



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2025 – 10:09 AM JST

PDB ID : 9IPW  
Title : Crystal structure of VHL-EloB-EloC in complex with a fragment compound  
7HC\_5(D3)  
Authors : Lee, B.I.; Kim, Y.  
Deposited on : 2024-07-11  
Resolution : 3.00 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

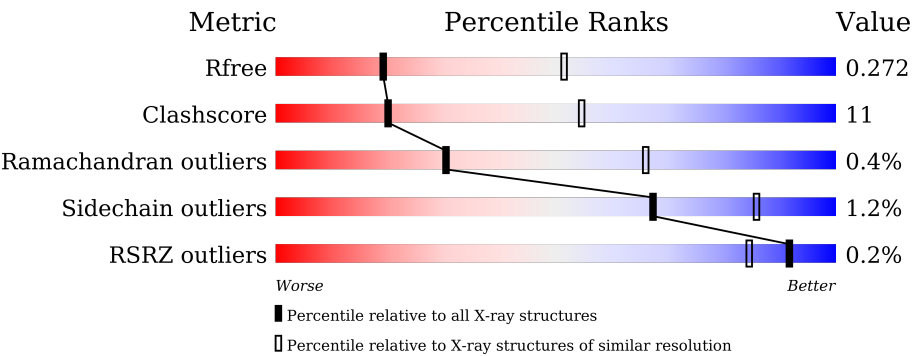
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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>%</div><div><div></div><div>71%</div><div>22%</div><div>7%</div></div></div>
1	D	104	<div><div></div><div>59%</div><div>23%</div><div>18%</div></div>
1	G	104	<div><div></div><div>65%</div><div>34%</div><div>.</div></div>
1	J	104	<div><div></div><div>70%</div><div>27%</div><div>..</div></div>
2	B	97	<div><div></div><div>58%</div><div>28%</div><div>14%</div></div>
2	E	97	<div><div></div><div>65%</div><div>21%</div><div>14%</div></div>

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Mol	Chain	Length	Quality of chain
2	H	97	<div><div></div><div>57%27%16%</div></div>
2	K	97	<div><div></div><div>72%13%14%</div></div>
3	C	162	<div><div></div><div>%50%28%•21%</div></div>
3	F	162	<div><div></div><div>57%26%•16%</div></div>
3	I	162	<div><div></div><div>64%21%•14%</div></div>
3	L	162	<div><div></div><div>%64%23%•12%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10223 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	97	Total	As	C	N	O	S	0	0	0
			775	2	493	130	146	4			
1	D	85	Total	As	C	N	O	S	0	0	0
			671	2	423	111	131	4			
1	G	103	Total	As	C	N	O	S	0	0	0
			819	2	518	136	158	5			
1	J	103	Total	As	C	N	O	S	0	0	0
			819	2	518	136	158	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			667	433	106	122	6			
2	E	83	Total	C	N	O	S	0	0	0
			665	429	107	124	5			
2	H	81	Total	C	N	O	S	0	0	0
			654	424	105	119	6			
2	K	83	Total	C	N	O	S	0	0	0
			669	435	106	121	7			

There are 4 discrepancies between the modelled and reference sequences:

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

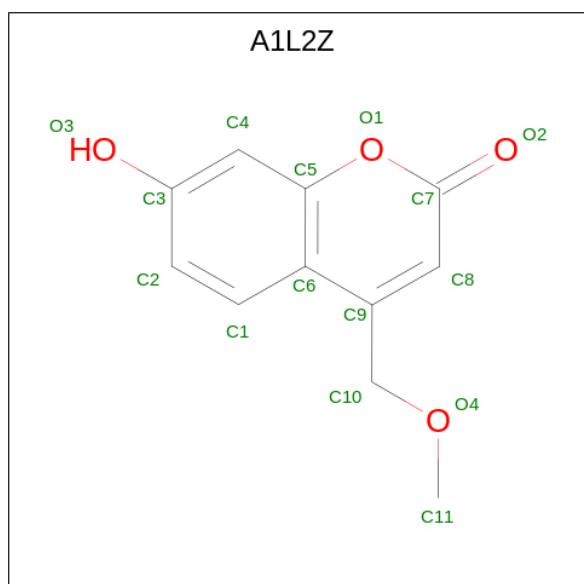
- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	128	Total	As	C	N	O	S	0	0	0
			1048	1	671	189	185	2			
3	F	136	Total	As	C	N	O	S	0	0	0
			1114	1	710	202	199	2			
3	I	139	Total	As	C	N	O	S	0	0	0
			1140	1	726	208	203	2			
3	L	142	Total	As	C	N	O	S	0	0	0
			1165	1	741	212	209	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337
I	52	GLY	-	expression tag	UNP P40337
I	53	SER	-	expression tag	UNP P40337
L	52	GLY	-	expression tag	UNP P40337
L	53	SER	-	expression tag	UNP P40337

- Molecule 4 is 7-Hydroxy-4-methoxymethylcoumarin (three-letter code: A1L2Z) (formula:  $C_{11}H_{10}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	C	O	0	0
			15	11	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	2	Total	O	0	0
			2	2		

### 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: Elongin-B



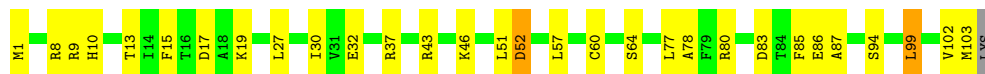
#### • Molecule 1: Elongin-B



#### • Molecule 1: Elongin-B



#### • Molecule 1: Elongin-B



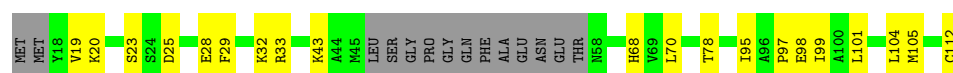
#### • Molecule 2: Elongin-C





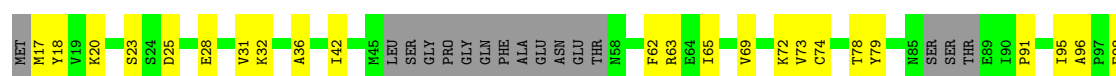
- Molecule 2: Elongin-C

Chain E: 65% 21% 14%



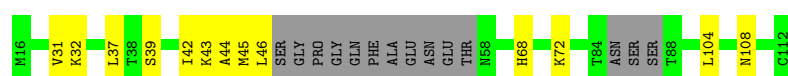
- Molecule 2: Elongin-C

Chain H: 57% 27% 16%



- Molecule 2: Elongin-C

Chain K: 72% 13% 14%



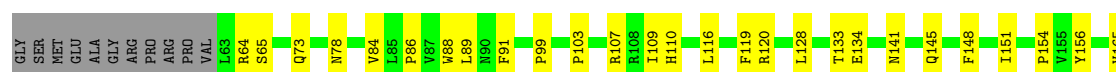
- Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain C: % 50% 28% 21%



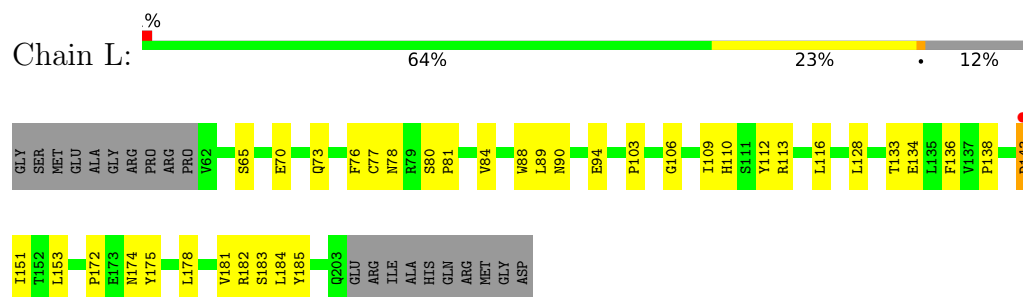
- Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F: 57% 26% 16%



- Molecule 3: von Hippel-Lindau disease tumor suppressor





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.44Å 94.44Å 361.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 3.00 49.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.06-3.00) 99.6 (49.06-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.206 , 0.273 0.208 , 0.272	Depositor DCC
$R_{free}$ test set	31951 reflections (5.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.43 % 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 1.1083e-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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, A1L2Z

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	0.55	0/770	0.80	0/1036
1	D	0.49	0/661	0.73	0/886
1	G	0.50	0/815	0.75	0/1099
1	J	0.51	0/815	0.75	0/1099
2	B	0.53	0/680	0.72	1/915 (0.1%)
2	E	0.50	0/679	0.69	1/916 (0.1%)
2	H	0.59	0/667	0.66	0/897
2	K	0.52	0/682	0.71	0/917
3	C	0.52	0/1064	0.78	0/1446
3	F	0.52	0/1134	0.73	0/1547
3	I	0.56	0/1158	0.75	0/1576
3	L	0.57	0/1185	0.79	0/1616
All	All	0.53	0/10310	0.74	2/13950 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	CYS	CA-CB-SG	7.25	127.04	114.00
2	E	112	CYS	CA-CB-SG	5.31	123.55	114.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	775	0	772	12	0
1	D	671	0	660	14	0
1	G	819	0	807	27	0
1	J	819	0	808	18	0
2	B	667	0	671	19	0
2	E	665	0	663	16	0
2	H	654	0	654	21	0
2	K	669	0	675	8	0
3	C	1048	0	1045	33	0
3	F	1114	0	1106	29	0
3	I	1140	0	1135	27	0
3	L	1165	0	1160	29	0
4	K	15	0	0	0	0
5	L	2	0	0	0	0
All	All	10223	0	10156	229	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 11.

All (229) 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:G:23:THR:HG22	1:G:26:GLU:HG3	1.52	0.91
3:F:193:ASN:HB3	3:F:196:LYS:HG3	1.59	0.85
3:I:90:ASN:HD21	3:I:94:GLU:HB3	1.43	0.83
3:L:181:VAL:HG12	3:L:183:SER:H	1.40	0.83
1:J:9:ARG:HB2	1:J:77:LEU:HB3	1.61	0.83
3:F:120:ARG:NH1	3:F:197:ASP:OD2	2.12	0.81
3:C:180:ILE:HD12	3:C:184:LEU:HB3	1.61	0.79
3:L:90:ASN:HD21	3:L:94:GLU:HB3	1.48	0.79
2:B:83:TYR:HB3	2:B:90:ILE:HD12	1.66	0.77
2:H:20:LYS:NZ	2:H:28:GLU:OE1	2.20	0.74
3:I:172:PRO:O	3:I:174:ASN:N	2.21	0.74
2:H:79:TYR:OH	2:H:91:PRO:O	2.06	0.72
3:L:90:ASN:ND2	3:L:94:GLU:HB3	2.07	0.70
3:C:178:LEU:O	3:C:185:TYR:OH	2.03	0.70
1:J:17:ASP:OD2	2:K:32:LYS:NZ	2.25	0.69
3:F:64:ARG:HD3	3:F:91:PHE:O	1.94	0.68
1:G:23:THR:HG22	1:G:26:GLU:CG	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:THR:O	2:B:45:MET:HG3	1.95	0.67
3:C:193:ASN:OD1	3:C:196:LYS:N	2.27	0.67
3:F:165:VAL:O	3:F:169:LEU:HD13	1.95	0.66
1:G:80:ARG:HA	1:G:85:PHE:HA	1.78	0.66
3:C:197:ASP:OD1	3:C:200:ARG:NH2	2.24	0.66
3:L:182:ARG:HA	3:L:185:TYR:HD2	1.62	0.65
3:F:180:ILE:HD12	3:F:184:LEU:HB3	1.78	0.65
3:I:133:THR:HG22	3:I:134:GLU:H	1.61	0.65
2:B:39:SER:HB3	2:B:42:ILE:HG13	1.78	0.64
1:A:7:ILE:HD11	1:A:27:LEU:HD11	1.80	0.64
3:I:181:VAL:HG22	3:I:183:SER:H	1.62	0.64
3:C:182:ARG:HA	3:C:185:TYR:HD2	1.62	0.64
2:K:104:LEU:HG	3:L:184:LEU:HD13	1.80	0.64
1:G:37:ARG:NH1	1:G:41:GLU:OE1	2.30	0.63
2:E:68:HIS:HD2	2:E:99:ILE:HG22	1.63	0.63
3:I:90:ASN:ND2	3:I:94:GLU:HB3	2.13	0.63
3:C:85:LEU:HB2	3:C:122:ALA:HB2	1.78	0.63
3:C:120:ARG:NH1	3:C:197:ASP:OD2	2.26	0.62
1:D:25:PHE:HB2	1:D:53:ASP:HB3	1.80	0.61
2:E:95:ILE:HB	3:F:165:VAL:HG21	1.81	0.61
2:H:17:MET:HG3	2:H:18:TYR:CD1	2.36	0.61
1:D:23:THR:H	1:D:26:GLU:HG3	1.65	0.60
3:F:73:GLN:OE1	3:F:110:HIS:ND1	2.34	0.60
3:L:182:ARG:HA	3:L:185:TYR:CD2	2.37	0.59
3:I:73:GLN:OE1	3:I:110:HIS:ND1	2.36	0.59
1:J:1:MET:HB3	1:J:64:SER:OG	2.04	0.58
1:A:9:ARG:HB2	1:A:77:LEU:HB3	1.86	0.58
1:D:46:LYS:HG3	1:D:62:PHE:CZ	2.38	0.58
2:K:108:ASN:ND2	3:L:184:LEU:HD21	2.18	0.58
3:L:73:GLN:OE1	3:L:110:HIS:ND1	2.34	0.58
3:C:72:SER:N	3:C:111:SER:O	2.38	0.57
3:C:69:ARG:HH11	3:C:69:ARG:HB2	1.69	0.57
1:G:27:LEU:HD22	1:G:57:LEU:HD21	1.87	0.56
1:A:1:MET:HB3	1:A:64:SER:HB3	1.88	0.56
3:F:141:ASN:ND2	3:F:145:GLN:O	2.39	0.56
1:G:10:HIS:CD2	1:G:89:CAS:HB2	2.39	0.56
3:C:154:PRO:HG2	3:C:156:TYR:CE1	2.40	0.56
3:L:76:PHE:O	3:L:106:GLY:HA2	2.06	0.56
1:J:15:PHE:HB2	2:K:31:VAL:HG12	1.88	0.56
3:I:64:ARG:HD2	3:I:91:PHE:O	2.06	0.55
2:B:58:ASN:O	2:B:58:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:GLN:O	3:C:134:GLU:N	2.40	0.55
1:G:26:GLU:O	1:G:30:ILE:HD13	2.05	0.55
1:G:23:THR:HG23	1:G:25:PHE:H	1.72	0.55
3:L:76:PHE:CZ	3:L:109:ILE:HD13	2.42	0.55
2:B:98:GLU:H	2:B:98:GLU:CD	2.09	0.55
3:F:133:THR:HG22	3:F:134:GLU:H	1.72	0.54
1:G:102:VAL:O	3:I:170:VAL:HG23	2.08	0.54
3:C:74:VAL:HG22	3:C:147:ILE:HB	1.88	0.54
1:D:43:ARG:HB3	1:D:45:TYR:HE1	1.73	0.54
1:D:69:PRO:HB3	2:E:78:THR:HG22	1.89	0.54
1:G:70:GLN:HB3	2:H:79:TYR:HD2	1.73	0.54
1:J:94:SER:OG	2:K:68:HIS:ND1	2.29	0.54
3:I:131:ASN:O	3:I:133:THR:N	2.41	0.53
1:J:8:ARG:HG2	1:J:13:THR:HG23	1.89	0.53
3:I:160:GLU:HA	3:I:163:LEU:HD12	1.90	0.53
2:H:31:VAL:HG11	2:H:74:CYS:HB3	1.91	0.53
1:J:9:ARG:NH2	1:J:10:HIS:CE1	2.77	0.53
3:L:84:VAL:HG21	3:L:151:ILE:HG21	1.91	0.52
2:E:105:MET:CE	3:F:180:ILE:HG22	2.39	0.52
1:D:28:LYS:HE3	1:D:44:LEU:HG	1.91	0.52
1:G:69:PRO:HB3	2:H:78:THR:HG22	1.91	0.52
3:I:182:ARG:HA	3:I:185:TYR:CD2	2.45	0.52
1:D:7:ILE:HD11	1:D:27:LEU:HD11	1.91	0.52
2:K:44:ALA:O	2:K:46:LEU:N	2.42	0.52
2:B:83:TYR:HB3	2:B:90:ILE:CD1	2.38	0.52
1:G:32:GLU:OE2	1:G:38:PRO:HA	2.10	0.51
2:K:37:LEU:HB3	2:K:43:LYS:HE3	1.92	0.51
2:E:29:PHE:CD2	2:E:70:LEU:HD23	2.45	0.51
1:J:27:LEU:HD12	1:J:30:ILE:HD12	1.93	0.51
3:F:180:ILE:HD12	3:F:184:LEU:CB	2.41	0.50
2:B:108:ASN:CG	3:C:184:LEU:HD11	2.32	0.50
3:F:86:PRO:HB3	3:F:119:PHE:CE2	2.45	0.50
1:A:38:PRO:HD2	1:A:41:GLU:OE1	2.11	0.50
1:D:56:THR:O	1:D:59:GLU:HB2	2.11	0.50
2:E:101:LEU:HD11	3:F:178:LEU:HD12	1.94	0.50
3:C:180:ILE:HD12	3:C:184:LEU:CB	2.39	0.50
3:F:84:VAL:HG21	3:F:151:ILE:HG21	1.94	0.50
3:L:78:ASN:ND2	3:L:103:PRO:HA	2.26	0.50
2:B:95:ILE:HB	3:C:165:VAL:HG21	1.94	0.50
1:J:19:LYS:O	1:J:57:LEU:HD12	2.12	0.50
3:C:182:ARG:HA	3:C:185:TYR:CD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:ILE:HB	3:I:165:VAL:HG21	1.93	0.49
1:J:52:ASP:OD1	1:J:52:ASP:N	2.45	0.48
3:L:89:LEU:HD12	3:L:116:LEU:HD23	1.95	0.48
2:H:104:LEU:HG	3:I:184:LEU:HD13	1.93	0.48
3:C:73:GLN:OE1	3:C:110:HIS:ND1	2.46	0.48
3:F:154:PRO:HG2	3:F:156:TYR:CE1	2.48	0.48
1:G:45:TYR:HB3	1:G:47:ASP:O	2.13	0.48
3:C:85:LEU:HB2	3:C:122:ALA:CB	2.43	0.48
1:D:24:VAL:HG23	1:D:55:LYS:O	2.14	0.48
1:D:24:VAL:HB	1:D:53:ASP:HA	1.95	0.48
1:G:56:THR:O	1:G:59:GLU:N	2.46	0.48
2:B:101:LEU:HD12	2:B:101:LEU:HA	1.62	0.48
1:D:42:GLN:HG2	1:D:77:LEU:HD11	1.96	0.48
3:I:154:PRO:HG2	3:I:156:TYR:CE1	2.49	0.47
3:I:182:ARG:HA	3:I:185:TYR:HD2	1.78	0.47
3:L:143:ASP:N	3:L:143:ASP:OD1	2.47	0.47
3:I:193:ASN:HB3	3:I:196:LYS:HB2	1.96	0.47
2:E:20:LYS:HD2	2:E:28:GLU:HB3	1.95	0.47
3:F:168:SER:O	3:F:169:LEU:HD12	2.15	0.47
3:L:133:THR:OG1	3:L:134:GLU:N	2.47	0.47
3:C:78:ASN:ND2	3:C:103:PRO:HA	2.30	0.47
3:I:67:ASN:OD1	3:I:69:ARG:HD3	2.14	0.47
3:I:117:TRP:HB2	3:I:136:PHE:HB3	1.96	0.47
3:L:70:GLU:OE1	3:L:113:ARG:NH1	2.47	0.47
3:L:172:PRO:HA	3:L:175:TYR:CE1	2.50	0.47
1:G:15:PHE:HB2	2:H:31:VAL:HG12	1.96	0.47
1:G:99:LEU:HG	2:H:98:GLU:HG3	1.97	0.47
2:H:62:PHE:HB3	2:H:65:ILE:HD12	1.97	0.47
2:B:88:THR:HB	2:B:89:GLU:H	1.44	0.47
2:E:23:SER:OG	2:E:25:ASP:OD1	2.33	0.47
2:E:32:LYS:HB3	2:E:32:LYS:HE2	1.60	0.47
2:E:97:PRO:HD2	2:E:98:GLU:OE2	2.15	0.46
3:F:65:SER:OG	3:F:88:TRP:NE1	2.49	0.46
2:H:101:LEU:HD23	2:H:101:LEU:HA	1.74	0.46
2:B:69:VAL:O	2:B:73:VAL:HG23	2.15	0.46
3:C:141:ASN:ND2	3:C:147:ILE:HG12	2.30	0.46
3:L:178:LEU:O	3:L:185:TYR:OH	2.24	0.46
3:F:174:ASN:O	3:F:177:ARG:HB3	2.16	0.46
2:H:69:VAL:O	2:H:73:VAL:HG23	2.16	0.46
3:C:162:CYS:O	3:C:166:VAL:HG23	2.15	0.46
2:H:72:LYS:HG3	2:H:99:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:VAL:HB	3:L:174:ASN:HB3	1.98	0.46
3:C:136:PHE:CE2	3:C:149:ALA:HB2	2.51	0.46
3:C:113:ARG:CZ	3:C:140:LEU:HB2	2.45	0.45
2:E:105:MET:HE2	3:F:180:ILE:HA	1.98	0.45
1:G:9:ARG:HB2	1:G:77:LEU:HD23	1.98	0.45
3:C:73:GLN:HB2	3:C:141:ASN:OD1	2.16	0.45
1:A:3:VAL:HG11	1:A:62:PHE:O	2.15	0.45
3:I:170:VAL:HG13	3:I:175:TYR:CD1	2.51	0.45
1:A:29:ARG:NH1	1:A:32:GLU:OE1	2.47	0.45
2:B:38:THR:HG21	2:B:80:LYS:HD3	1.98	0.45
1:D:50:LEU:HG	1:D:51:LEU:N	2.30	0.45
1:G:103:MET:HE3	3:I:169:LEU:HD13	1.99	0.45
1:J:80:ARG:HA	1:J:85:PHE:HA	1.99	0.45
3:L:81:PRO:HD2	3:L:153:LEU:HG	1.99	0.45
3:I:130:VAL:O	3:I:131:ASN:HB2	2.16	0.45
3:C:181:VAL:HG13	3:C:183:SER:H	1.81	0.44
3:L:136:PHE:CE2	3:L:149:ALA:HB2	2.53	0.44
3:C:73:GLN:OE1	3:C:110:HIS:CE1	2.70	0.44
2:E:68:HIS:CD2	2:E:99:ILE:HG22	2.48	0.44
1:J:32:GLU:HG3	1:J:37:ARG:O	2.17	0.44
1:J:99:LEU:HD22	1:J:103:MET:HB2	2.00	0.44
3:L:128:LEU:HA	3:L:128:LEU:HD23	1.75	0.44
2:E:19:VAL:CG1	2:E:33:ARG:HG3	2.48	0.44
3:F:181:VAL:HG22	3:F:183:SER:H	1.82	0.44
1:A:46:LYS:O	1:A:47:ASP:HB2	2.17	0.43
3:F:99:PRO:O	3:F:107:ARG:NH1	2.47	0.43
3:I:133:THR:HG22	3:I:134:GLU:N	2.31	0.43
2:H:72:LYS:HG3	2:H:99:ILE:CD1	2.47	0.43
2:B:62:PHE:CD1	2:B:65:ILE:HD12	2.53	0.43
2:E:105:MET:HE3	3:F:180:ILE:HG22	2.00	0.43
3:F:172:PRO:HA	3:F:175:TYR:CZ	2.54	0.43
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.78	0.43
2:H:17:MET:HG3	2:H:18:TYR:CE1	2.53	0.43
3:C:129:LEU:O	3:C:151:ILE:HA	2.19	0.43
2:K:39:SER:HB3	2:K:42:ILE:HD12	1.99	0.43
1:G:36:LYS:O	1:G:37:ARG:HG2	2.18	0.43
3:C:89:LEU:HD12	3:C:116:LEU:HD13	2.00	0.43
1:G:41:GLU:O	1:G:80:ARG:N	2.50	0.43
2:H:18:TYR:CE2	2:H:32:LYS:HG3	2.54	0.43
1:D:44:LEU:HD23	1:D:44:LEU:HA	1.78	0.43
2:H:96:ALA:HB3	2:H:99:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:65:SER:OG	3:L:88:TRP:NE1	2.52	0.43
3:L:181:VAL:HG12	3:L:183:SER:N	2.22	0.43
3:F:78:ASN:ND2	3:F:103:PRO:HA	2.34	0.42
3:F:89:LEU:HD12	3:F:116:LEU:HB3	2.01	0.42
3:I:153:LEU:HD23	3:I:153:LEU:HA	1.78	0.42
1:A:10:HIS:O	1:A:91:GLU:HB2	2.20	0.42
1:J:86:GLU:HG3	1:J:87:ALA:O	2.19	0.42
2:B:34:GLU:H	2:B:34:GLU:CD	2.21	0.42
2:H:23:SER:OG	2:H:25:ASP:OD1	2.30	0.42
3:C:86:PRO:HB3	3:C:119:PHE:CE2	2.54	0.42
1:G:5:LEU:HD23	1:G:73:ALA:HB3	2.01	0.42
1:A:4:PHE:CE1	1:A:69:PRO:HG3	2.55	0.42
3:F:171:LYS:C	3:F:173:GLU:H	2.21	0.42
1:G:27:LEU:HA	1:G:27:LEU:HD12	1.84	0.42
1:J:46:LYS:HB2	1:J:51:LEU:HD21	2.02	0.42
1:A:80:ARG:HA	1:A:85:PHE:HA	2.02	0.42
3:L:109:ILE:O	3:L:109:ILE:HG13	2.16	0.42
3:I:89:LEU:HD12	3:I:116:LEU:HB3	2.02	0.41
1:D:9:ARG:HD2	1:D:10:HIS:CE1	2.55	0.41
3:I:65:SER:OG	3:I:89:LEU:O	2.37	0.41
2:B:69:VAL:HG21	2:B:102:GLU:HB3	2.02	0.41
3:C:100:THR:O	3:C:107:ARG:NH2	2.54	0.41
1:G:24:VAL:HG23	1:G:55:LYS:O	2.19	0.41
1:G:41:GLU:O	1:G:85:PHE:HE1	2.03	0.41
3:C:69:ARG:HB2	3:C:69:ARG:NH1	2.33	0.41
2:E:104:LEU:HG	3:F:184:LEU:HD13	2.03	0.41
3:F:84:VAL:HG22	3:F:128:LEU:HD13	2.02	0.41
2:H:62:PHE:CG	2:H:65:ILE:HD12	2.55	0.41
3:I:113:ARG:HH11	3:I:113:ARG:HG2	1.85	0.41
3:L:112:TYR:O	3:L:138:PRO:HB2	2.19	0.41
1:A:34:ILE:HD11	2:B:18:TYR:CZ	2.55	0.41
2:B:76:TYR:HA	2:B:93:PHE:CE1	2.55	0.41
3:F:109:ILE:HD12	3:F:109:ILE:O	2.21	0.41
2:B:25:ASP:OD1	2:B:25:ASP:N	2.44	0.41
3:I:165:VAL:O	3:I:169:LEU:HD12	2.20	0.41
3:L:143:ASP:OD1	3:L:145:GLN:HB2	2.21	0.41
1:A:37:ARG:NH1	1:A:41:GLU:HB3	2.35	0.41
2:E:29:PHE:HD2	2:E:70:LEU:HD23	1.85	0.41
1:G:16:THR:OG1	1:G:17:ASP:N	2.53	0.41
1:G:19:LYS:O	1:G:57:LEU:HD12	2.21	0.41
1:J:46:LYS:HD2	1:J:60:CAS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:77:CAS:AS	3:L:106:GLY:HA3	2.81	0.41
2:H:36:ALA:HB1	2:H:42:ILE:HG21	2.02	0.40
3:C:181:VAL:HG13	3:C:183:SER:N	2.37	0.40
2:B:45:MET:HE2	2:B:60:VAL:HG13	2.03	0.40
1:G:23:THR:HG23	1:G:25:PHE:N	2.36	0.40
3:L:76:PHE:CE2	3:L:109:ILE:HD13	2.56	0.40
1:J:43:ARG:HB2	1:J:78:ALA:HB3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	91/104 (88%)	83 (91%)	8 (9%)	0	100	100
1	D	77/104 (74%)	70 (91%)	6 (8%)	1 (1%)	10	39
1	G	99/104 (95%)	88 (89%)	11 (11%)	0	100	100
1	J	99/104 (95%)	91 (92%)	7 (7%)	1 (1%)	13	46
2	B	77/97 (79%)	75 (97%)	2 (3%)	0	100	100
2	E	79/97 (81%)	74 (94%)	5 (6%)	0	100	100
2	H	75/97 (77%)	68 (91%)	7 (9%)	0	100	100
2	K	77/97 (79%)	71 (92%)	5 (6%)	1 (1%)	10	39
3	C	119/162 (74%)	106 (89%)	12 (10%)	1 (1%)	16	51
3	F	133/162 (82%)	123 (92%)	10 (8%)	0	100	100
3	I	132/162 (82%)	120 (91%)	12 (9%)	0	100	100
3	L	139/162 (86%)	130 (94%)	8 (6%)	1 (1%)	19	54
All	All	1197/1452 (82%)	1099 (92%)	93 (8%)	5 (0%)	30	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	45	MET
3	L	143	ASP
3	C	67	ASN
1	D	97	PRO
1	J	83	ASP

### 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	84/90 (93%)	83 (99%)	1 (1%)	67	86
1	D	73/90 (81%)	73 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	J	89/90 (99%)	87 (98%)	2 (2%)	47	76
2	B	75/86 (87%)	75 (100%)	0	100	100
2	E	75/86 (87%)	74 (99%)	1 (1%)	65	85
2	H	73/86 (85%)	72 (99%)	1 (1%)	62	83
2	K	75/86 (87%)	74 (99%)	1 (1%)	65	85
3	C	119/147 (81%)	116 (98%)	3 (2%)	42	73
3	F	126/147 (86%)	124 (98%)	2 (2%)	58	82
3	I	129/147 (88%)	127 (98%)	2 (2%)	58	82
3	L	132/147 (90%)	131 (99%)	1 (1%)	79	90
All	All	1139/1292 (88%)	1125 (99%)	14 (1%)	67	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
3	C	64	ARG
3	C	120	ARG
3	C	148	PHE
2	E	43	LYS
3	F	148	PHE

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Mol	Chain	Res	Type
3	F	183	SER
2	H	63	ARG
3	I	69	ARG
3	I	183	SER
1	J	52	ASP
1	J	99	LEU
2	K	72	LYS
3	L	80	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	132	GLN
2	K	27	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	$\# Z  > 2$
3	CAS	I	77	3	5,8,9	0.97	0	1,9,11	0.37	0
1	CAS	A	60	1	5,8,9	0.91	0	1,9,11	0.84	0
1	CAS	D	89	1	5,8,9	1.02	0	1,9,11	0.01	0
3	CAS	F	77	3	5,8,9	0.82	0	1,9,11	0.56	0
1	CAS	D	60	1	5,8,9	1.03	0	1,9,11	0.74	0
1	CAS	A	89	1	5,8,9	0.85	0	1,9,11	0.11	0
3	CAS	C	77	3	5,8,9	0.81	0	1,9,11	0.69	0
3	CAS	L	77	3	5,8,9	0.96	0	1,9,11	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CAS	J	89	1	5,8,9	0.99	0	1,9,11	0.22	0
1	CAS	G	60	1	5,8,9	0.87	0	1,9,11	2.50	1 (100%)
1	CAS	J	60	1	5,8,9	0.83	0	1,9,11	1.59	0
1	CAS	G	89	1	5,8,9	0.96	0	1,9,11	0.53	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	CAS	I	77	3	-	0/0/7/9	-
1	CAS	A	60	1	-	0/0/7/9	-
1	CAS	D	89	1	-	0/0/7/9	-
3	CAS	F	77	3	-	0/0/7/9	-
1	CAS	D	60	1	-	0/0/7/9	-
1	CAS	A	89	1	-	0/0/7/9	-
3	CAS	C	77	3	-	0/0/7/9	-
3	CAS	L	77	3	-	0/0/7/9	-
1	CAS	J	89	1	-	0/0/7/9	-
1	CAS	G	60	1	-	0/0/7/9	-
1	CAS	J	60	1	-	0/0/7/9	-
1	CAS	G	89	1	-	0/0/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	60	CAS	CA-CB-SG	-2.50	103.92	114.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	77	CAS	1	0
1	J	60	CAS	1	0
1	G	89	CAS	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	A1L2Z	K	201	-	16,16,16	1.49	4 (25%)	20,22,22	1.37	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1L2Z	K	201	-	-	1/3/3/3	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	201	A1L2Z	C8-C7	-3.06	1.38	1.44
4	K	201	A1L2Z	C10-C9	2.36	1.53	1.51
4	K	201	A1L2Z	O1-C5	-2.28	1.35	1.38
4	K	201	A1L2Z	C8-C9	2.05	1.39	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	201	A1L2Z	O1-C7-O2	4.08	121.64	116.44
4	K	201	A1L2Z	O2-C7-C8	-3.19	119.32	125.84

There are no chirality outliers.

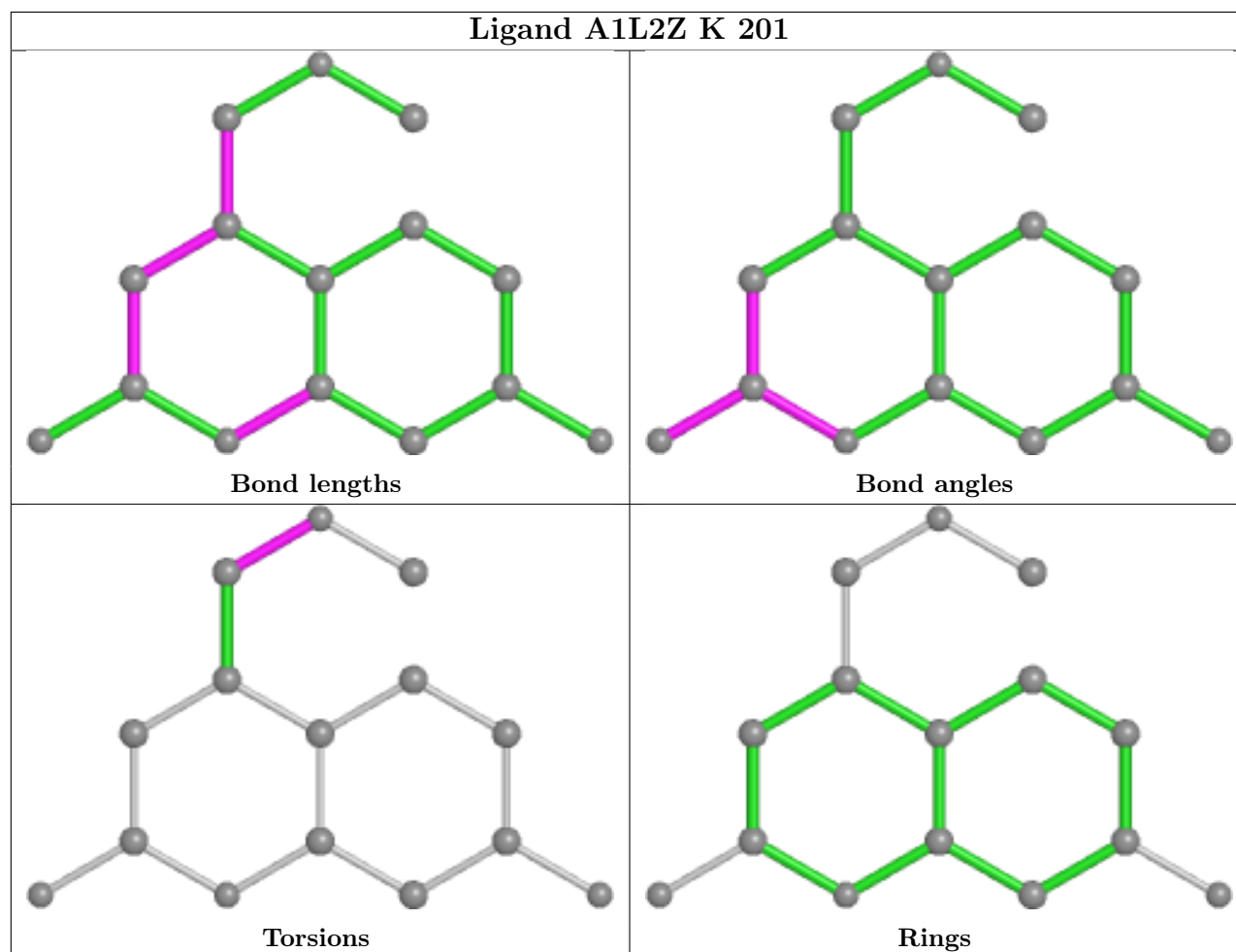
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	201	A1L2Z	C9-C10-O4-C11

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	95/104 (91%)	-0.64	1 (1%) 77 58	30, 42, 62, 72	0
1	D	83/104 (79%)	-0.29	0 100 100	40, 60, 77, 90	0
1	G	101/104 (97%)	-0.45	0 100 100	39, 55, 74, 87	0
1	J	101/104 (97%)	-0.72	0 100 100	28, 44, 66, 86	0
2	B	83/97 (85%)	-0.52	0 100 100	34, 45, 64, 74	0
2	E	83/97 (85%)	-0.45	0 100 100	38, 56, 70, 80	0
2	H	81/97 (83%)	-0.33	0 100 100	39, 52, 67, 75	0
2	K	83/97 (85%)	-0.61	0 100 100	31, 42, 66, 69	0
3	C	127/162 (78%)	-0.28	1 (0%) 82 66	36, 51, 75, 105	0
3	F	135/162 (83%)	-0.27	0 100 100	37, 57, 84, 99	0
3	I	138/162 (85%)	-0.48	0 100 100	33, 48, 81, 96	0
3	L	141/162 (87%)	-0.59	1 (0%) 84 68	27, 41, 70, 88	0
All	All	1251/1452 (86%)	-0.47	3 (0%) 92 84	27, 49, 75, 105	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	178	LEU	4.6
1	A	100	PRO	2.3
3	L	143	ASP	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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( $\text{\AA}^2$ )	Q<0.9
1	CAS	D	89	9/10	0.77	0.16	76,79,101,133	0
1	CAS	A	89	9/10	0.88	0.12	44,51,106,119	0
1	CAS	J	89	9/10	0.89	0.13	46,48,92,104	0
1	CAS	G	89	9/10	0.92	0.13	48,50,92,93	0
3	CAS	C	77	9/10	0.95	0.10	50,55,90,91	0
3	CAS	F	77	9/10	0.96	0.08	53,57,78,94	0
1	CAS	D	60	9/10	0.96	0.09	45,49,67,94	0
1	CAS	A	60	9/10	0.96	0.08	38,43,52,87	0
1	CAS	J	60	9/10	0.97	0.12	40,44,57,85	0
1	CAS	G	60	9/10	0.97	0.10	52,57,68,85	0
3	CAS	L	77	9/10	0.97	0.07	37,41,57,84	0
3	CAS	I	77	9/10	0.98	0.06	43,45,65,82	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

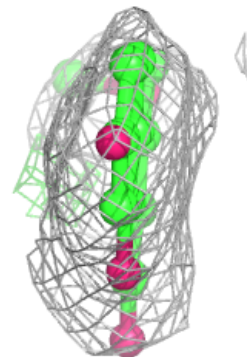
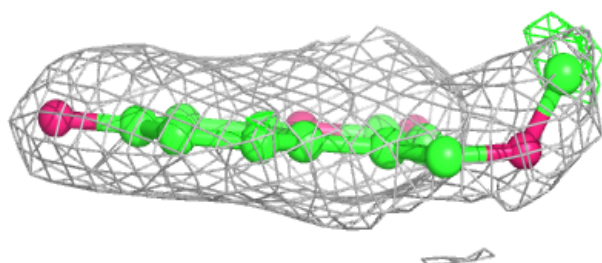
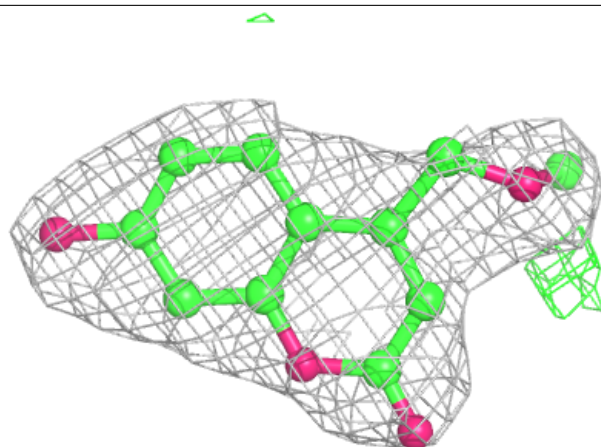
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	A1L2Z	K	201	15/15	0.81	0.14	41,50,61,63	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 A1L2Z K 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.