



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2025 – 04:11 PM EDT

PDB ID : 9OIM / pdb\_00009oim  
Title : The von Hippel Lindau-ElonginB-ElonginC (VCB) complex with fragment 9  
Authors : Amporndanai, K.; Katinas, J.M.; Chopra, A.; Fesik, S.W.  
Deposited on : 2025-05-06  
Resolution : 2.61 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 : 2022.3.0, CSD as543be (2022)  
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

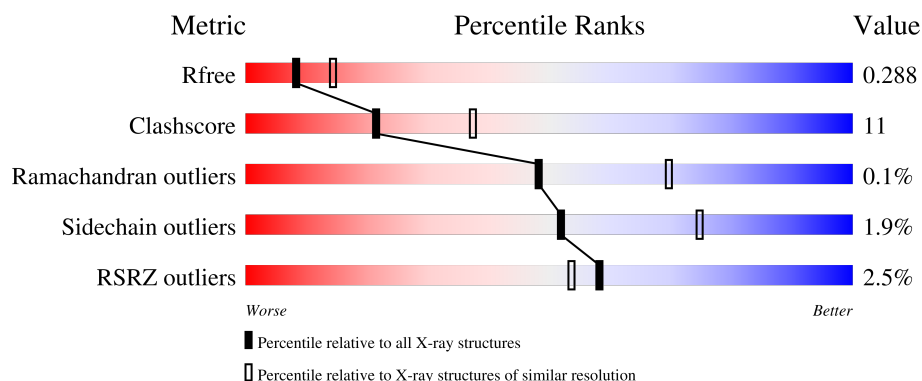
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (2.64-2.60)

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	A	104	<div> <div>2%</div> <div>67%</div> <div>32%</div> <div>.</div> </div>
1	D	104	<div> <div>3%</div> <div>69%</div> <div>26%</div> <div>..</div> </div>
1	J	104	<div> <div>2%</div> <div>73%</div> <div>25%</div> <div>..</div> </div>
2	B	98	<div> <div>2%</div> <div>66%</div> <div>21%</div> <div>12%</div> </div>
2	E	98	<div> <div>5%</div> <div>63%</div> <div>24%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	98	<div><div><div></div><div></div><div></div></div><div>4%76%14%10%</div></div>
2	K	98	<div><div><div></div><div></div><div></div></div><div>3%65%24%10%</div></div>
3	C	180	<div><div><div></div><div></div><div></div></div><div>%59%18%•22%</div></div>
3	F	180	<div><div><div></div><div></div><div></div></div><div>%61%19%•20%</div></div>
3	I	180	<div><div><div></div><div></div><div></div></div><div>2%62%17%21%</div></div>
3	L	180	<div><div><div></div><div></div><div></div></div><div>%59%19%••21%</div></div>
4	G	104	<div><div><div></div><div></div><div></div></div><div>2%73%26%•</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10365 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 Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	103	Total	As	C	N	O	S	0	0	0
			794	1	507	133	148	5			
1	D	100	Total	As	C	N	O	S	0	0	0
			746	1	479	122	140	4			
1	J	103	Total	As	C	N	O	S	0	0	0
			800	1	508	132	154	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			679	439	108	126	6			
2	E	87	Total	C	N	O	S	0	0	0
			676	439	109	123	5			
2	H	88	Total	C	N	O	S	0	0	0
			679	441	108	124	6			
2	K	88	Total	C	N	O	S	0	0	0
			676	439	107	125	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	MET	-	initiating methionine	UNP Q15369
B	16	GLY	-	expression tag	UNP Q15369
E	15	MET	-	initiating methionine	UNP Q15369
E	16	GLY	-	expression tag	UNP Q15369
H	15	MET	-	initiating methionine	UNP Q15369
H	16	GLY	-	expression tag	UNP Q15369
K	15	MET	-	initiating methionine	UNP Q15369
K	16	GLY	-	expression tag	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	141	Total	As	C	N	O	S	0	0	0
			1091	1	697	191	200	2			
3	F	144	Total	As	C	N	O	S	0	0	0
			1124	1	720	201	200	2			
3	I	143	Total	As	C	N	O	S	0	0	0
			1113	1	712	198	200	2			
3	L	143	Total	As	C	N	O	S	0	0	0
			1132	1	722	205	202	2			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	34	MET	-	expression tag	UNP P40337
C	35	GLY	-	expression tag	UNP P40337
C	36	SER	-	expression tag	UNP P40337
C	37	SER	-	expression tag	UNP P40337
C	38	HIS	-	expression tag	UNP P40337
C	39	HIS	-	expression tag	UNP P40337
C	40	HIS	-	expression tag	UNP P40337
C	41	HIS	-	expression tag	UNP P40337
C	42	HIS	-	expression tag	UNP P40337
C	43	HIS	-	expression tag	UNP P40337
C	44	SER	-	expression tag	UNP P40337
C	45	SER	-	expression tag	UNP P40337
C	46	GLY	-	expression tag	UNP P40337
C	47	LEU	-	expression tag	UNP P40337
C	48	VAL	-	expression tag	UNP P40337
C	49	PRO	-	expression tag	UNP P40337
C	50	ARG	-	expression tag	UNP P40337
C	51	GLY	-	expression tag	UNP P40337
C	52	SER	-	expression tag	UNP P40337
C	53	HIS	-	expression tag	UNP P40337
F	34	MET	-	expression tag	UNP P40337
F	35	GLY	-	expression tag	UNP P40337
F	36	SER	-	expression tag	UNP P40337
F	37	SER	-	expression tag	UNP P40337
F	38	HIS	-	expression tag	UNP P40337
F	39	HIS	-	expression tag	UNP P40337
F	40	HIS	-	expression tag	UNP P40337
F	41	HIS	-	expression tag	UNP P40337
F	42	HIS	-	expression tag	UNP P40337
F	43	HIS	-	expression tag	UNP P40337
F	44	SER	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
F	45	SER	-	expression tag	UNP P40337
F	46	GLY	-	expression tag	UNP P40337
F	47	LEU	-	expression tag	UNP P40337
F	48	VAL	-	expression tag	UNP P40337
F	49	PRO	-	expression tag	UNP P40337
F	50	ARG	-	expression tag	UNP P40337
F	51	GLY	-	expression tag	UNP P40337
F	52	SER	-	expression tag	UNP P40337
F	53	HIS	-	expression tag	UNP P40337
I	34	MET	-	expression tag	UNP P40337
I	35	GLY	-	expression tag	UNP P40337
I	36	SER	-	expression tag	UNP P40337
I	37	SER	-	expression tag	UNP P40337
I	38	HIS	-	expression tag	UNP P40337
I	39	HIS	-	expression tag	UNP P40337
I	40	HIS	-	expression tag	UNP P40337
I	41	HIS	-	expression tag	UNP P40337
I	42	HIS	-	expression tag	UNP P40337
I	43	HIS	-	expression tag	UNP P40337
I	44	SER	-	expression tag	UNP P40337
I	45	SER	-	expression tag	UNP P40337
I	46	GLY	-	expression tag	UNP P40337
I	47	LEU	-	expression tag	UNP P40337
I	48	VAL	-	expression tag	UNP P40337
I	49	PRO	-	expression tag	UNP P40337
I	50	ARG	-	expression tag	UNP P40337
I	51	GLY	-	expression tag	UNP P40337
I	52	SER	-	expression tag	UNP P40337
I	53	HIS	-	expression tag	UNP P40337
L	34	MET	-	expression tag	UNP P40337
L	35	GLY	-	expression tag	UNP P40337
L	36	SER	-	expression tag	UNP P40337
L	37	SER	-	expression tag	UNP P40337
L	38	HIS	-	expression tag	UNP P40337
L	39	HIS	-	expression tag	UNP P40337
L	40	HIS	-	expression tag	UNP P40337
L	41	HIS	-	expression tag	UNP P40337
L	42	HIS	-	expression tag	UNP P40337
L	43	HIS	-	expression tag	UNP P40337
L	44	SER	-	expression tag	UNP P40337
L	45	SER	-	expression tag	UNP P40337
L	46	GLY	-	expression tag	UNP P40337

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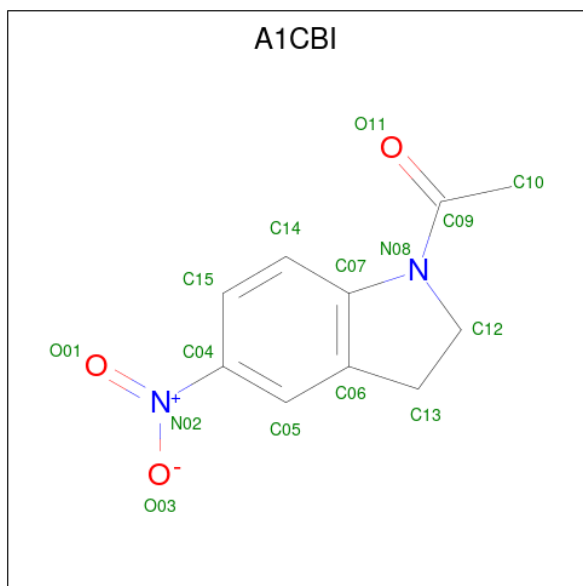
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Chain	Residue	Modelled	Actual	Comment	Reference
L	47	LEU	-	expression tag	UNP P40337
L	48	VAL	-	expression tag	UNP P40337
L	49	PRO	-	expression tag	UNP P40337
L	50	ARG	-	expression tag	UNP P40337
L	51	GLY	-	expression tag	UNP P40337
L	52	SER	-	expression tag	UNP P40337
L	53	HIS	-	expression tag	UNP P40337

- Molecule 4 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	G	103	Total	As	C	N	O	S	0	0	0
			788	2	503	131	148	4			

- Molecule 5 is 1-[5-[oxidanyl(oxidanylidene)- $\text{N}^{\{4\}}$ -azanyl]-2,3-dihydroindol-1-yl]ethanone (CCD ID: A1CBI) (formula:  $\text{C}_{10}\text{H}_{10}\text{N}_2\text{O}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			15	10	2	3		
5	E	1	Total	C	N	O	0	0
			15	10	2	3		
5	H	1	Total	C	N	O	0	0
			15	10	2	3		
5	K	1	Total	C	N	O	0	0
			15	10	2	3		

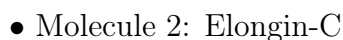
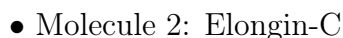
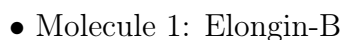
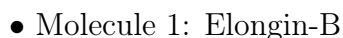
- Molecule 6 is water.

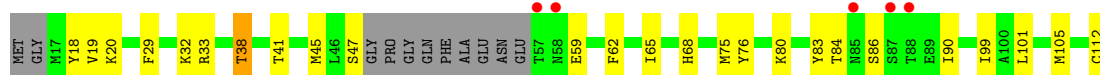
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	O 1	0	0
6	C	1	Total 1	O 1	0	0
6	I	1	Total 1	O 1	0	0
6	K	1	Total 1	O 1	0	0
6	L	3	Total 3	O 3	0	0



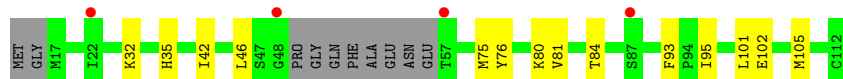
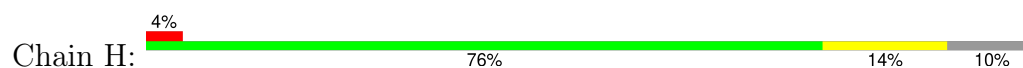


- Molecule 1: Elongin-B

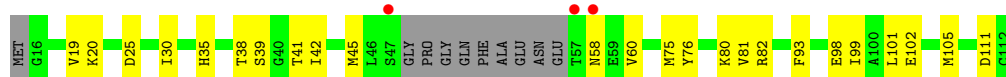




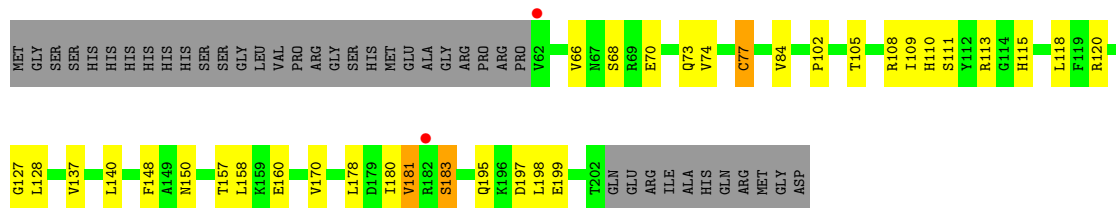
• Molecule 2: Elongin-C



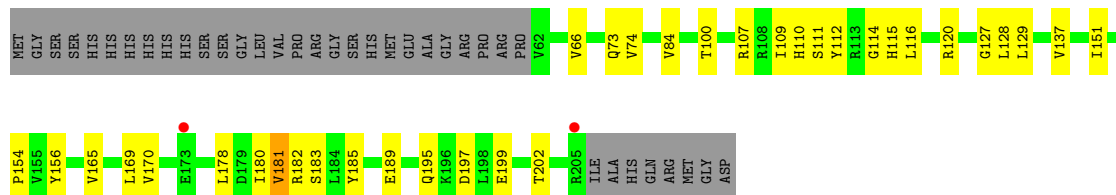
• Molecule 2: Elongin-C



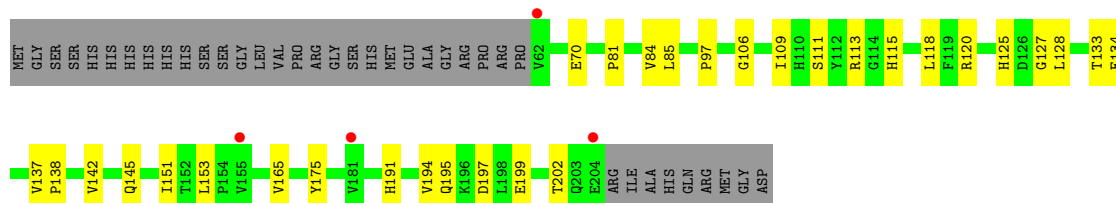
• Molecule 3: von Hippel-Lindau disease tumor suppressor



• Molecule 3: von Hippel-Lindau disease tumor suppressor



• Molecule 3: von Hippel-Lindau disease tumor suppressor



- Chain L:  59% 19% 21%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.39Å 93.39Å 362.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.61 48.83 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.4 (48.83-2.61) 94.4 (48.83-2.61)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.225 , 0.283 0.229 , 0.288	Depositor DCC
$R_{free}$ test set	2461 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.5	Xtrriage
Anisotropy	0.305	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 27.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8607e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: A1CBI, CAS

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	0.45	0/800	0.68	0/1082
1	D	0.37	0/751	0.56	0/1019
1	J	0.48	0/806	0.69	0/1091
2	B	0.49	0/693	0.66	0/936
2	E	0.42	0/690	0.63	0/932
2	H	0.39	0/693	0.61	0/936
2	K	0.43	0/690	0.64	0/933
3	C	0.45	0/1110	0.69	0/1524
3	F	0.42	0/1144	0.63	0/1568
3	I	0.42	0/1132	0.66	0/1551
3	L	0.50	0/1151	0.69	1/1574 (0.1%)
4	G	0.40	0/784	0.59	0/1062
All	All	0.44	0/10444	0.65	1/14208 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	113	ARG	CG-CD-NE	5.06	123.14	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	77	CAS	Mainchain

## 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	794	0	786	21	0
1	D	746	0	715	24	0
1	J	800	0	783	19	0
2	B	679	0	670	15	0
2	E	676	0	663	22	0
2	H	679	0	663	9	0
2	K	676	0	660	21	0
3	C	1091	0	1034	24	0
3	F	1124	0	1081	23	0
3	I	1113	0	1074	19	1
3	L	1132	0	1103	23	1
4	G	788	0	760	18	0
5	B	15	0	0	1	1
5	E	15	0	0	1	1
5	H	15	0	0	0	0
5	K	15	0	0	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
6	L	3	0	0	0	0
All	All	10365	0	9992	217	2

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 11.

All (217) 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)
3:C:157:THR:OG1	3:C:160:GLU:HG3	1.75	0.86
4:G:23:THR:HG22	4:G:26:GLU:HG3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HD3	1:A:50:LEU:HD11	1.61	0.82
2:H:102:GLU:HA	2:H:105:MET:HE2	1.64	0.79
2:B:19:VAL:HG13	2:B:33:ARG:HG2	1.64	0.78
3:C:157:THR:HG1	3:C:160:GLU:HG3	1.51	0.76
2:K:38:THR:HG23	2:K:80:LYS:HD3	1.70	0.73
3:C:77:CAS:SG	3:C:148:PHE:HE1	2.13	0.71
2:B:105:MET:SD	3:C:180:ILE:HG22	2.31	0.71
3:F:170:VAL:HG21	3:F:178:LEU:HD21	1.73	0.71
3:C:108:ARG:NH2	2:K:41:THR:OG1	2.23	0.71
2:E:86:SER:HB3	2:E:90:ILE:HD11	1.71	0.70
3:L:90:ASN:OD1	3:L:94:GLU:HB3	1.92	0.70
2:B:68:HIS:HD2	2:B:99:ILE:HG22	1.56	0.70
3:L:113:ARG:HH11	3:L:113:ARG:HG2	1.57	0.70
2:E:83:TYR:HB3	2:E:90:ILE:HG13	1.75	0.69
1:A:41:GLU:OE2	1:A:80:ARG:NH2	2.26	0.68
2:E:101:LEU:HD11	3:F:178:LEU:HD23	1.74	0.68
1:J:99:LEU:HD22	1:J:103:MET:HB2	1.73	0.68
4:G:23:THR:N	4:G:26:GLU:OE1	2.25	0.68
1:J:9:ARG:HB2	1:J:77:LEU:HB3	1.75	0.67
3:I:115:HIS:O	3:I:138:PRO:HD2	1.95	0.67
1:D:23:THR:HG22	1:D:26:GLU:HG3	1.75	0.66
2:B:105:MET:HE3	5:B:201:A1CBI:C15	2.26	0.66
2:E:41:THR:O	2:E:45:MET:HG3	1.97	0.65
2:E:68:HIS:HD2	2:E:99:ILE:HG22	1.63	0.64
3:F:120:ARG:NH2	3:F:197:ASP:OD2	2.30	0.64
3:I:133:THR:HG22	3:I:134:GLU:H	1.61	0.63
3:F:165:VAL:O	3:F:169:LEU:HD23	2.00	0.62
2:B:17:MET:HE2	2:B:33:ARG:HD3	1.82	0.62
1:J:80:ARG:HA	1:J:85:PHE:HA	1.81	0.61
2:E:105:MET:HE3	5:E:201:A1CBI:C15	2.31	0.61
3:L:112:TYR:O	3:L:138:PRO:HG2	2.00	0.61
3:C:181:VAL:HG23	3:C:183:SER:H	1.64	0.61
3:I:85:LEU:HD11	3:I:97:PRO:HB3	1.83	0.61
1:J:34:ILE:HG21	2:K:30:ILE:HG21	1.82	0.61
1:J:8:ARG:HG3	1:J:74:THR:HG23	1.83	0.60
3:I:84:VAL:HG22	3:I:128:LEU:HD13	1.83	0.60
3:F:195:GLN:O	3:F:199:GLU:HG3	2.03	0.59
1:J:71:ALA:HA	2:K:75:MET:HE3	1.83	0.59
1:A:9:ARG:HB2	1:A:77:LEU:HB3	1.85	0.58
3:L:195:GLN:O	3:L:199:GLU:HG3	2.03	0.58
3:I:120:ARG:HD3	3:I:127:GLY:HA2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:120:ARG:HD3	3:F:127:GLY:HA2	1.85	0.58
3:I:175:TYR:OH	3:I:191:HIS:NE2	2.28	0.58
2:E:105:MET:SD	3:F:180:ILE:HG22	2.44	0.58
2:H:35:HIS:CE1	2:H:81:VAL:HG11	2.39	0.58
1:D:8:ARG:HG2	1:D:13:THR:HG23	1.85	0.57
3:C:120:ARG:HD3	3:C:127:GLY:HA2	1.85	0.57
2:E:47:SER:O	2:E:47:SER:OG	2.17	0.57
2:K:102:GLU:HA	2:K:105:MET:HE2	1.86	0.57
2:B:41:THR:O	2:B:45:MET:HG3	2.05	0.57
3:I:195:GLN:O	3:I:199:GLU:HG3	2.05	0.56
1:J:19:LYS:O	1:J:22:SER:HB3	2.05	0.56
2:H:80:LYS:NZ	2:H:84:THR:OG1	2.30	0.56
1:A:80:ARG:HA	1:A:85:PHE:HA	1.88	0.56
1:A:62:PHE:CZ	1:A:75:VAL:HG22	2.40	0.56
2:E:19:VAL:HG13	2:E:33:ARG:HG2	1.89	0.55
4:G:4:PHE:CE1	4:G:69:PRO:HG3	2.42	0.54
3:F:73:GLN:OE1	3:F:110:HIS:ND1	2.41	0.54
1:A:7:ILE:HD11	1:A:27:LEU:HD21	1.90	0.54
2:B:19:VAL:CG1	2:B:33:ARG:HG2	2.36	0.54
3:C:120:ARG:NH2	3:C:197:ASP:OD2	2.41	0.54
3:C:195:GLN:O	3:C:199:GLU:HG3	2.08	0.53
2:K:38:THR:CG2	2:K:80:LYS:HD3	2.36	0.53
4:G:72:PRO:HD2	2:H:75:MET:HE2	1.91	0.53
2:K:20:LYS:HE2	2:K:30:ILE:HD11	1.90	0.53
3:L:89:LEU:HD12	3:L:116:LEU:HD23	1.91	0.53
1:A:8:ARG:HG3	1:A:74:THR:HG23	1.90	0.53
3:I:84:VAL:HG22	3:I:128:LEU:CD1	2.39	0.53
1:J:46:LYS:O	1:J:49:GLN:HB2	2.09	0.53
1:A:29:ARG:NH1	1:A:32:GLU:OE1	2.39	0.52
1:A:51:LEU:HD22	1:A:60:CYS:SG	2.50	0.52
3:C:73:GLN:OE1	3:C:110:HIS:ND1	2.43	0.52
1:D:28:LYS:HE3	1:D:53:ASP:OD1	2.10	0.52
3:L:84:VAL:HG22	3:L:128:LEU:HD13	1.92	0.51
2:K:45:MET:HE3	2:K:60:VAL:HG11	1.92	0.51
3:F:84:VAL:HG21	3:F:151:ILE:HG21	1.92	0.51
1:D:46:LYS:HZ1	1:D:61:GLY:HA3	1.76	0.51
2:H:95:ILE:HB	3:I:165:VAL:HG21	1.92	0.50
1:D:46:LYS:NZ	1:D:60:CYS:O	2.44	0.50
1:D:79:PHE:H	1:D:86:GLU:CD	2.19	0.50
3:F:66:VAL:HG22	3:F:114:GLY:HA3	1.91	0.50
3:F:185:TYR:O	3:F:189:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LEU:HD22	1:D:60:CYS:SG	2.52	0.50
1:D:28:LYS:HB3	1:D:39:PRO:HB3	1.94	0.49
3:L:84:VAL:HG21	3:L:151:ILE:HG21	1.93	0.49
1:A:86:GLU:HG3	1:A:87:ALA:O	2.12	0.49
3:L:115:HIS:O	3:L:138:PRO:HD2	2.11	0.49
4:G:23:THR:HG22	4:G:26:GLU:CG	2.39	0.49
3:I:120:ARG:NH2	3:I:197:ASP:OD2	2.45	0.49
2:H:76:TYR:HA	2:H:93:PHE:CE1	2.47	0.49
1:J:72:PRO:HD2	2:K:75:MET:HE3	1.94	0.49
3:L:113:ARG:HH11	3:L:113:ARG:CG	2.25	0.49
4:G:9:ARG:HB2	4:G:77:LEU:HB3	1.93	0.49
2:E:83:TYR:HB3	2:E:90:ILE:CG1	2.42	0.49
2:K:105:MET:HE3	5:K:201:A1CBI:C15	2.43	0.49
1:D:23:THR:HG23	1:D:26:GLU:H	1.77	0.49
1:D:23:THR:CG2	1:D:26:GLU:HG3	2.41	0.48
3:F:154:PRO:HD2	3:F:156:TYR:CZ	2.48	0.48
1:A:80:ARG:HH11	1:A:83:ASP:H	1.61	0.48
2:H:42:ILE:O	2:H:46:LEU:HG	2.13	0.48
1:A:7:ILE:HB	1:A:14:ILE:HB	1.95	0.48
3:I:118:LEU:HD11	3:I:194:VAL:HG13	1.95	0.48
2:B:46:LEU:HD22	2:B:58:ASN:HB3	1.96	0.48
3:C:102:PRO:HD2	3:C:105:THR:OG1	2.13	0.48
4:G:27:LEU:HD22	4:G:57:LEU:HD21	1.97	0.47
3:F:74:VAL:HB	3:F:109:ILE:HD11	1.96	0.47
3:C:109:ILE:CD1	3:C:111:SER:HB2	2.44	0.47
1:A:37:ARG:NH2	1:A:80:ARG:O	2.47	0.47
2:E:19:VAL:CG1	2:E:33:ARG:HG2	2.44	0.47
2:K:25:ASP:OD1	2:K:25:ASP:N	2.40	0.47
3:L:84:VAL:HG22	3:L:128:LEU:CD1	2.45	0.47
1:A:19:LYS:O	1:A:22:SER:HB3	2.14	0.47
3:C:115:HIS:O	3:C:137:VAL:HA	2.15	0.47
4:G:101:ASP:OD2	4:G:101:ASP:N	2.48	0.47
1:J:8:ARG:HD2	1:J:13:THR:OG1	2.15	0.47
1:D:28:LYS:NZ	1:D:42:GLN:O	2.48	0.47
2:B:72:LYS:NZ	2:B:94:PRO:O	2.37	0.46
2:B:98:GLU:H	2:B:98:GLU:CD	2.22	0.46
1:D:99:LEU:HD12	1:D:100:PRO:HD2	1.97	0.46
3:L:73:GLN:OE1	3:L:110:HIS:ND1	2.48	0.46
3:L:109:ILE:C	3:L:109:ILE:HD12	2.40	0.46
1:A:30:ILE:O	1:A:34:ILE:HG13	2.15	0.46
3:C:74:VAL:HB	3:C:109:ILE:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:103:MET:HE1	2:K:101:LEU:HG	1.97	0.46
3:F:84:VAL:HG22	3:F:128:LEU:CD1	2.45	0.46
2:K:39:SER:HB3	2:K:42:ILE:HB	1.97	0.46
2:K:76:TYR:HA	2:K:93:PHE:CE1	2.51	0.46
2:K:98:GLU:CD	2:K:98:GLU:H	2.24	0.46
3:L:170:VAL:HG21	3:L:178:LEU:HD21	1.98	0.46
3:I:84:VAL:HG21	3:I:151:ILE:HG21	1.98	0.46
1:A:99:LEU:HD12	1:A:100:PRO:HD2	1.98	0.46
3:I:115:HIS:O	3:I:137:VAL:HA	2.16	0.46
1:A:4:PHE:CE1	1:A:69:PRO:HG3	2.51	0.45
1:A:7:ILE:HD13	1:A:75:VAL:HB	1.98	0.45
2:E:101:LEU:HD23	2:E:101:LEU:HA	1.80	0.45
2:B:101:LEU:HD11	3:C:178:LEU:HD22	1.98	0.45
3:I:120:ARG:HD2	3:I:125:HIS:O	2.16	0.45
2:K:35:HIS:CE1	2:K:81:VAL:HG11	2.52	0.45
1:A:91:GLU:HG3	1:A:92:PRO:HD2	1.99	0.45
3:C:170:VAL:HG21	3:C:178:LEU:HD21	1.97	0.45
3:L:129:LEU:O	3:L:151:ILE:HA	2.16	0.45
2:K:19:VAL:HG12	2:K:58:ASN:HA	1.98	0.45
1:A:43:ARG:HD3	1:A:50:LEU:CD1	2.42	0.45
3:C:84:VAL:HG22	3:C:128:LEU:HD13	1.99	0.45
4:G:8:ARG:HG2	4:G:13:THR:HG23	1.99	0.45
3:C:113:ARG:NH1	3:C:140:LEU:HD13	2.32	0.45
4:G:80:ARG:HA	4:G:85:PHE:HA	1.98	0.45
2:B:20:LYS:HD3	2:B:28:GLU:OE2	2.17	0.44
3:L:139:SER:H	3:L:147:ILE:HD13	1.81	0.44
4:G:7:ILE:HD13	4:G:31:VAL:CG2	2.47	0.44
1:D:42:GLN:HA	1:D:78:ALA:O	2.18	0.44
2:E:76:TYR:CE2	2:E:80:LYS:HD2	2.53	0.44
3:F:181:VAL:HG23	3:F:183:SER:H	1.82	0.44
4:G:80:ARG:HB2	4:G:85:PHE:CE1	2.52	0.44
1:D:15:PHE:HE1	2:E:29:PHE:HD1	1.66	0.44
1:J:4:PHE:HZ	2:K:82:ARG:HD3	1.83	0.44
1:D:29:ARG:HH21	1:D:39:PRO:CG	2.31	0.44
3:C:102:PRO:HB2	3:C:105:THR:HG21	2.00	0.44
3:L:85:LEU:HD11	3:L:97:PRO:HB2	2.00	0.44
2:B:103:LEU:HD11	3:C:158:LEU:HD21	2.00	0.43
2:B:25:ASP:OD1	2:B:25:ASP:N	2.49	0.43
2:B:111:ASP:O	2:B:112:CYS:HB2	2.18	0.43
1:D:29:ARG:HH21	1:D:39:PRO:CD	2.31	0.43
4:G:10:HIS:O	4:G:91:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:THR:HG23	2:E:80:LYS:NZ	2.34	0.43
4:G:30:ILE:O	4:G:34:ILE:HG13	2.18	0.43
3:L:130:VAL:HG21	3:L:136:PHE:HB2	2.01	0.43
3:L:116:LEU:HD12	3:L:137:VAL:HG22	2.00	0.43
1:A:8:ARG:NH2	1:A:91:GLU:O	2.51	0.43
3:F:129:LEU:O	3:F:151:ILE:HA	2.18	0.43
4:G:23:THR:HG23	4:G:25:PHE:H	1.83	0.43
4:G:24:VAL:HG21	4:G:51:LEU:HB3	2.01	0.43
3:C:68:SER:O	3:C:70:GLU:HG3	2.19	0.43
3:C:108:ARG:NE	2:K:111:ASP:HB2	2.34	0.43
1:J:96:PRO:HB3	2:K:99:ILE:HG22	2.01	0.43
3:L:79:ARG:HD2	3:L:150:ASN:OD1	2.19	0.43
3:F:182:ARG:HA	3:F:185:TYR:CD2	2.54	0.43
4:G:103:MET:HE1	2:H:101:LEU:HG	2.01	0.42
1:D:4:PHE:CE1	1:D:69:PRO:HG3	2.54	0.42
2:E:62:PHE:CD2	2:E:65:ILE:HD12	2.54	0.42
1:D:103:MET:HG2	3:F:170:VAL:CG2	2.49	0.42
2:E:20:LYS:HE3	2:E:59:GLU:OE2	2.20	0.42
2:E:18:TYR:CE2	2:E:32:LYS:HG2	2.54	0.42
1:J:45:TYR:HA	1:J:49:GLN:O	2.19	0.42
3:I:109:ILE:C	3:I:109:ILE:HD12	2.45	0.42
1:J:8:ARG:HA	1:J:12:THR:O	2.20	0.42
3:C:77:CAS:SG	3:C:148:PHE:CE1	3.04	0.42
1:J:7:ILE:O	1:J:13:THR:HA	2.20	0.42
1:D:29:ARG:HH21	1:D:39:PRO:HD2	1.85	0.42
3:F:109:ILE:CD1	3:F:111:SER:HB2	2.50	0.41
3:F:154:PRO:HG2	3:F:156:TYR:CE1	2.55	0.41
1:J:35:LEU:HD23	1:J:35:LEU:HA	1.79	0.41
1:J:37:ARG:HD2	1:J:41:GLU:OE1	2.20	0.41
1:D:86:GLU:HG3	1:D:87:ALA:O	2.20	0.41
2:E:80:LYS:O	2:E:84:THR:HG23	2.20	0.41
3:F:112:TYR:HB2	3:F:115:HIS:CD2	2.55	0.41
3:L:176:ARG:HH21	3:L:189:GLU:CD	2.28	0.41
3:I:81:PRO:HD2	3:I:153:LEU:HG	2.03	0.41
3:L:118:LEU:HD21	3:L:198:LEU:HD21	2.02	0.41
1:D:71:ALA:HA	2:E:75:MET:HE3	2.02	0.41
2:E:38:THR:HG23	2:E:80:LYS:HZ3	1.85	0.41
4:G:32:GLU:CD	4:G:39:PRO:HD3	2.45	0.41
3:F:100:THR:O	3:F:107:ARG:NH2	2.44	0.41
3:I:70:GLU:CD	3:I:113:ARG:HE	2.29	0.41
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:142:VAL:O	3:I:145:GLN:HB2	2.21	0.41
3:L:109:ILE:CD1	3:L:111:SER:HB2	2.50	0.41
3:L:118:LEU:HD11	3:L:194:VAL:HG13	2.02	0.41
1:D:72:PRO:HD2	2:E:75:MET:HE3	2.03	0.41
1:D:42:GLN:HB3	1:D:77:LEU:HD11	2.03	0.40
1:D:46:LYS:HZ3	1:D:46:LYS:HG2	1.77	0.40
2:H:32:LYS:HE3	2:H:32:LYS:HB2	1.86	0.40
1:J:70:GLN:O	2:K:75:MET:HE2	2.20	0.40
3:F:116:LEU:HD23	3:F:137:VAL:HG22	2.01	0.40
3:I:109:ILE:HD11	3:I:111:SER:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:106:GLY:O	5:B:201:A1CBI:C10[1_545]	1.38	0.82
3:I:106:GLY:O	5:E:201:A1CBI:C10[1_545]	1.38	0.82

## 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	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
1	D	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
1	J	100/104 (96%)	95 (95%)	4 (4%)	1 (1%)	13	26
2	B	82/98 (84%)	79 (96%)	3 (4%)	0	100	100
2	E	83/98 (85%)	80 (96%)	3 (4%)	0	100	100
2	H	84/98 (86%)	83 (99%)	1 (1%)	0	100	100
2	K	84/98 (86%)	84 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	138/180 (77%)	135 (98%)	3 (2%)	0	100	100
3	F	141/180 (78%)	138 (98%)	3 (2%)	0	100	100
3	I	140/180 (78%)	136 (97%)	4 (3%)	0	100	100
3	L	140/180 (78%)	135 (96%)	5 (4%)	0	100	100
4	G	99/104 (95%)	93 (94%)	6 (6%)	0	100	100
All	All	1286/1528 (84%)	1242 (97%)	43 (3%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	81	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/91 (92%)	83 (99%)	1 (1%)	67	84
1	D	76/91 (84%)	73 (96%)	3 (4%)	27	51
1	J	86/91 (94%)	84 (98%)	2 (2%)	45	69
2	B	75/86 (87%)	74 (99%)	1 (1%)	65	83
2	E	72/86 (84%)	70 (97%)	2 (3%)	38	63
2	H	72/86 (84%)	72 (100%)	0	100	100
2	K	72/86 (84%)	72 (100%)	0	100	100
3	C	117/163 (72%)	112 (96%)	5 (4%)	25	47
3	F	120/163 (74%)	118 (98%)	2 (2%)	56	77
3	I	120/163 (74%)	119 (99%)	1 (1%)	79	91
3	L	123/163 (76%)	120 (98%)	3 (2%)	44	68
4	G	80/90 (89%)	79 (99%)	1 (1%)	65	83
All	All	1097/1359 (81%)	1076 (98%)	21 (2%)	52	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
2	B	92	GLU
3	C	66	VAL
3	C	118	LEU
3	C	150	ASN
3	C	181	VAL
3	C	183	SER
1	D	46	LYS
1	D	64	SER
1	D	84	THR
2	E	38	THR
2	E	112	CYS
3	F	181	VAL
3	F	202	THR
4	G	88	LEU
3	I	202	THR
1	J	46	LYS
1	J	64	SER
3	L	66	VAL
3	L	113	ARG
3	L	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	61	ASN
3	F	96	GLN
3	F	174	ASN
3	F	191	HIS
4	G	65	GLN
2	H	35	HIS
2	H	61	ASN
2	H	108	ASN
3	L	115	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CAS	A	89	1	5,8,9	0.73	0	1,9,11	0.06	0
1	CAS	D	89	1	5,8,9	0.67	0	1,9,11	0.18	0
4	CAS	G	89	4	5,8,9	0.60	0	1,9,11	0.17	0
4	CAS	G	60	4	5,8,9	0.70	0	1,9,11	0.08	0
3	CAS	F	77	3	5,8,9	0.72	0	1,9,11	0.54	0
1	CAS	J	89	1	5,8,9	0.85	0	1,9,11	0.10	0
3	CAS	L	77	3	5,8,9	0.76	0	1,9,11	1.12	0
3	CAS	C	77	3	5,8,9	1.05	0	1,9,11	0.40	0
3	CAS	I	77	3	5,8,9	0.75	0	1,9,11	0.71	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
1	CAS	A	89	1	-	0/0/7/9	-
1	CAS	D	89	1	-	0/0/7/9	-
4	CAS	G	89	4	-	0/0/7/9	-
4	CAS	G	60	4	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-
1	CAS	J	89	1	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
3	CAS	I	77	3	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	77	CAS	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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$
5	A1CBI	H	201	-	16,16,16	2.52	3 (18%)	21,23,23	2.01	3 (14%)
5	A1CBI	B	201	-	16,16,16	2.57	3 (18%)	21,23,23	2.08	5 (23%)
5	A1CBI	K	201	-	16,16,16	2.18	2 (12%)	21,23,23	3.24	6 (28%)
5	A1CBI	E	201	-	16,16,16	2.22	3 (18%)	21,23,23	1.94	3 (14%)

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
5	A1CBI	H	201	-	-	0/6/17/17	0/2/2/2
5	A1CBI	B	201	-	-	0/6/17/17	0/2/2/2
5	A1CBI	K	201	-	-	0/6/17/17	0/2/2/2
5	A1CBI	E	201	-	-	0/6/17/17	0/2/2/2

All (11) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	201	A1CBI	C09-N08	7.65	1.46	1.36
5	B	201	A1CBI	C09-N08	7.61	1.46	1.36
5	K	201	A1CBI	C09-N08	6.28	1.44	1.36
5	E	201	A1CBI	C09-N08	6.21	1.44	1.36
5	B	201	A1CBI	C07-N08	5.58	1.50	1.39
5	H	201	A1CBI	C07-N08	5.26	1.49	1.39
5	K	201	A1CBI	C07-N08	4.69	1.48	1.39
5	E	201	A1CBI	C07-N08	4.69	1.48	1.39
5	E	201	A1CBI	O01-N02	-3.18	1.17	1.22
5	B	201	A1CBI	O01-N02	-2.79	1.18	1.22
5	H	201	A1CBI	O01-N02	-2.02	1.19	1.22

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	201	A1CBI	C07-N08-C09	-11.14	122.16	126.05
5	E	201	A1CBI	C07-N08-C09	-6.75	123.69	126.05
5	K	201	A1CBI	C06-C07-N08	-6.28	106.58	109.69
5	B	201	A1CBI	C07-N08-C09	6.08	128.18	126.05
5	H	201	A1CBI	C06-C07-N08	-5.52	106.96	109.69
5	K	201	A1CBI	C05-C04-N02	-4.52	114.84	118.74
5	H	201	A1CBI	C05-C04-N02	-4.37	114.97	118.74
5	B	201	A1CBI	C12-N08-C07	-4.13	106.47	109.29
5	H	201	A1CBI	C15-C04-N02	4.08	122.90	119.34
5	E	201	A1CBI	C06-C07-N08	-3.14	108.14	109.69
5	B	201	A1CBI	C15-C04-N02	3.06	122.01	119.34
5	K	201	A1CBI	C15-C04-N02	2.86	121.84	119.34
5	B	201	A1CBI	C14-C07-C06	-2.68	119.05	121.62
5	E	201	A1CBI	C12-N08-C09	2.52	128.16	121.30
5	K	201	A1CBI	C15-C04-C05	2.49	123.31	120.11
5	K	201	A1CBI	C12-N08-C09	2.47	128.05	121.30
5	B	201	A1CBI	C06-C07-N08	-2.12	108.64	109.69

There are no chirality outliers.

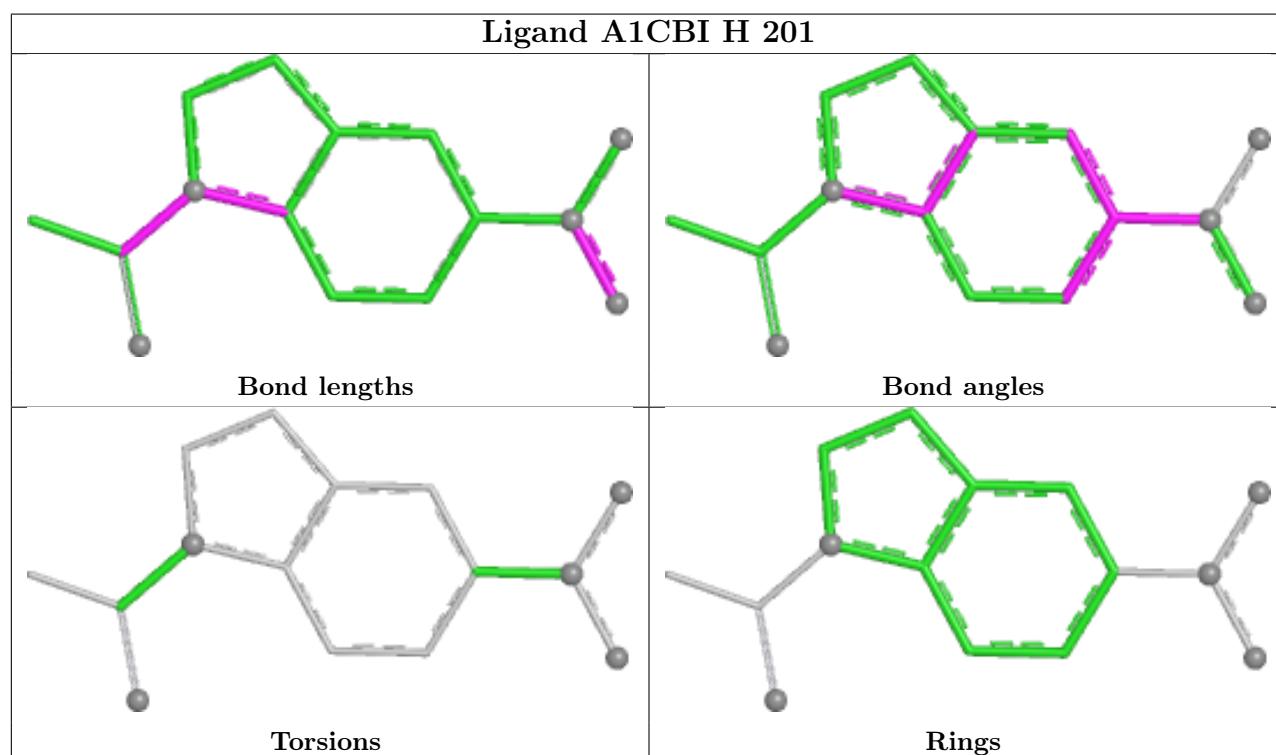
There are no torsion outliers.

There are no ring outliers.

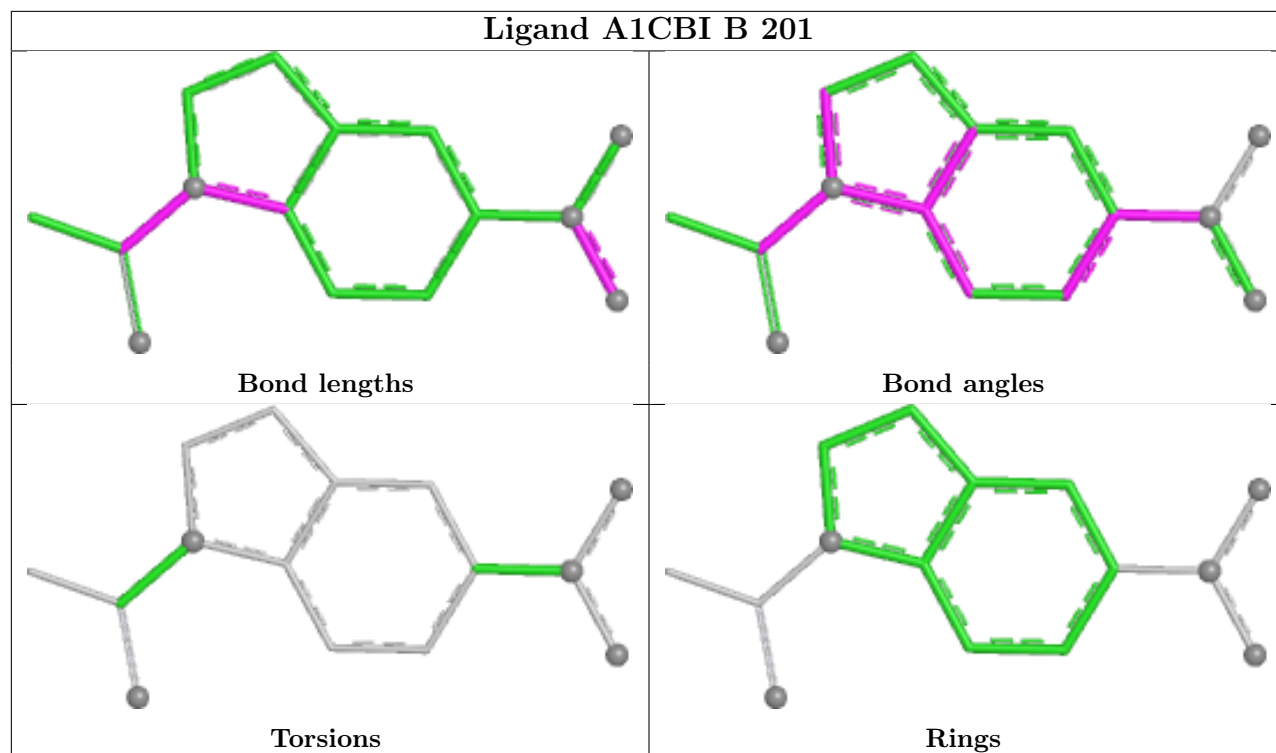
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	201	A1CBI	1	1
5	K	201	A1CBI	1	0
5	E	201	A1CBI	1	1

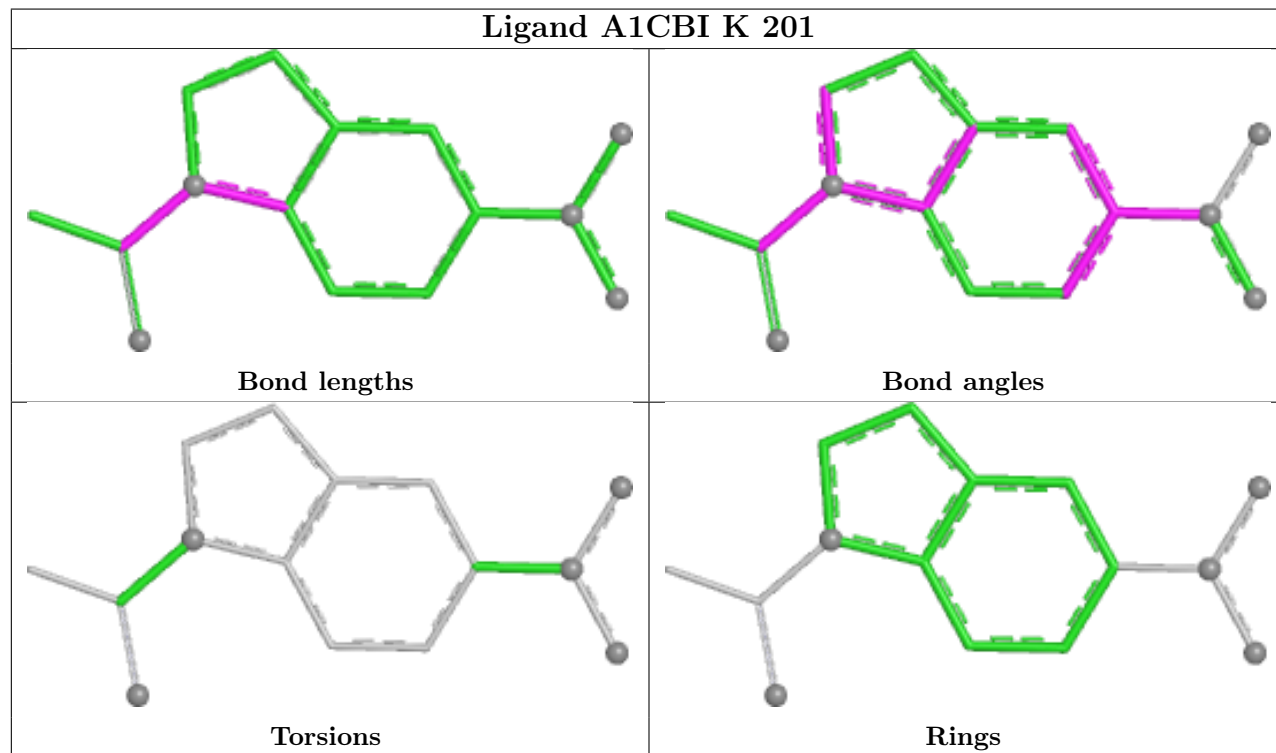
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

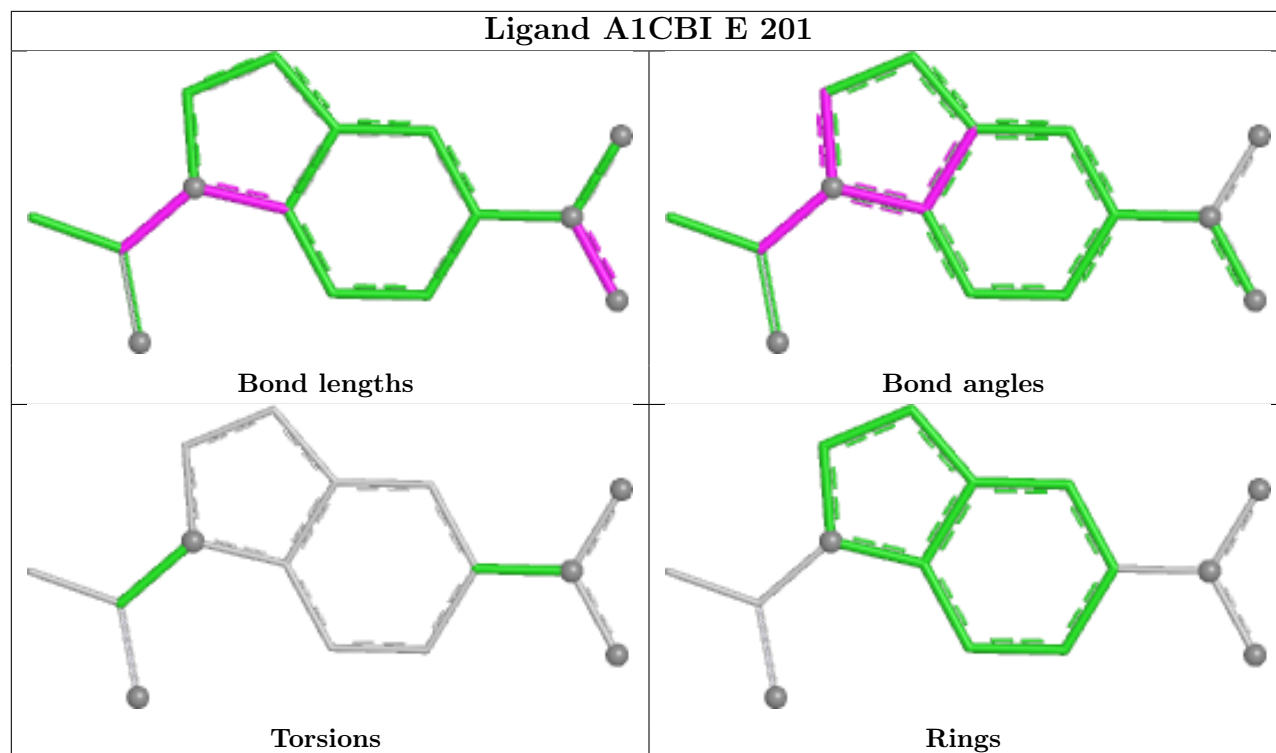


## Ligand A1CBI B 201



## Ligand A1CBI K 201





## 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	A	102/104 (98%)	-0.09	2 (1%) 64 60	42, 52, 88, 104	0
1	D	99/104 (95%)	0.52	3 (3%) 52 47	51, 76, 97, 117	0
1	J	102/104 (98%)	0.04	2 (1%) 64 60	43, 58, 77, 97	0
2	B	86/98 (87%)	-0.06	2 (2%) 61 56	42, 52, 78, 108	0
2	E	87/98 (88%)	0.33	5 (5%) 30 26	47, 66, 89, 99	0
2	H	88/98 (89%)	0.33	4 (4%) 39 34	48, 65, 100, 120	0
2	K	88/98 (89%)	-0.03	3 (3%) 48 43	42, 52, 87, 103	0
3	C	140/180 (77%)	0.03	2 (1%) 73 69	44, 57, 82, 104	0
3	F	143/180 (79%)	0.06	2 (1%) 73 69	45, 61, 89, 117	0
3	I	142/180 (78%)	0.01	4 (2%) 55 50	46, 56, 87, 103	0
3	L	142/180 (78%)	-0.18	2 (1%) 73 69	41, 48, 72, 94	0
4	G	101/104 (97%)	0.40	2 (1%) 64 60	54, 73, 92, 115	0
All	All	1320/1528 (86%)	0.09	33 (2%) 58 54	41, 59, 92, 120	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	1	MET	4.7
2	B	112	CYS	4.7
2	K	47	SER	4.5
1	D	83	ASP	4.2
2	H	48	GLY	4.2
2	E	57	THR	4.0
1	D	49	GLN	3.5
3	I	155	VAL	3.5
2	H	57	THR	3.2
3	I	62	VAL	3.2
3	C	62	VAL	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	K	57	THR	3.0
1	J	81	ALA	3.0
2	E	58	ASN	3.0
1	A	82	ASP	2.9
1	A	101	ASP	2.7
1	J	1	MET	2.7
3	L	204	GLU	2.6
3	F	173	GLU	2.6
2	K	58	ASN	2.6
2	H	87	SER	2.5
2	B	88	THR	2.5
2	H	22	ILE	2.5
3	I	204	GLU	2.4
3	F	205	ARG	2.4
1	D	65	GLN	2.4
2	E	87	SER	2.4
3	L	62	VAL	2.3
2	E	88	THR	2.3
2	E	85	ASN	2.2
4	G	66	THR	2.0
3	C	182	ARG	2.0
3	I	181	VAL	2.0

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

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
1	CAS	D	89	9/10	0.74	0.17	92,96,123,148	0
4	CAS	G	89	9/10	0.81	0.15	65,74,89,128	0
4	CAS	G	60	9/10	0.85	0.22	68,74,87,142	0
1	CAS	A	89	9/10	0.87	0.13	62,64,97,124	0
3	CAS	F	77	9/10	0.89	0.13	68,71,95,110	0
1	CAS	J	89	9/10	0.92	0.11	57,61,82,101	0
3	CAS	I	77	9/10	0.93	0.10	50,52,80,105	0
3	CAS	C	77	9/10	0.95	0.10	53,54,82,93	0
3	CAS	L	77	9/10	0.96	0.07	45,49,68,85	0

## 6.3 Carbohydrates [i](#)

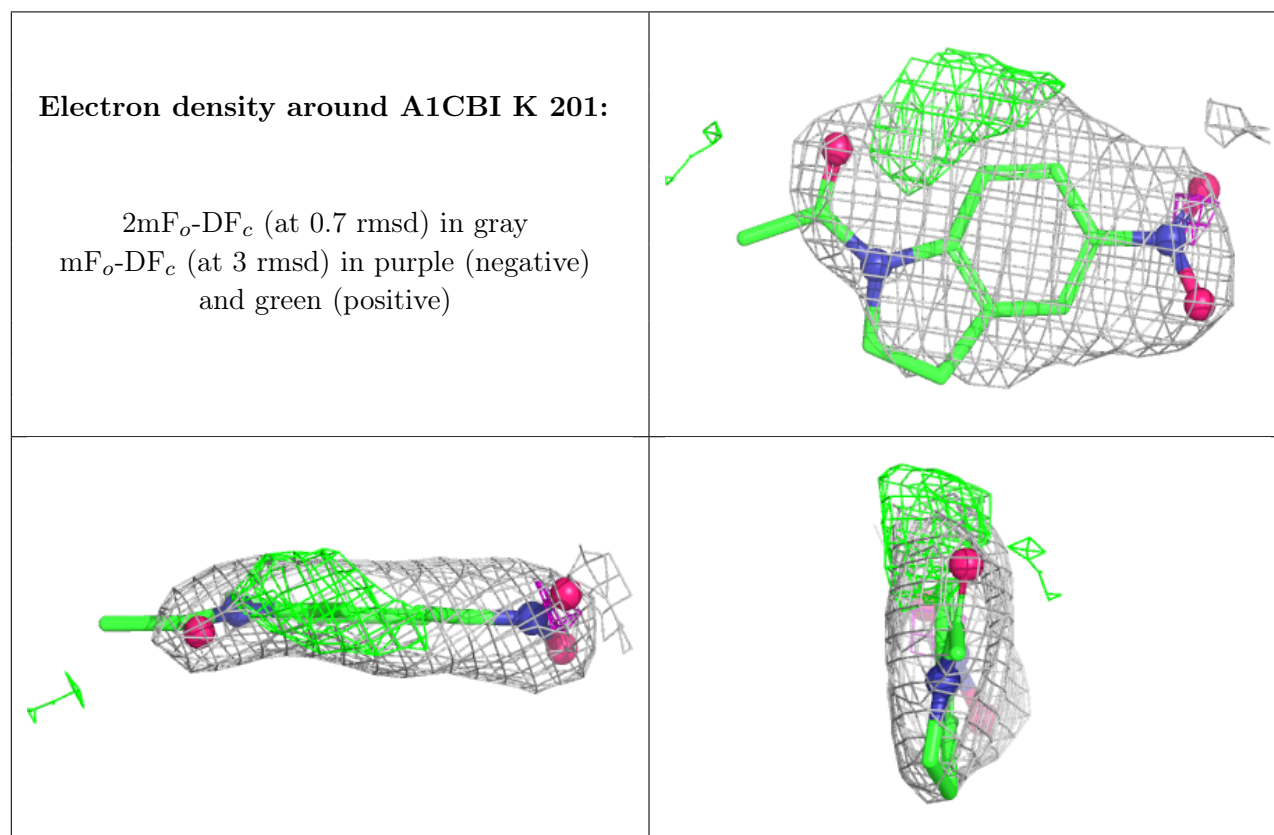
There are no oligosaccharides in this entry.

## 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, 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.

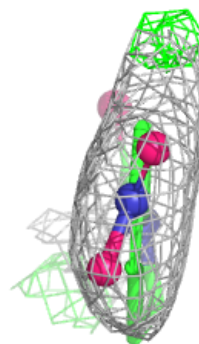
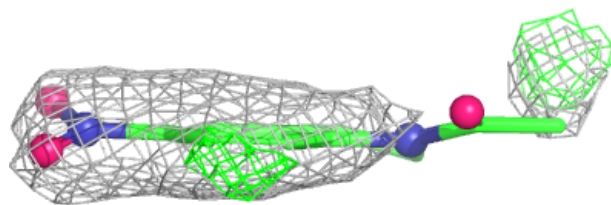
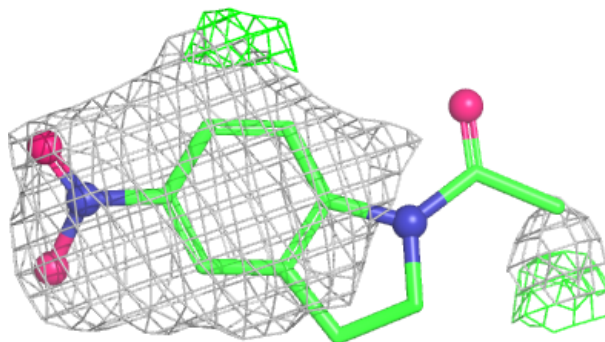
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	A1CBI	K	201	15/15	0.74	0.19	56,60,69,73	15
5	A1CBI	H	201	15/15	0.78	0.20	60,68,76,76	15
5	A1CBI	B	201	15/15	0.78	0.18	70,71,72,77	15
5	A1CBI	E	201	15/15	0.84	0.17	70,70,73,78	15

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.

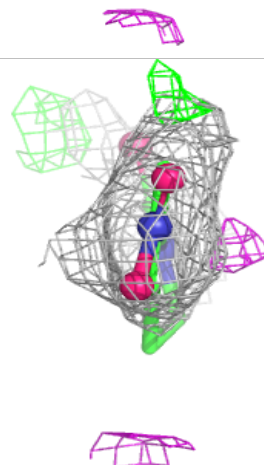
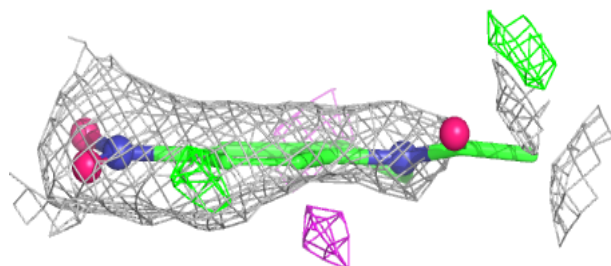
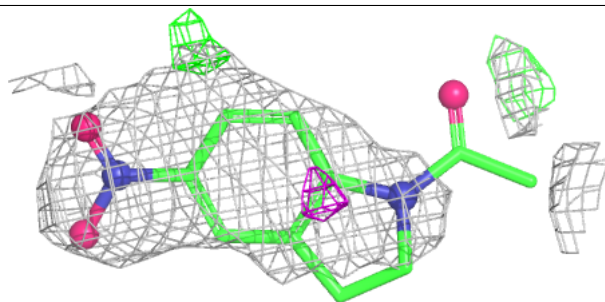


**Electron density around A1CBI H 201:**

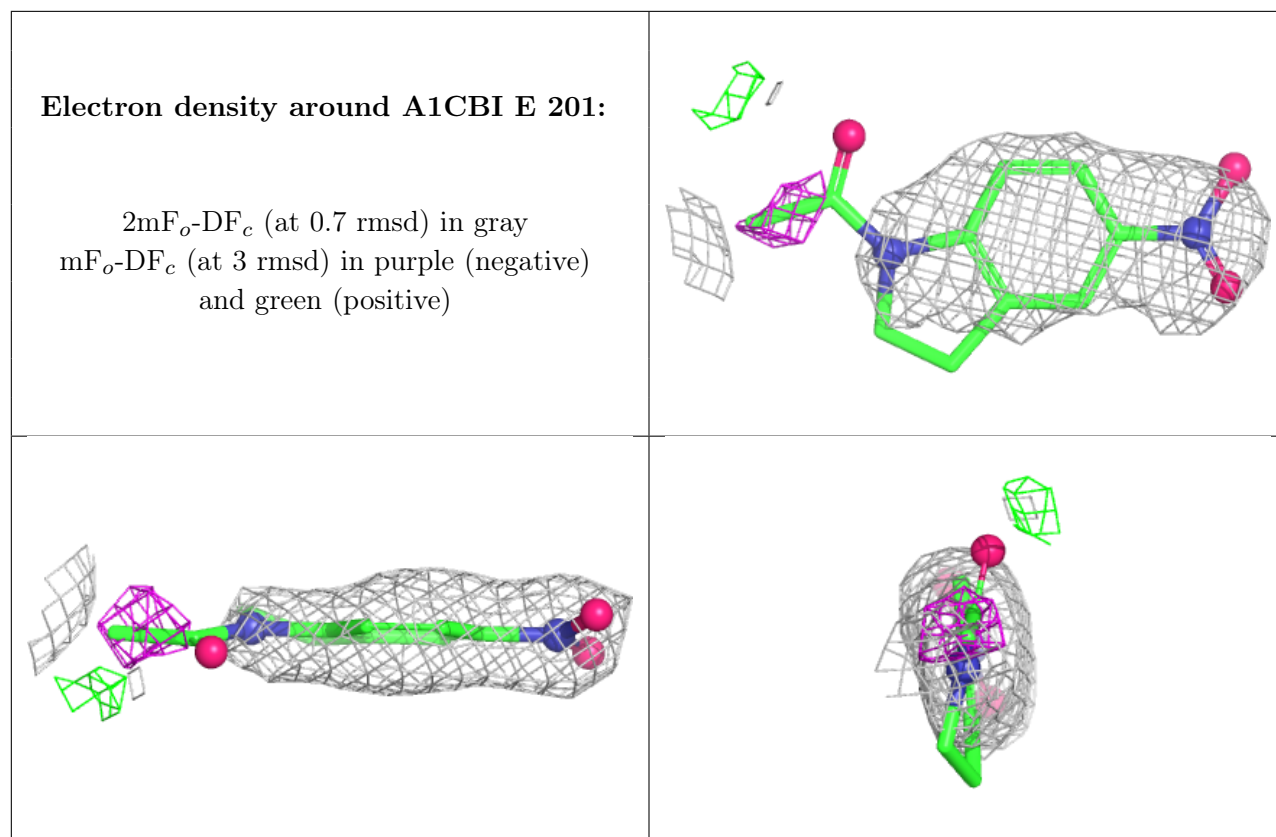
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around A1CBI B 201:**

$2mF_o-DF_c$  (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.