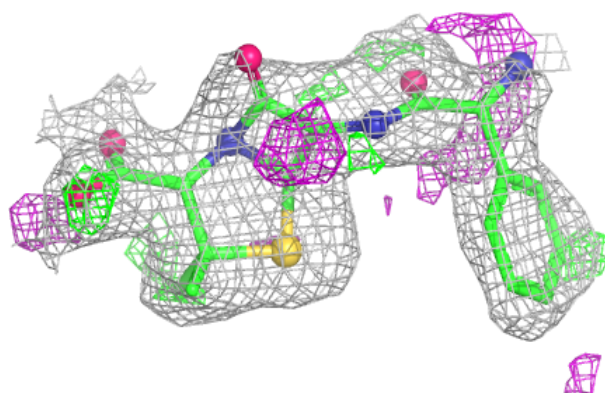


Electron density around AIC A 5001:

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

**Electron density around AIC C 5003:**

$2mF_o-DF_c$ (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.