



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 02:03 pm BST

PDB ID : 9HL7 / pdb\_00009hl7  
Title : Protein Kinase CK2 and small molecule ligands  
Authors : Krimm, I.; Gelin, I.; Guichou, J.F.  
Deposited on : 2024-12-04  
Resolution : 2.28 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

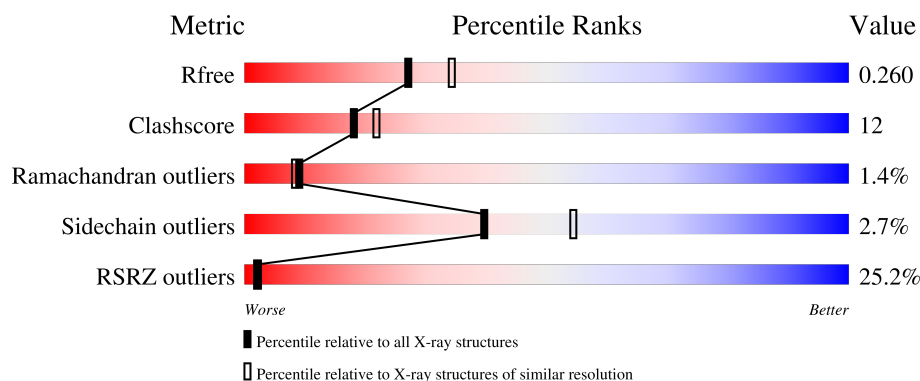
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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))
$R_{free}$	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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  $\geq 3$ , 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	B	359	<div> <div>23%</div> <div>68%</div> <div>23%</div> <div>8%</div> </div>
1	C	359	<div> <div>24%</div> <div>67%</div> <div>24%</div> <div>8%</div> </div>

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	SO4	C	409	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5818 atoms, of which 24 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	331	Total	C	N	O	S	0	2	0
			2796	1792	492	501	11			
1	C	331	Total	C	N	O	S	0	2	0
			2790	1789	489	501	11			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP P68400
B	-20	HIS	-	expression tag	UNP P68400
B	-19	HIS	-	expression tag	UNP P68400
B	-18	HIS	-	expression tag	UNP P68400
B	-17	HIS	-	expression tag	UNP P68400
B	-16	HIS	-	expression tag	UNP P68400
B	-15	HIS	-	expression tag	UNP P68400
B	-14	SER	-	expression tag	UNP P68400
B	-13	SER	-	expression tag	UNP P68400
B	-12	GLY	-	expression tag	UNP P68400
B	-11	VAL	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	LEU	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	THR	-	expression tag	UNP P68400
B	-6	GLU	-	expression tag	UNP P68400
B	-5	ASN	-	expression tag	UNP P68400
B	-4	LEU	-	expression tag	UNP P68400
B	-3	TYR	-	expression tag	UNP P68400
B	-2	PHE	-	expression tag	UNP P68400
B	-1	GLN	-	expression tag	UNP P68400
B	0	SER	-	expression tag	UNP P68400
C	-21	MET	-	initiating methionine	UNP P68400
C	-20	HIS	-	expression tag	UNP P68400
C	-19	HIS	-	expression tag	UNP P68400

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP P68400
C	-17	HIS	-	expression tag	UNP P68400
C	-16	HIS	-	expression tag	UNP P68400
C	-15	HIS	-	expression tag	UNP P68400
C	-14	SER	-	expression tag	UNP P68400
C	-13	SER	-	expression tag	UNP P68400
C	-12	GLY	-	expression tag	UNP P68400
C	-11	VAL	-	expression tag	UNP P68400
C	-10	ASP	-	expression tag	UNP P68400
C	-9	LEU	-	expression tag	UNP P68400
C	-8	GLY	-	expression tag	UNP P68400
C	-7	THR	-	expression tag	UNP P68400
C	-6	GLU	-	expression tag	UNP P68400
C	-5	ASN	-	expression tag	UNP P68400
C	-4	LEU	-	expression tag	UNP P68400
C	-3	TYR	-	expression tag	UNP P68400
C	-2	PHE	-	expression tag	UNP P68400
C	-1	GLN	-	expression tag	UNP P68400
C	0	SER	-	expression tag	UNP P68400

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



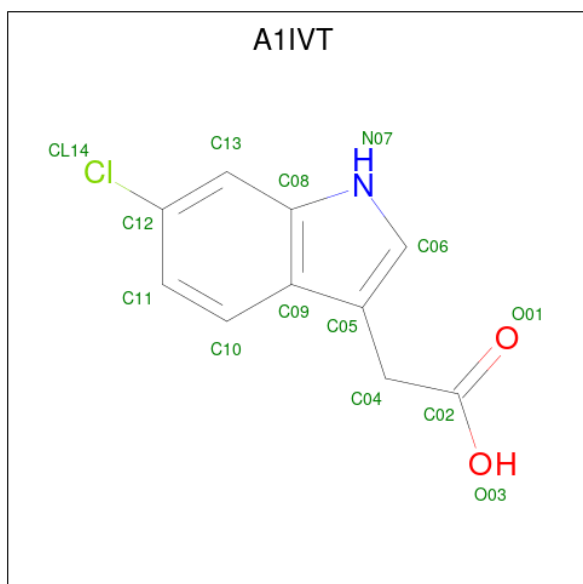
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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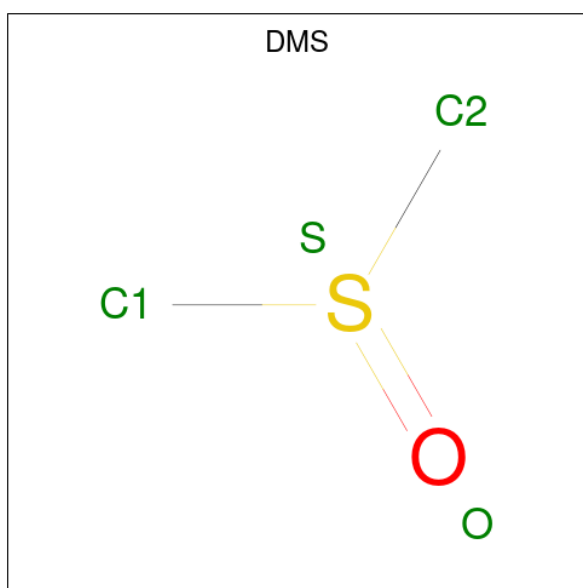
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

- Molecule 3 is 2-(6-chloranyl-1 {H}-indol-3-yl)ethanoic acid (CCD ID: A1IVT) (formula:  $C_{10}H_8ClNO_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			14	10	1	1	2		
3	B	1	Total	C	Cl	N	O	0	0
			14	10	1	1	2		
3	C	1	Total	C	Cl	N	O	0	0
			14	10	1	1	2		
3	C	1	Total	C	Cl	N	O	0	0
			14	10	1	1	2		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula:  $C_2H_6OS$ ).



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

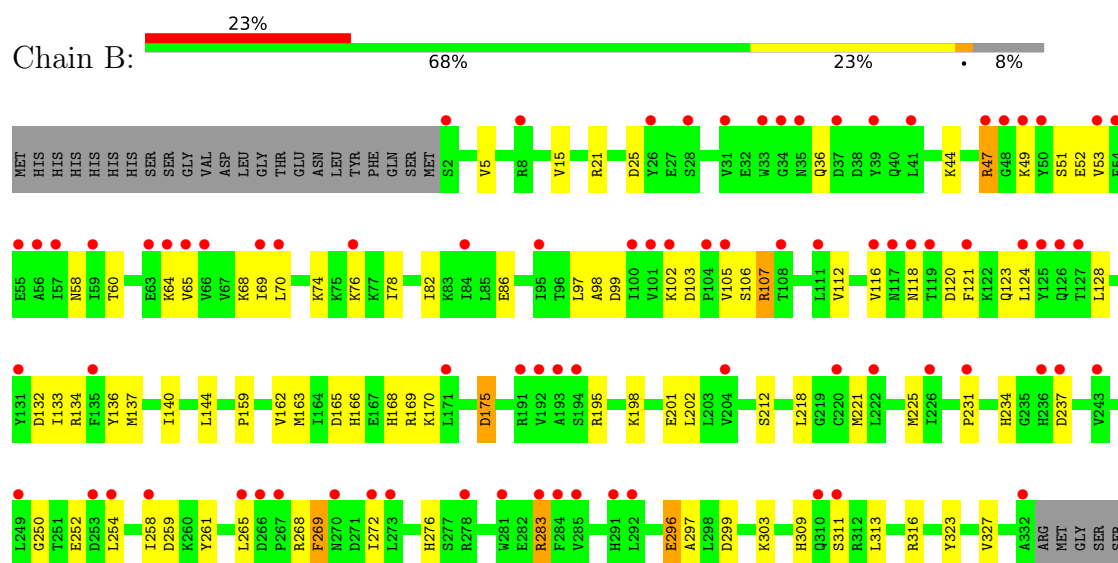
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	32	Total	O	0	0
			32	32		
5	C	34	Total	O	0	0
			34	34		

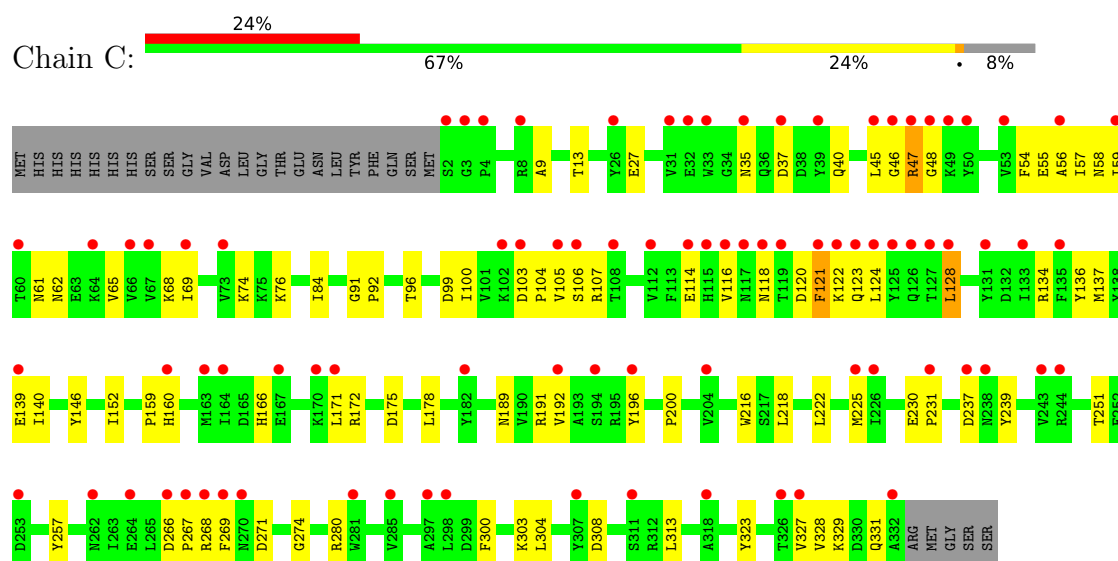
### 3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha



- Molecule 1: Casein kinase II subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.95Å 126.95Å 124.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.77 – 2.28 56.77 – 2.28	Depositor EDS
% Data completeness (in resolution range)	93.3 (56.77-2.28) 92.1 (56.77-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, $R_{free}$	0.216 , 0.265 0.217 , 0.260	Depositor DCC
$R_{free}$ test set	2889 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k 0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5818	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, DMS, A1IVT

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	B	0.38	0/2877	0.56	0/3892
1	C	0.39	0/2871	0.59	0/3885
All	All	0.38	0/5748	0.57	0/7777

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	B	2796	0	2735	66	0
1	C	2790	0	2724	69	0
2	B	35	0	0	0	0
2	C	35	0	0	4	0
3	B	28	0	0	5	0
3	C	28	0	0	4	0
4	B	4	6	6	0	0
4	C	12	18	18	1	0
5	B	32	0	0	0	0
5	C	34	0	0	0	0
All	All	5794	24	5483	135	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 12.

All (135) 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:C:74:LYS:H	1:C:74:LYS:HD2	1.35	0.90
1:B:128:LEU:HD22	1:B:132:ASP:HB3	1.61	0.82
1:B:64:LYS:H	1:B:64:LYS:HD3	1.42	0.82
1:B:303:LYS:HB3	1:B:313:LEU:HD13	1.66	0.75
1:B:175:ASP:HA	3:B:403:A1IVT:O03	1.87	0.75
1:B:74:LYS:HE2	1:B:76:LYS:HE2	1.71	0.70
1:B:102:LYS:HD3	1:B:107:ARG:HD3	1.74	0.70
1:B:120:ASP:HB3	1:B:163:MET:CE	2.23	0.69
1:C:121:PHE:CE2	1:C:225:MET:HE1	2.29	0.68
1:B:64:LYS:H	1:B:64:LYS:CD	2.07	0.66
1:B:195:ARG:HD3	1:B:237:ASP:C	2.21	0.65
1:C:121:PHE:HE2	1:C:140:ILE:HD11	1.62	0.65
1:B:132:ASP:OD1	1:B:169:ARG:NH2	2.30	0.65
1:C:124:LEU:O	1:C:128:LEU:HD22	1.97	0.65
1:B:124:LEU:HD11	1:B:166:HIS:CD2	2.31	0.65
1:C:47[B]:ARG:HG3	1:C:47[B]:ARG:HH11	1.63	0.64
1:C:84:ILE:HG23	1:C:152:ILE:HD13	1.79	0.63
1:C:137:MET:HE2	1:C:222:LEU:HB2	1.81	0.63
1:B:64:LYS:HD3	1:B:64:LYS:N	2.13	0.62
1:C:280:ARG:HB2	2:C:409:SO4:O1	2.00	0.62
1:B:47:ARG:HG3	1:B:53:VAL:CG2	2.30	0.62
1:C:136:TYR:HH	1:C:166:HIS:HD1	1.46	0.62
1:C:268:ARG:HH11	1:C:268:ARG:HG3	1.64	0.62
1:C:40:GLN:HG3	1:C:59:ILE:CG2	2.30	0.61
1:B:107:ARG:HD2	2:C:404:SO4:O1	2.01	0.61
1:B:303:LYS:HB3	1:B:313:LEU:CD1	2.30	0.60
1:B:137:MET:HE1	1:B:218:LEU:HG	1.82	0.60
1:C:121:PHE:CZ	1:C:225:MET:HE1	2.37	0.60
1:C:46:GLY:HA2	1:C:47[A]:ARG:NH1	2.16	0.60
1:B:124:LEU:HD11	1:B:166:HIS:HD2	1.67	0.59
1:C:121:PHE:CE2	1:C:140:ILE:HD11	2.38	0.59
1:C:45:LEU:HD13	1:C:55:GLU:N	2.17	0.59
1:C:175:ASP:HA	3:C:402:A1IVT:O01	2.03	0.59
1:B:116:VAL:HG12	3:B:403:A1IVT:CL14	2.40	0.58
1:C:91:GLY:HA3	1:C:146:TYR:CE2	2.39	0.58
1:B:82:ILE:CG2	1:B:86:GLU:OE1	2.52	0.57
1:B:296[A]:GLU:H	1:B:296[A]:GLU:CD	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ARG:HA	1:B:198:LYS:HD2	1.86	0.56
1:C:300:PHE:CZ	1:C:304:LEU:HD11	2.41	0.56
1:B:165:ASP:OD2	1:B:168:HIS:ND1	2.31	0.56
1:C:122:LYS:HD2	1:C:160:HIS:CE1	2.41	0.56
1:C:47[A]:ARG:CZ	1:C:47[A]:ARG:H	2.19	0.55
1:C:46:GLY:HA2	1:C:47[A]:ARG:HH12	1.72	0.55
1:B:47:ARG:HG3	1:B:53:VAL:HG21	1.89	0.54
1:C:96:THR:HB	1:C:114[A]:GLU:HG3	1.90	0.54
1:B:70:LEU:HD13	1:B:78:ILE:HG12	1.88	0.54
1:B:116:VAL:CG1	3:B:403:A1IVT:CL14	2.92	0.54
1:C:303:LYS:HB3	1:C:313:LEU:HG	1.89	0.54
1:C:47[B]:ARG:HG3	1:C:47[B]:ARG:NH1	2.23	0.54
1:C:137:MET:CE	1:C:222:LEU:HB2	2.38	0.54
1:B:128:LEU:HD22	1:B:132:ASP:CB	2.34	0.53
1:C:280:ARG:HD2	2:C:409:SO4:O1	2.09	0.53
1:B:82:ILE:HG22	1:B:86:GLU:OE1	2.09	0.53
1:C:96:THR:HB	1:C:114[A]:GLU:CG	2.39	0.52
1:C:189:ASN:HA	4:C:411:DMS:H12	1.91	0.52
1:C:122:LYS:HE2	1:C:230:GLU:OE2	2.10	0.52
1:B:120:ASP:HB3	1:B:163:MET:HE1	1.92	0.52
1:C:40:GLN:HG3	1:C:59:ILE:HG21	1.91	0.51
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.46	0.50
1:C:54:PHE:CE1	1:C:69:ILE:HD12	2.47	0.50
1:B:21:ARG:HG3	1:B:25:ASP:HB2	1.93	0.50
1:C:116:VAL:HB	3:C:402:A1IVT:CL14	2.48	0.50
1:C:92:PRO:HD2	1:C:146:TYR:CG	2.47	0.50
1:B:159:PRO:HD3	1:B:221:MET:HG2	1.95	0.49
1:B:44:LYS:NZ	1:B:52:GLU:OE2	2.33	0.49
1:B:254:LEU:O	1:B:258:ILE:HG12	2.12	0.49
1:C:268:ARG:HG3	1:C:268:ARG:NH1	2.26	0.49
1:B:165:ASP:HB3	1:B:170:LYS:HB3	1.93	0.49
1:B:297:ALA:HB2	1:B:323:TYR:CE1	2.48	0.49
1:C:134:ARG:HG2	1:C:323:TYR:CZ	2.48	0.49
1:C:45:LEU:HD11	1:C:55:GLU:HB2	1.95	0.48
1:B:250:GLY:HA2	1:B:276:HIS:O	2.13	0.48
1:B:51:SER:HB2	1:B:69:ILE:O	2.13	0.48
1:B:252:GLU:HA	1:B:252:GLU:OE1	2.13	0.48
1:B:316:ARG:HD3	1:B:316:ARG:O	2.14	0.48
1:B:121:PHE:HB2	1:B:162:VAL:HB	1.96	0.47
1:C:99:ASP:C	1:C:100:ILE:HG13	2.39	0.47
1:B:283[B]:ARG:HG2	1:B:283[B]:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LYS:H	1:C:74:LYS:CD	2.08	0.46
1:B:231:PRO:HG2	1:B:234:HIS:HB2	1.97	0.46
1:C:56:ALA:HB3	1:C:65:VAL:HG23	1.97	0.46
1:B:82:ILE:HG23	1:B:86:GLU:OE1	2.14	0.46
1:C:121:PHE:HB3	1:C:159:PRO:HB3	1.96	0.46
1:B:136:TYR:O	1:B:140:ILE:HG13	2.16	0.46
1:B:36:GLN:OE1	1:B:103:ASP:HA	2.16	0.46
1:B:299:ASP:OD2	1:B:303:LYS:HE2	2.15	0.45
1:C:104:PRO:HG2	3:C:403:A1IVT:C04	2.46	0.45
1:B:265:LEU:HD22	1:B:269:PHE:CD2	2.51	0.45
1:B:68:LYS:HD3	3:B:403:A1IVT:C04	2.47	0.45
1:C:91:GLY:HA3	1:C:146:TYR:CD2	2.51	0.45
1:B:269:PHE:HA	1:B:272:ILE:CG1	2.47	0.45
1:C:27:GLU:HG2	1:C:76:LYS:HG2	1.97	0.45
1:B:201:GLU:HG2	1:B:202:LEU:N	2.32	0.44
1:C:120:ASP:CG	1:C:123:GLN:OE1	2.60	0.44
1:B:105:VAL:HG13	1:B:106:SER:H	1.81	0.44
1:C:9:ALA:O	1:C:13:THR:HG22	2.17	0.44
1:C:251:THR:HG21	1:C:274:GLY:O	2.18	0.44
1:C:139:GLU:HB2	1:C:171:LEU:HD13	2.00	0.44
1:C:191:ARG:HA	1:C:191:ARG:HD2	1.82	0.44
1:B:5:VAL:HB	1:B:261:TYR:HA	2.00	0.43
1:C:237:ASP:OD1	1:C:239:TYR:N	2.50	0.43
1:C:68:LYS:HD2	3:C:402:A1IVT:C04	2.48	0.43
1:B:49:LYS:HD2	1:B:49:LYS:HA	1.71	0.43
1:C:96:THR:H	1:C:114[B]:GLU:HG2	1.82	0.43
1:C:269:PHE:O	1:C:271:ASP:N	2.52	0.43
1:C:266:ASP:OD1	1:C:267:PRO:HD2	2.18	0.43
1:B:269:PHE:HA	1:B:272:ILE:HG13	2.01	0.43
1:C:257:TYR:CE1	1:C:308:ASP:HA	2.53	0.43
1:C:35:ASN:OD1	1:C:37:ASP:HB2	2.18	0.42
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.91	0.42
1:C:171:LEU:C	1:C:171:LEU:HD23	2.44	0.42
1:C:47[B]:ARG:HB2	1:C:48:GLY:H	1.61	0.42
1:C:230:GLU:HA	1:C:231:PRO:HA	1.90	0.42
1:C:137:MET:HE2	1:C:222:LEU:HD13	2.01	0.42
1:C:116:VAL:HG21	1:C:172:ARG:HG3	2.01	0.42
1:B:212:SER:OG	1:B:309:HIS:HB2	2.20	0.42
1:B:58:ASN:OD1	1:B:60:THR:OG1	2.27	0.42
1:B:98:ALA:O	1:B:99:ASP:HB2	2.20	0.41
1:C:327:VAL:O	1:C:331:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:TYR:CD2	1:C:231:PRO:HG3	2.55	0.41
1:B:144:LEU:HD23	1:B:144:LEU:HA	1.85	0.41
1:B:105:VAL:HG13	1:B:106:SER:N	2.36	0.41
1:B:97:LEU:HD12	1:B:112:VAL:O	2.21	0.41
1:C:9:ALA:O	1:C:13:THR:CG2	2.68	0.41
1:C:178:LEU:HD22	1:C:192:VAL:HB	2.03	0.41
1:C:280:ARG:CB	2:C:409:SO4:O1	2.68	0.41
1:B:47:ARG:HG3	1:B:53:VAL:HG23	2.02	0.40
1:B:133:ILE:HD13	1:B:225:MET:HB3	2.03	0.40
1:C:58:ASN:CG	1:C:61:ASN:HD21	2.30	0.40
1:B:170:LYS:HB2	1:B:170:LYS:HE3	1.93	0.40
1:C:103:ASP:OD1	1:C:104:PRO:HD2	2.21	0.40
1:B:116:VAL:HG13	3:B:403:A1IVT:CL14	2.58	0.40
1:C:200:PRO:HD3	1:C:216:TRP:CE2	2.57	0.40
1:B:120:ASP:HB3	1:B:163:MET:HE2	2.03	0.40
1:C:218:LEU:HA	1:C:218:LEU:HD12	1.89	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	B	331/359 (92%)	306 (92%)	18 (5%)	7 (2%)	5	4
1	C	331/359 (92%)	307 (93%)	22 (7%)	2 (1%)	22	25
All	All	662/718 (92%)	613 (93%)	40 (6%)	9 (1%)	9	8

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	ASN
1	C	118	ASN

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Mol	Chain	Res	Type
1	B	123	GLN
1	B	268	ARG
1	C	62	ASN
1	B	175	ASP
1	B	269	PHE
1	B	47	ARG
1	B	107	ARG

### 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	B	303/329 (92%)	294 (97%)	9 (3%)	36	50
1	C	302/329 (92%)	292 (97%)	10 (3%)	33	46
All	All	605/658 (92%)	586 (97%)	19 (3%)	40	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	VAL
1	B	65	VAL
1	B	259	ASP
1	B	283[A]	ARG
1	B	283[B]	ARG
1	B	296[A]	GLU
1	B	296[B]	GLU
1	B	311	SER
1	B	327	VAL
1	C	47[A]	ARG
1	C	47[B]	ARG
1	C	57	ILE
1	C	105	VAL
1	C	106	SER
1	C	107	ARG
1	C	121	PHE

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Mol	Chain	Res	Type
1	C	128	LEU
1	C	328	VAL
1	C	329	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	HIS
1	B	166	HIS
1	B	262	ASN
1	C	29	HIS
1	C	61	ASN
1	C	160	HIS
1	C	310	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	405	-	4,4,4	0.17	0	6,6,6	0.33	0
2	SO4	B	406	-	4,4,4	0.21	0	6,6,6	0.18	0
2	SO4	C	401	-	4,4,4	0.21	0	6,6,6	0.36	0
2	SO4	C	407	-	4,4,4	0.27	0	6,6,6	0.17	0
2	SO4	B	409	-	4,4,4	0.28	0	6,6,6	0.41	0
4	DMS	B	410	-	3,3,3	0.73	0	3,3,3	0.58	0
4	DMS	C	411	-	3,3,3	0.76	0	3,3,3	1.01	0
2	SO4	B	408	-	4,4,4	0.30	0	6,6,6	0.63	0
2	SO4	C	409	-	4,4,4	0.20	0	6,6,6	0.46	0
2	SO4	C	404	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	C	406	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	B	405	-	4,4,4	0.22	0	6,6,6	0.06	0
2	SO4	B	407	-	4,4,4	0.19	0	6,6,6	0.46	0
3	A1IVT	B	404	-	14,15,15	1.64	3 (21%)	16,21,21	2.11	5 (31%)
2	SO4	B	401	-	4,4,4	0.21	0	6,6,6	0.28	0
3	A1IVT	C	403	-	14,15,15	1.78	3 (21%)	16,21,21	1.63	2 (12%)
3	A1IVT	C	402	-	14,15,15	2.17	3 (21%)	16,21,21	1.88	3 (18%)
4	DMS	C	412	-	3,3,3	0.76	0	3,3,3	0.75	0
4	DMS	C	410	-	3,3,3	0.70	0	3,3,3	0.68	0
3	A1IVT	B	403	-	14,15,15	1.66	3 (21%)	16,21,21	1.96	5 (31%)
2	SO4	C	408	-	4,4,4	0.25	0	6,6,6	0.55	0
2	SO4	B	402	-	4,4,4	0.22	0	6,6,6	0.31	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	A1IVT	B	403	-	-	0/4/4/4	0/2/2/2
3	A1IVT	C	403	-	-	0/4/4/4	0/2/2/2
3	A1IVT	C	402	-	-	0/4/4/4	0/2/2/2
3	A1IVT	B	404	-	-	0/4/4/4	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	A1IVT	C04-C02	5.21	1.62	1.51
3	C	403	A1IVT	C04-C02	4.38	1.60	1.51
3	C	402	A1IVT	C06-N07	3.61	1.44	1.36
3	B	404	A1IVT	C04-C05	-3.49	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	A1IVT	C13-C08	-3.29	1.36	1.41
3	C	402	A1IVT	C12-CL14	3.06	1.81	1.74
3	B	403	A1IVT	C06-N07	2.80	1.42	1.36
3	B	403	A1IVT	C04-C02	2.72	1.56	1.51
3	C	403	A1IVT	C12-CL14	2.50	1.79	1.74
3	C	403	A1IVT	C06-N07	2.48	1.41	1.36
3	B	404	A1IVT	C06-N07	2.29	1.41	1.36
3	B	403	A1IVT	C12-CL14	2.01	1.78	1.74

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	A1IVT	C12-C13-C08	-5.83	114.58	119.50
3	B	403	A1IVT	C12-C13-C08	-5.75	114.65	119.50
3	B	404	A1IVT	C12-C13-C08	-4.91	115.36	119.50
3	C	403	A1IVT	C12-C13-C08	-4.59	115.62	119.50
3	B	404	A1IVT	C13-C12-CL14	-4.19	114.40	119.64
3	B	404	A1IVT	C11-C12-C13	2.96	125.49	121.99
3	B	403	A1IVT	C13-C12-CL14	-2.72	116.23	119.64
3	B	403	A1IVT	C11-C12-C13	2.39	124.82	121.99
3	C	402	A1IVT	O01-C02-C04	-2.39	116.23	123.04
3	B	404	A1IVT	O01-C02-C04	-2.31	116.44	123.04
3	C	403	A1IVT	O01-C02-C04	-2.23	116.69	123.04
3	C	402	A1IVT	C13-C08-C09	2.15	123.92	121.16
3	B	403	A1IVT	C13-C08-C09	2.13	123.90	121.16
3	B	404	A1IVT	O03-C02-O01	2.08	128.48	123.30
3	B	403	A1IVT	C04-C05-C09	2.02	130.47	126.50

There are no chirality outliers.

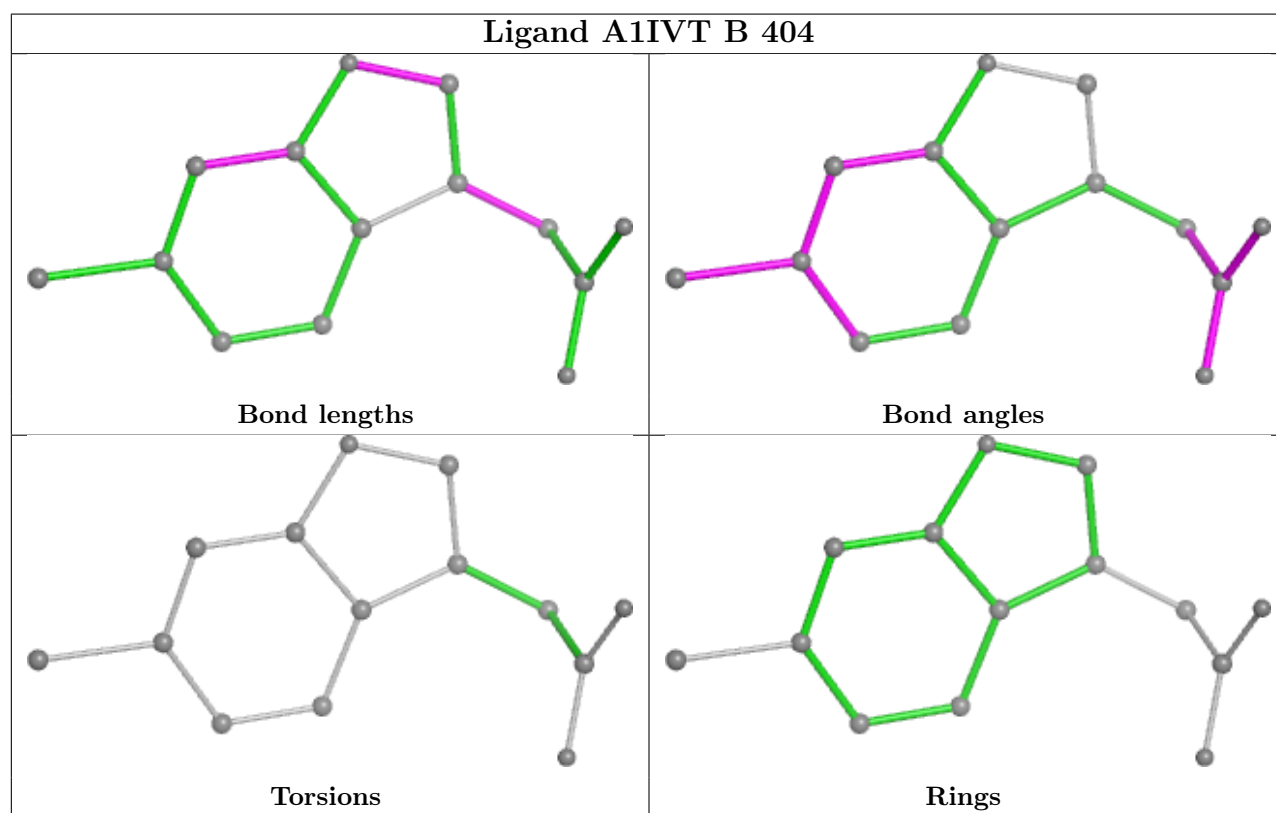
There are no torsion outliers.

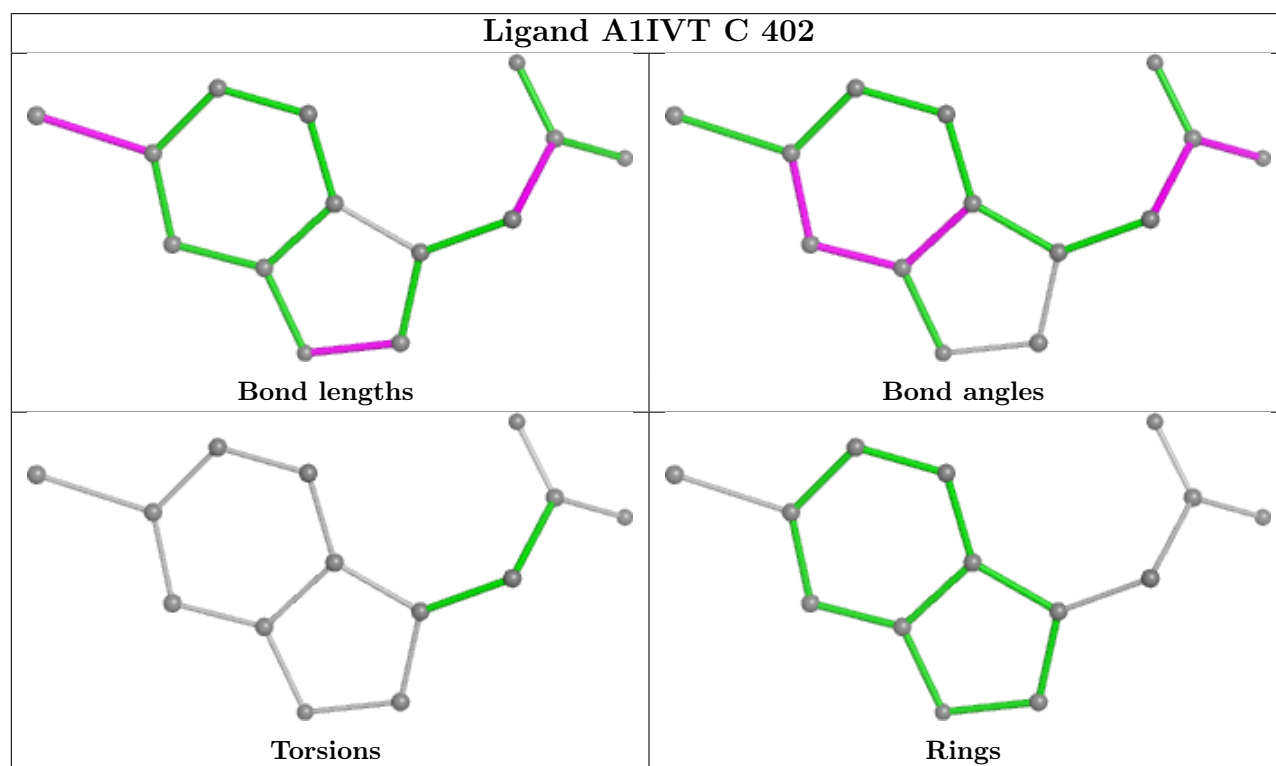
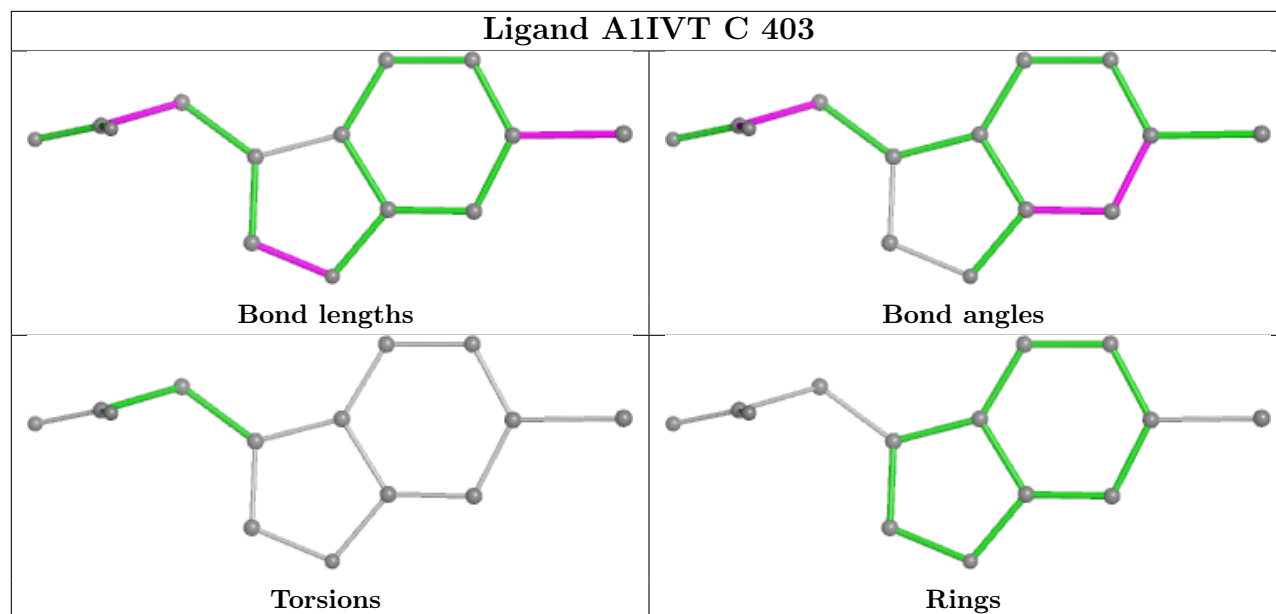
There are no ring outliers.

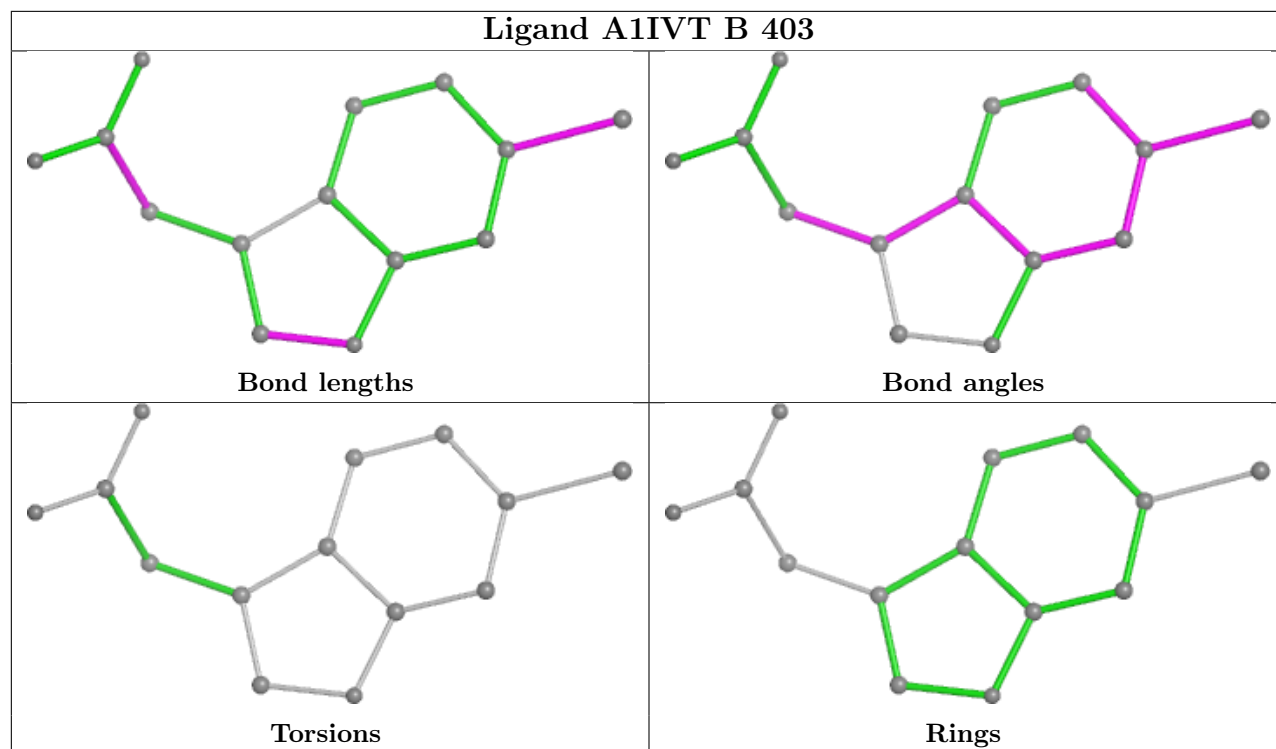
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	411	DMS	1	0
2	C	409	SO4	3	0
2	C	404	SO4	1	0
3	C	403	A1IVT	1	0
3	C	402	A1IVT	3	0
3	B	403	A1IVT	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	B	331/359 (92%)	1.44	81 (24%)	2 2	42, 69, 115, 167	3 (0%)
1	C	331/359 (92%)	1.46	86 (25%)	2 2	45, 68, 108, 156	2 (0%)
All	All	662/718 (92%)	1.45	167 (25%)	2 2	42, 69, 113, 167	5 (0%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	116	VAL	5.5
1	B	105	VAL	5.4
1	C	266	ASP	5.2
1	C	103	ASP	5.2
1	B	266	ASP	5.1
1	C	118	ASN	4.6
1	B	125	TYR	4.3
1	B	119	THR	4.2
1	B	34	GLY	4.2
1	C	125	TYR	4.1
1	B	116	VAL	4.1
1	C	126	GLN	4.1
1	C	121	PHE	4.1
1	C	105	VAL	4.1
1	B	124	LEU	4.0
1	C	127	THR	3.9
1	C	50	TYR	3.9
1	C	332	ALA	3.8
1	C	231	PRO	3.8
1	C	128	LEU	3.7
1	B	249	LEU	3.7
1	C	124	LEU	3.7
1	B	101	VAL	3.6
1	B	171	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	64	LYS	3.5
1	B	48	GLY	3.5
1	C	326	THR	3.4
1	B	47	ARG	3.4
1	B	117	ASN	3.4
1	C	270	ASN	3.4
1	C	108	THR	3.3
1	C	49	LYS	3.3
1	B	283[A]	ARG	3.3
1	C	170	LYS	3.3
1	B	193	ALA	3.3
1	B	126	GLN	3.3
1	B	65	VAL	3.2
1	C	285	VAL	3.2
1	B	8	ARG	3.2
1	B	66	VAL	3.2
1	C	135	PHE	3.2
1	C	311	SER	3.2
1	C	106	SER	3.2
1	B	267	PRO	3.1
1	B	272	ILE	3.1
1	C	253	ASP	3.1
1	C	26	TYR	3.1
1	C	164	ILE	3.1
1	B	332	ALA	3.1
1	B	56	ALA	3.1
1	B	49	LYS	3.1
1	B	2	SER	3.0
1	B	311	SER	3.0
1	B	63	GLU	3.0
1	C	67	VAL	3.0
1	B	50	TYR	3.0
1	C	117	ASN	3.0
1	C	163	MET	3.0
1	C	64	LYS	3.0
1	B	192	VAL	3.0
1	B	59	ILE	2.9
1	C	269	PHE	2.9
1	B	222	LEU	2.9
1	B	127	THR	2.9
1	B	265	LEU	2.8
1	B	53	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	114[A]	GLU	2.8
1	C	318	ALA	2.8
1	B	237	ASP	2.8
1	C	139	GLU	2.8
1	B	204	VAL	2.8
1	C	47[A]	ARG	2.8
1	C	112	VAL	2.8
1	B	121	PHE	2.7
1	C	268	ARG	2.7
1	B	253	ASP	2.7
1	C	3	GLY	2.7
1	C	119	THR	2.7
1	C	56	ALA	2.7
1	C	59	ILE	2.7
1	C	225	MET	2.7
1	B	291	HIS	2.7
1	B	70	LEU	2.6
1	B	254	LEU	2.6
1	B	118	ASN	2.6
1	B	270	ASN	2.6
1	B	33	TRP	2.6
1	B	41	LEU	2.6
1	C	33	TRP	2.6
1	C	69	ILE	2.6
1	C	238	ASN	2.6
1	C	226	ILE	2.5
1	B	226	ILE	2.5
1	B	292	LEU	2.5
1	C	122	LYS	2.5
1	B	231	PRO	2.5
1	B	57	ILE	2.5
1	B	54	PHE	2.5
1	C	262	ASN	2.5
1	B	285	VAL	2.4
1	C	2	SER	2.4
1	C	60	THR	2.4
1	B	100	ILE	2.4
1	C	160	HIS	2.4
1	B	220	CYS	2.4
1	B	310	GLN	2.4
1	C	102	LYS	2.4
1	B	26	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	35	ASN	2.4
1	C	171	LEU	2.4
1	C	53	VAL	2.3
1	C	192	VAL	2.3
1	C	4	PRO	2.3
1	C	32	GLU	2.3
1	C	123	GLN	2.3
1	C	133	ILE	2.3
1	C	39	TYR	2.3
1	C	131	TYR	2.3
1	B	284	PHE	2.3
1	C	8	ARG	2.3
1	B	191	ARG	2.3
1	B	84	ILE	2.3
1	B	194	SER	2.3
1	C	264	GLU	2.2
1	B	243	VAL	2.2
1	C	31	VAL	2.2
1	C	243	VAL	2.2
1	B	135	PHE	2.2
1	B	104	PRO	2.2
1	B	278	ARG	2.2
1	C	244	ARG	2.2
1	B	281	TRP	2.2
1	C	167	GLU	2.2
1	C	115	HIS	2.2
1	C	37	ASP	2.2
1	B	95	ILE	2.2
1	C	281	TRP	2.2
1	B	236	HIS	2.2
1	B	28	SER	2.1
1	B	69	ILE	2.1
1	C	46	GLY	2.1
1	C	45	LEU	2.1
1	B	108	THR	2.1
1	C	196	TYR	2.1
1	C	307	TYR	2.1
1	C	204	VAL	2.1
1	C	194	SER	2.1
1	B	35	ASN	2.1
1	C	298	LEU	2.1
1	C	66	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	76	LYS	2.1
1	B	111	LEU	2.1
1	C	297	ALA	2.1
1	B	131	TYR	2.1
1	C	73	VAL	2.1
1	C	237	ASP	2.1
1	C	48	GLY	2.1
1	B	273	LEU	2.1
1	C	267	PRO	2.1
1	B	55	GLU	2.0
1	B	31	VAL	2.0
1	C	182	TYR	2.0
1	B	102	LYS	2.0
1	C	327	VAL	2.0
1	B	39	TYR	2.0
1	B	37	ASP	2.0
1	B	258	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	408	5/5	0.54	0.27	74,78,82,87	5
2	SO4	B	406	5/5	0.59	0.17	93,94,96,102	5
2	SO4	B	407	5/5	0.70	0.15	84,87,91,96	0
2	SO4	C	405	5/5	0.70	0.17	82,86,89,95	5
4	DMS	B	410	4/4	0.70	0.18	70,84,100,100	0
2	SO4	B	405	5/5	0.71	0.13	98,99,109,112	0

*Continued on next page...*

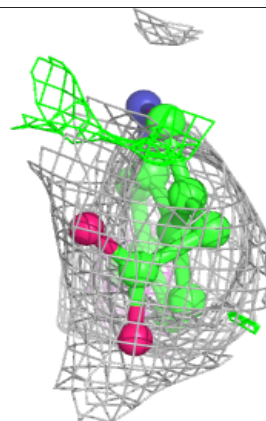
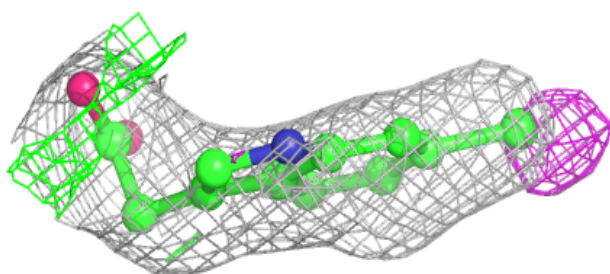
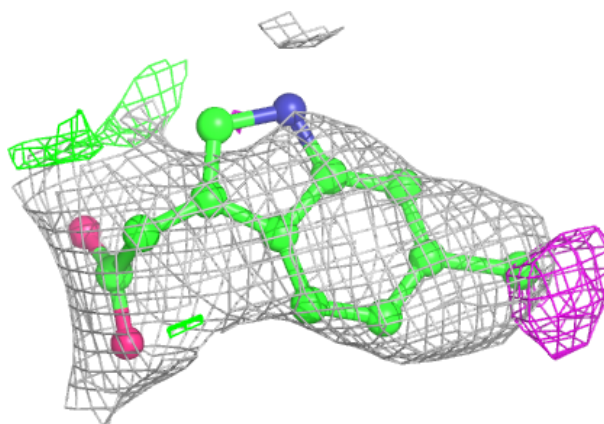
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	404	5/5	0.71	0.15	105,106,109,116	0
2	SO4	C	409	5/5	0.75	0.17	71,74,80,81	5
2	SO4	C	406	5/5	0.75	0.10	108,115,120,121	0
3	A1IVT	B	404	14/14	0.79	0.17	83,86,87,89	0
3	A1IVT	C	402	14/14	0.81	0.19	63,71,81,107	0
2	SO4	C	408	5/5	0.81	0.14	79,79,85,91	0
4	DMS	C	411	4/4	0.81	0.16	76,92,94,96	0
3	A1IVT	B	403	14/14	0.82	0.19	64,71,83,97	0
3	A1IVT	C	403	14/14	0.83	0.16	77,82,85,89	0
4	DMS	C	412	4/4	0.85	0.21	77,93,100,100	0
2	SO4	B	409	5/5	0.86	0.17	65,67,68,73	5
4	DMS	C	410	4/4	0.87	0.20	70,84,93,93	0
2	SO4	B	401	5/5	0.88	0.13	73,75,80,81	5
2	SO4	B	402	5/5	0.91	0.10	72,72,77,79	0
2	SO4	C	401	5/5	0.92	0.09	70,73,73,73	0
2	SO4	C	407	5/5	0.93	0.09	77,81,86,87	0

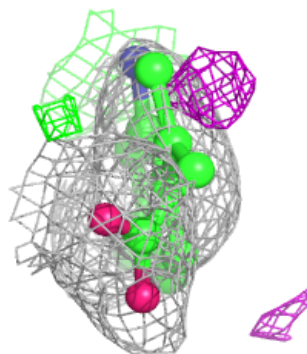
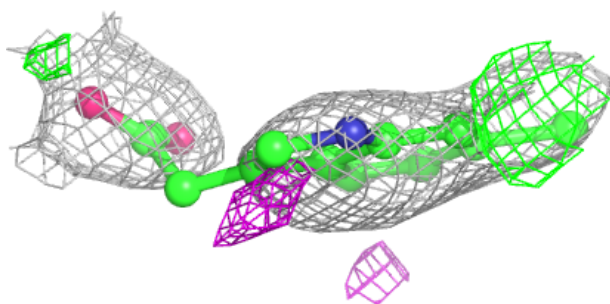
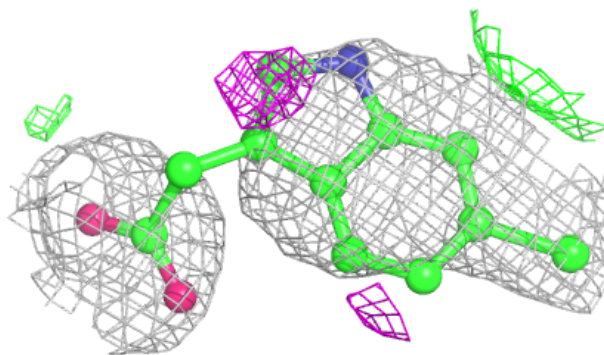
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A1IVT B 404:**

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

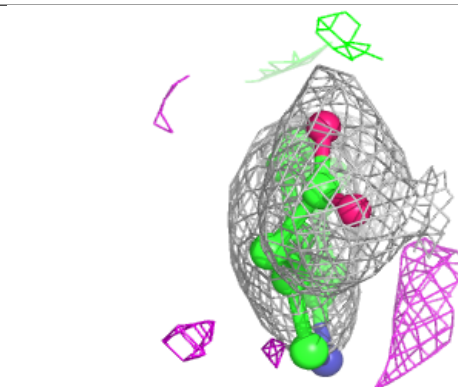
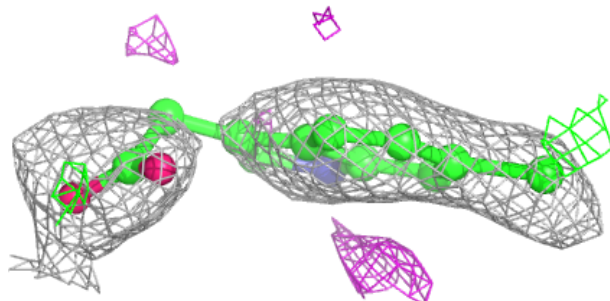
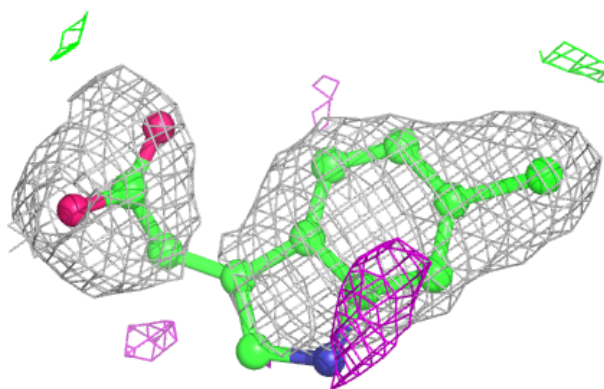
**Electron density around A1IVT C 402:**

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

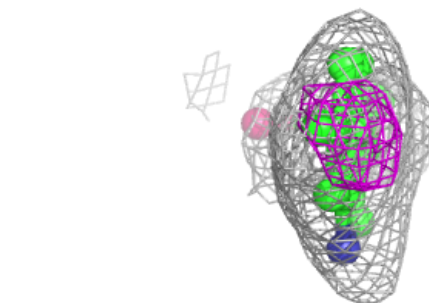
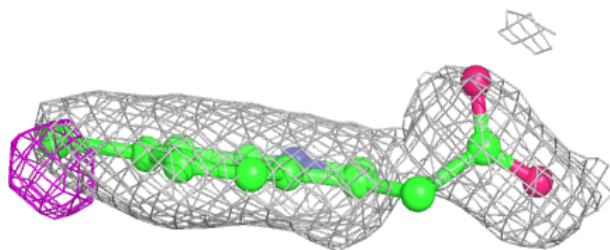
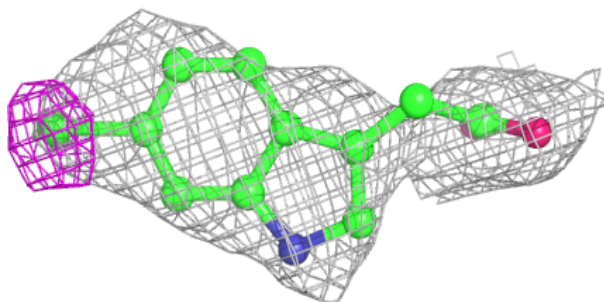


**Electron density around A1IVT B 403:**

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

**Electron density around A1IVT C 403:**

$2mF_o - DF_c$  (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.