



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:21 PM EDT

PDB ID : 4B95 / pdb_00004b95
Title : pVHL-EloB-EloB-EloC complex_(2S,4R)-1-(2-chlorophenyl)carbonyl-N-[(4-chlorophenyl)methyl]-4-oxidanyl-pyrrolidine-2-carboxamide bound
Authors : Buckley, D.L.; Gustafson, J.L.; VanMolle, I.; Roth, A.G.; SeopTae, H.; Gareiss, P.C.; Jorgensen, W.L.; Ciulli, A.; Crews, C.M.
Deposited on : 2012-08-31
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

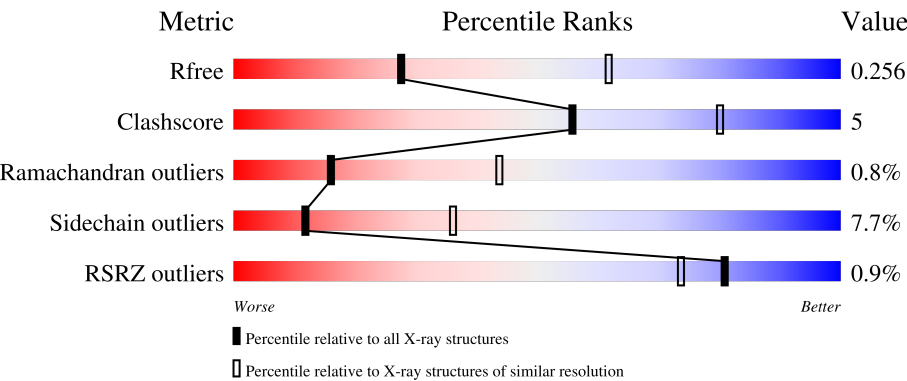
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	118	% 73% 15% • 11%
1	D	118	2% 63% 16% •• 19%
1	G	118	76% 10% • 13%
1	J	118	3% 77% 9% 14%

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Mol	Chain	Length	Quality of chain
2	B	97	68% 21% • 10%
2	E	97	67% 20% • 10%
2	H	97	% 69% 20% • 10%
2	K	97	% 69% 19% • 11%
3	C	162	69% 12% • 17%
3	F	162	% 74% 10% • 14%
3	I	162	73% 15% • 11%
3	L	162	% 69% 15% •• 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10217 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 TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	1
			782	499	134	145	4			
1	D	95	Total	C	N	O	S	0	0	0
			676	431	111	131	3			
1	G	103	Total	C	N	O	S	0	0	0
			759	485	125	145	4			
1	J	102	Total	C	N	O	S	0	0	0
			769	492	126	147	4			

- Molecule 2 is a protein called TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	1	0
			696	449	111	130	6			
2	E	87	Total	C	N	O	S	0	0	0
			667	431	104	126	6			
2	H	87	Total	C	N	O	S	0	0	0
			654	423	104	122	5			
2	K	86	Total	C	N	O	S	0	0	0
			666	432	107	120	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15369
B	17	MET	-	expression tag	UNP Q15369
E	16	MET	-	expression tag	UNP Q15369
E	17	MET	-	expression tag	UNP Q15369
H	16	MET	-	expression tag	UNP Q15369
H	17	MET	-	expression tag	UNP Q15369
K	16	MET	-	expression tag	UNP Q15369

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Chain	Residue	Modelled	Actual	Comment	Reference
K	17	MET	-	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	134	Total	C	N	O	S	0	0	0
			1008	649	177	180	2			
3	F	139	Total	C	N	O	S	0	0	0
			1050	672	183	193	2			
3	I	144	Total	C	N	O	S	0	0	0
			1079	695	187	195	2			
3	L	140	Total	C	N	O	S	0	1	0
			1110	713	196	199	2			

There are 8 discrepancies between the modelled and reference sequences:

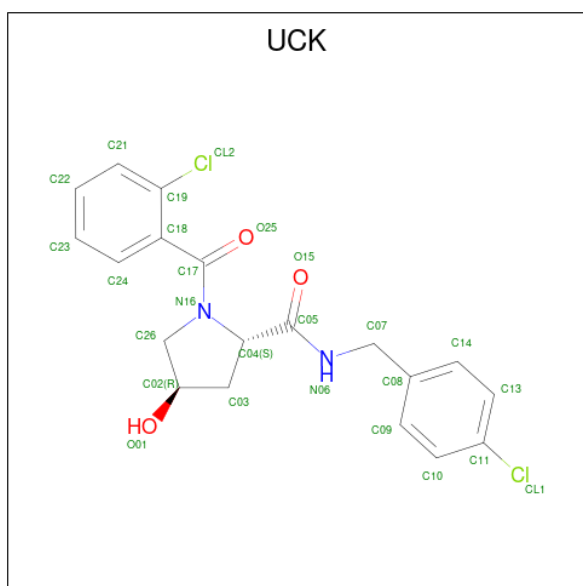
Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337
I	52	GLY	-	expression tag	UNP P40337
I	53	SER	-	expression tag	UNP P40337
L	52	GLY	-	expression tag	UNP P40337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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 5 is (2S,4R)-1-(2-chlorophenyl)carbonyl-N-[(4-chlorophenyl)methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: UCK) (formula: $C_{19}H_{18}Cl_2N_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Cl	N	O	0	0
			26	19	2	2	3		
5	F	1	Total	C	Cl	N	O	0	0
			26	19	2	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	Cl	N	O	
			26	19	2	2	3	
5	L	1	Total	C	Cl	N	O	
			26	19	2	2	3	

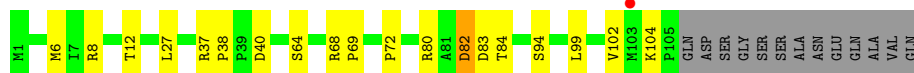
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O		
			12	12	0	0
6	B	21	Total	O		
			21	21	0	0
6	C	21	Total	O		
			21	21	0	0
6	D	14	Total	O		
			14	14	0	0
6	E	13	Total	O		
			13	13	0	0
6	F	22	Total	O		
			22	22	0	0
6	G	19	Total	O		
			19	19	0	0
6	H	9	Total	O		
			9	9	0	0
6	I	13	Total	O		
			13	13	0	0
6	J	22	Total	O		
			22	22	0	0
6	K	14	Total	O		
			14	14	0	0
6	L	13	Total	O		
			13	13	0	0

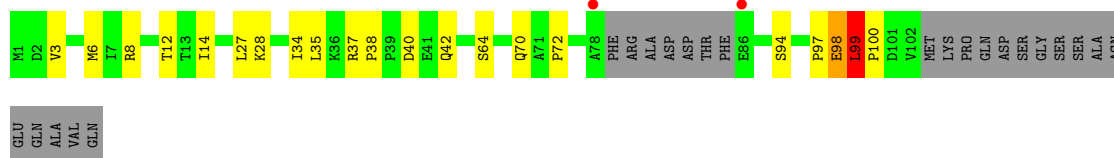
3 Residue-property plots [i](#)

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

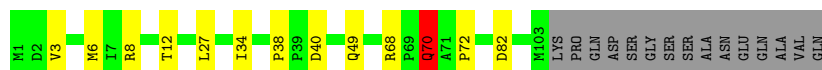
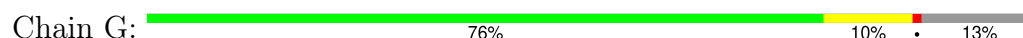
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



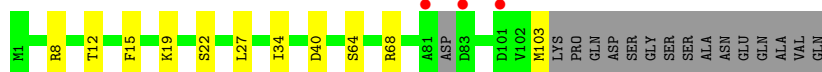
- Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



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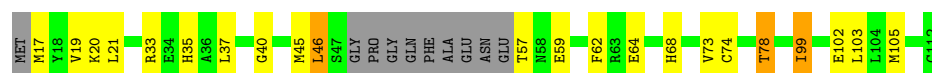


- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



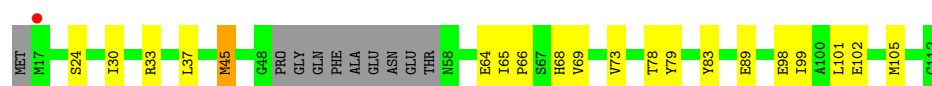
- Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain E: 



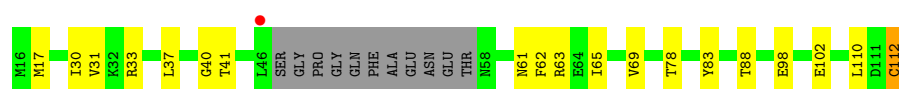
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain H: 



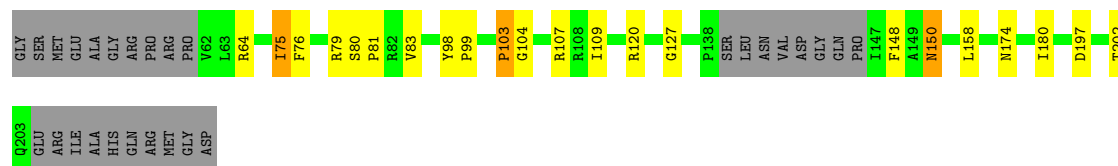
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

Chain K: 



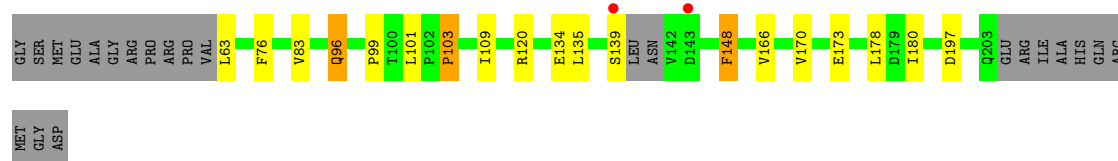
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain C: 



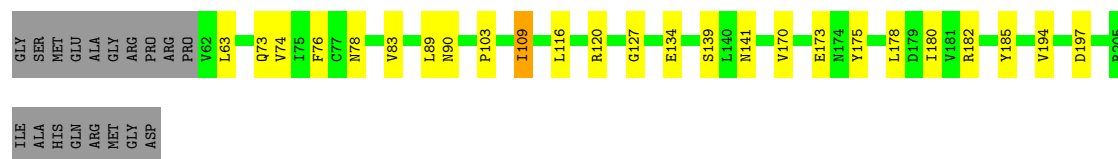
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain F: 

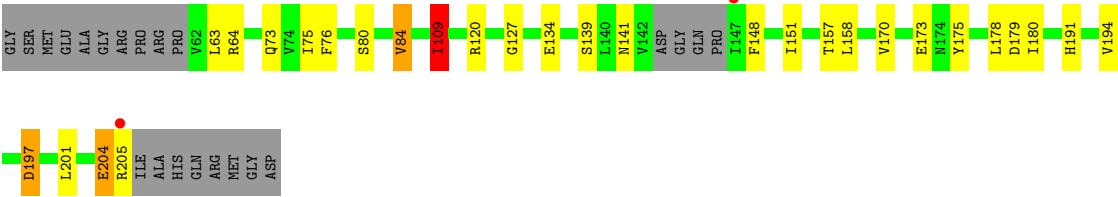


• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

Chain I: 



• 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, α , β , γ	93.04Å 93.04Å 362.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.59 – 2.80 27.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (27.59-2.80) 95.4 (27.59-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.80Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.185 , 0.236 0.202 , 0.256	Depositor DCC
R_{free} test set	1960 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10217	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 28.70 % 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 1.7596e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.89	1/798 (0.1%)	1.26	2/1085 (0.2%)
1	D	0.95	1/688 (0.1%)	1.40	6/939 (0.6%)
1	G	0.79	0/775	1.28	3/1058 (0.3%)
1	J	0.80	0/784	1.25	1/1064 (0.1%)
2	B	0.82	0/710	1.32	4/959 (0.4%)
2	E	0.85	0/681	1.38	3/923 (0.3%)
2	H	0.92	0/667	1.31	2/906 (0.2%)
2	K	0.88	0/680	1.47	7/920 (0.8%)
3	C	0.86	1/1035 (0.1%)	1.31	3/1422 (0.2%)
3	F	0.88	0/1078	1.33	3/1482 (0.2%)
3	I	0.89	0/1109	1.29	3/1528 (0.2%)
3	L	0.90	1/1138 (0.1%)	1.34	4/1557 (0.3%)
All	All	0.87	4/10143 (0.0%)	1.33	41/13843 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	80	SER	CA-C	5.70	1.57	1.52
1	A	104	LYS	C-N	-5.60	1.25	1.34
3	C	80	SER	CA-C	5.53	1.57	1.52
1	D	98	GLU	CA-C	5.31	1.59	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	178	LEU	N-CA-C	12.71	126.33	111.71
1	D	99	LEU	CA-C-N	8.95	128.68	119.64
1	D	99	LEU	C-N-CA	8.95	128.68	119.64
3	F	96	GLN	CB-CA-C	7.93	118.98	110.17
2	K	62	PHE	CA-C-N	7.27	134.78	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	62	PHE	C-N-CA	7.27	134.78	121.70
1	D	100	PRO	N-CA-CB	7.25	110.20	103.46
2	K	65	ILE	N-CA-C	6.86	114.34	107.55
3	F	103	PRO	N-CA-C	6.79	126.46	112.47
3	I	76	PHE	CA-CB-CG	6.56	120.36	113.80
2	K	62	PHE	CA-CB-CG	6.38	120.18	113.80
3	L	76	PHE	CA-CB-CG	6.34	120.14	113.80
3	F	76	PHE	CA-CB-CG	6.29	120.09	113.80
2	E	73	VAL	N-CA-C	-6.16	104.74	110.53
3	C	76	PHE	CA-CB-CG	6.12	119.92	113.80
2	K	40	GLY	CA-C-N	6.02	128.27	120.44
2	K	40	GLY	C-N-CA	6.02	128.27	120.44
1	A	8	ARG	N-CA-C	5.94	118.58	108.90
2	B	86	SER	N-CA-C	5.78	120.83	113.55
3	C	202	THR	N-CA-C	-5.75	105.18	114.09
1	D	8	ARG	N-CA-C	5.73	118.25	108.90
1	J	8	ARG	N-CA-C	5.55	117.94	108.90
3	I	78	ASN	CA-CB-CG	5.48	118.08	112.60
1	G	70	GLN	CA-CB-CG	5.42	124.94	114.10
1	D	99	LEU	N-CA-C	5.35	121.64	109.81
1	D	38	PRO	N-CA-C	5.32	116.27	110.58
3	L	84	VAL	N-CA-C	5.28	116.19	108.58
3	C	64	ARG	N-CA-C	5.24	117.84	110.14
2	E	40	GLY	CA-C-N	5.21	127.21	120.44
2	E	40	GLY	C-N-CA	5.21	127.21	120.44
2	K	83	TYR	N-CA-C	5.19	119.32	112.89
2	B	65	ILE	N-CA-C	5.18	112.99	107.76
1	G	38	PRO	N-CA-C	5.14	116.08	110.58
1	G	8	ARG	N-CA-C	5.13	117.27	108.90
3	I	90	ASN	CA-CB-CG	5.13	117.73	112.60
2	B	40	GLY	CA-C-N	5.12	127.40	120.44
2	B	40	GLY	C-N-CA	5.12	127.40	120.44
1	A	38	PRO	N-CA-C	5.11	116.05	110.58
3	L	109	ILE	CA-CB-CG2	5.08	119.14	110.50
2	H	83	TYR	N-CA-C	5.08	119.19	112.89
2	H	73	VAL	N-CA-C	-5.00	105.83	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	782	0	760	7	0
1	D	676	0	624	7	0
1	G	759	0	712	3	0
1	J	769	0	748	4	0
2	B	696	0	686	10	0
2	E	667	0	635	11	0
2	H	654	0	621	10	0
2	K	666	0	645	10	0
3	C	1008	0	934	16	0
3	F	1050	0	977	7	0
3	I	1079	0	1004	10	0
3	L	1110	0	1076	13	0
4	B	4	0	3	0	0
5	C	26	0	18	3	0
5	F	26	0	18	2	0
5	I	26	0	18	0	0
5	L	26	0	18	1	0
6	A	12	0	0	0	0
6	B	21	0	0	2	0
6	C	21	0	0	0	0
6	D	14	0	0	0	0
6	E	13	0	0	1	0
6	F	22	0	0	0	0
6	G	19	0	0	0	0
6	H	9	0	0	0	0
6	I	13	0	0	0	0
6	J	22	0	0	0	0
6	K	14	0	0	0	0
6	L	13	0	0	0	0
All	All	10217	0	9497	91	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 5.

All (91) 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)
2:E:57:THR:HA	2:E:59:GLU:H	1.35	0.92
3:C:104:GLY:O	2:K:63:ARG:HB3	1.80	0.82
3:L:120[B]:ARG:CD	3:L:127:GLY:HA2	2.20	0.70
3:L:120[B]:ARG:HD2	3:L:127:GLY:HA2	1.73	0.69
3:L:109:ILE:HG12	5:L:1206:UCK:C13	2.25	0.67
2:E:19:VAL:HG11	2:E:46:LEU:HD21	1.78	0.64
2:E:99:ILE:HD13	2:E:103:LEU:HB2	1.80	0.63
3:C:99:PRO:HB2	3:C:107:ARG:HH12	1.63	0.63
1:A:102:VAL:HG23	3:C:174:ASN:HB3	1.81	0.62
2:H:101:LEU:HD11	3:I:178:LEU:HD22	1.83	0.60
3:I:170:VAL:HG11	3:I:178:LEU:HD11	1.83	0.60
1:D:34:ILE:HG22	1:D:35:LEU:HD12	1.84	0.59
2:B:102:GLU:HA	2:B:105:MET:HE2	1.85	0.59
1:A:102:VAL:CG2	3:C:174:ASN:HB3	2.33	0.58
3:C:75:ILE:HD12	2:K:41:THR:HG23	1.85	0.58
3:I:73:GLN:H	3:I:141:ASN:HD21	1.51	0.57
3:F:83:VAL:HG22	3:F:103:PRO:HD3	1.87	0.56
1:A:94:SER:H	2:B:67:SER:HB2	1.71	0.56
2:E:102:GLU:HA	2:E:105:MET:HE2	1.88	0.56
1:G:70:GLN:HG3	2:H:79:TYR:CD1	2.40	0.55
3:F:166:VAL:O	3:F:170:VAL:HG12	2.06	0.55
2:H:102:GLU:HA	2:H:105:MET:HE2	1.88	0.55
3:C:79:ARG:HE	3:C:150:ASN:HD21	1.54	0.54
3:I:83:VAL:HG22	3:I:103:PRO:HD3	1.89	0.54
3:L:73:GLN:H	3:L:141:ASN:HD21	1.55	0.54
1:D:34:ILE:HG22	1:D:35:LEU:CD1	2.38	0.53
3:I:74:VAL:HB	3:I:109:ILE:HD13	1.89	0.53
3:C:107:ARG:NH1	5:C:1206:UCK:CL1	2.79	0.53
2:K:112:CYS:OXT	3:L:157:THR:HB	2.09	0.53
1:D:28:LYS:HA	1:D:42:GLN:HE22	1.73	0.52
3:F:148:PHE:CZ	2:H:45:MET:HG3	2.44	0.52
3:C:98:TYR:OH	5:C:1206:UCK:H262	2.10	0.52
3:L:120[A]:ARG:HD2	3:L:194:VAL:HG22	1.92	0.52
1:D:94:SER:O	2:E:68:HIS:HB3	2.10	0.51
2:K:61:ASN:O	2:K:63:ARG:NE	2.32	0.51
6:B:2019:HOH:O	3:C:81:PRO:HD3	2.09	0.51
3:F:170:VAL:HG11	3:F:178:LEU:HD11	1.92	0.51
3:I:74:VAL:HB	3:I:109:ILE:CD1	2.41	0.51
2:B:72:LYS:HE3	6:B:2015:HOH:O	2.11	0.50
1:J:34:ILE:HG21	2:K:30:ILE:HG21	1.92	0.50
2:K:112:CYS:HB3	3:L:158:LEU:HB3	1.93	0.50
3:C:99:PRO:HD2	5:C:1206:UCK:CL1	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:170:VAL:HG13	3:I:175:TYR:CE1	2.49	0.48
2:B:20:LYS:HB3	2:B:59:GLU:HG2	1.95	0.48
3:C:79:ARG:NE	3:C:150:ASN:HD21	2.11	0.47
3:C:120:ARG:HD3	3:C:127:GLY:HA2	1.97	0.47
3:F:134:GLU:HB3	3:F:135:LEU:HD22	1.96	0.47
1:J:19:LYS:O	1:J:22:SER:HB3	2.14	0.47
1:D:6:MET:HE2	1:D:72:PRO:HG2	1.97	0.47
1:A:6:MET:HE2	1:A:72:PRO:HG2	1.97	0.47
2:E:64:GLU:HB2	6:E:2004:HOH:O	2.15	0.47
3:L:120[A]:ARG:HH22	3:L:197:ASP:CG	2.23	0.47
3:L:175:TYR:HE2	3:L:191:HIS:HE1	1.62	0.46
2:K:33:ARG:O	2:K:37:LEU:HG	2.16	0.46
1:J:103:MET:HG2	3:L:170:VAL:HG22	1.97	0.46
2:B:37:LEU:HD22	2:B:43:LYS:HG3	1.98	0.45
3:I:120:ARG:HD3	3:I:127:GLY:HA2	1.98	0.45
2:E:20:LYS:HB3	2:E:59:GLU:HG2	1.98	0.45
2:H:33:ARG:O	2:H:37:LEU:HG	2.17	0.45
1:A:82:ASP:HA	1:A:83:ASP:HA	1.88	0.44
3:F:99:PRO:HD2	5:F:1206:UCK:CL1	2.54	0.44
3:F:109:ILE:HG13	5:F:1206:UCK:C13	2.48	0.44
3:L:84:VAL:HG21	3:L:151:ILE:HG21	2.00	0.44
3:L:120[B]:ARG:HD3	3:L:127:GLY:HA2	1.98	0.44
3:C:79:ARG:HG3	3:C:150:ASN:ND2	2.33	0.43
1:G:34:ILE:HG21	2:H:30:ILE:HG21	1.99	0.43
1:A:69:PRO:HG2	2:B:82[A]:ARG:HG2	2.01	0.43
2:H:66:PRO:HD2	2:H:69:VAL:HB	2.01	0.43
2:K:69:VAL:HG21	2:K:102:GLU:HB3	2.01	0.43
2:B:21:LEU:HD22	2:B:62:PHE:HE2	1.84	0.43
2:B:33:ARG:O	2:B:37:LEU:HG	2.18	0.43
2:H:65:ILE:HA	2:H:66:PRO:HD3	1.95	0.42
2:E:21:LEU:HD22	2:E:62:PHE:HE2	1.84	0.42
3:I:89:LEU:HD12	3:I:116:LEU:HB3	2.01	0.42
2:H:68:HIS:HD2	2:H:99:ILE:HG22	1.85	0.42
2:B:112:CYS:OXT	3:C:158:LEU:N	2.49	0.42
3:C:83:VAL:HG22	3:C:103:PRO:HD3	2.00	0.42
3:C:79:ARG:HE	3:C:150:ASN:ND2	2.17	0.42
1:J:15:PHE:HB2	2:K:31:VAL:HG12	2.02	0.42
1:D:99:LEU:HD13	1:D:99:LEU:HA	1.90	0.42
2:B:98:GLU:H	2:B:98:GLU:CD	2.28	0.41
2:E:33:ARG:O	2:E:37:LEU:HG	2.20	0.41
1:D:14:ILE:HD11	1:D:35:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:NH2	1:A:80:ARG:O	2.54	0.40
3:I:182:ARG:HA	3:I:185:TYR:HD2	1.86	0.40
3:L:204:GLU:HA	3:L:205:ARG:HA	1.88	0.40
2:E:35:HIS:HD2	2:E:78:THR:HG22	1.86	0.40
2:E:74:CYS:O	2:E:78:THR:HG23	2.21	0.40
1:G:6:MET:HE2	1:G:72:PRO:HG2	2.03	0.40
2:H:98:GLU:CD	2:H:98:GLU:H	2.29	0.40
2:K:98:GLU:H	2:K:98:GLU:CD	2.29	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	103/118 (87%)	97 (94%)	4 (4%)	2 (2%)	6	22
1	D	91/118 (77%)	85 (93%)	3 (3%)	3 (3%)	3	11
1	G	101/118 (86%)	95 (94%)	5 (5%)	1 (1%)	12	38
1	J	98/118 (83%)	95 (97%)	3 (3%)	0	100	100
2	B	84/97 (87%)	79 (94%)	4 (5%)	1 (1%)	10	34
2	E	83/97 (86%)	80 (96%)	3 (4%)	0	100	100
2	H	83/97 (86%)	77 (93%)	5 (6%)	1 (1%)	10	34
2	K	82/97 (84%)	76 (93%)	6 (7%)	0	100	100
3	C	130/162 (80%)	122 (94%)	7 (5%)	1 (1%)	16	44
3	F	135/162 (83%)	127 (94%)	8 (6%)	0	100	100
3	I	142/162 (88%)	135 (95%)	7 (5%)	0	100	100
3	L	137/162 (85%)	128 (93%)	8 (6%)	1 (1%)	18	47
All	All	1269/1508 (84%)	1196 (94%)	63 (5%)	10 (1%)	16	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	99	LEU
2	H	89	GLU
1	A	84	THR
2	B	88	THR
1	G	82	ASP
3	L	179	ASP
1	A	82	ASP
1	D	98	GLU
3	C	103	PRO
1	D	97	PRO

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	80/103 (78%)	74 (92%)	6 (8%)	12	37
1	D	65/103 (63%)	57 (88%)	8 (12%)	4	16
1	G	76/103 (74%)	69 (91%)	7 (9%)	8	27
1	J	81/103 (79%)	76 (94%)	5 (6%)	16	45
2	B	77/86 (90%)	73 (95%)	4 (5%)	21	53
2	E	71/86 (83%)	66 (93%)	5 (7%)	14	40
2	H	67/86 (78%)	63 (94%)	4 (6%)	17	47
2	K	70/86 (81%)	65 (93%)	5 (7%)	13	39
3	C	102/148 (69%)	96 (94%)	6 (6%)	18	48
3	F	110/148 (74%)	101 (92%)	9 (8%)	10	33
3	I	111/148 (75%)	103 (93%)	8 (7%)	13	39
3	L	120/148 (81%)	108 (90%)	12 (10%)	7	24
All	All	1030/1348 (76%)	951 (92%)	79 (8%)	12	36

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	27	LEU
1	A	40	ASP
1	A	64	SER
1	A	68	ARG
1	A	99	LEU
2	B	45	MET
2	B	78	THR
2	B	80	LYS
2	B	112	CYS
3	C	75	ILE
3	C	109	ILE
3	C	148	PHE
3	C	150	ASN
3	C	180	ILE
3	C	197	ASP
1	D	3	VAL
1	D	12	THR
1	D	27	LEU
1	D	37	ARG
1	D	40	ASP
1	D	64	SER
1	D	70	GLN
1	D	99	LEU
2	E	17	MET
2	E	45	MET
2	E	46	LEU
2	E	78	THR
2	E	99	ILE
3	F	63	LEU
3	F	96	GLN
3	F	101	LEU
3	F	120	ARG
3	F	139	SER
3	F	148	PHE
3	F	173	GLU
3	F	180	ILE
3	F	197	ASP
1	G	3	VAL
1	G	12	THR
1	G	27	LEU
1	G	40	ASP
1	G	49	GLN

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Mol	Chain	Res	Type
1	G	68	ARG
1	G	70	GLN
2	H	24	SER
2	H	45	MET
2	H	64	GLU
2	H	78	THR
3	I	63	LEU
3	I	109	ILE
3	I	134	GLU
3	I	139	SER
3	I	173	GLU
3	I	180	ILE
3	I	194	VAL
3	I	197	ASP
1	J	12	THR
1	J	27	LEU
1	J	40	ASP
1	J	64	SER
1	J	68	ARG
2	K	17	MET
2	K	78	THR
2	K	88	THR
2	K	110	LEU
2	K	112	CYS
3	L	63	LEU
3	L	64	ARG
3	L	75	ILE
3	L	109	ILE
3	L	134	GLU
3	L	139	SER
3	L	148	PHE
3	L	173	GLU
3	L	180	ILE
3	L	197	ASP
3	L	201	LEU
3	L	204	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	58	ASN
3	C	150	ASN

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Mol	Chain	Res	Type
3	C	191	HIS
1	D	42	GLN
1	D	70	GLN
2	E	61	ASN
3	F	150	ASN
3	F	174	ASN
3	F	191	HIS
1	G	10	HIS
2	H	27	HIS
3	I	141	ASN
3	I	193	ASN
1	J	10	HIS
2	K	58	ASN
3	L	141	ASN
3	L	150	ASN
3	L	191	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	UCK	L	1206	-	28,28,28	2.40	9 (32%)	39,39,39	1.16	5 (12%)
5	UCK	F	1206	-	28,28,28	2.48	7 (25%)	39,39,39	1.20	5 (12%)
5	UCK	I	1206	-	28,28,28	2.57	8 (28%)	39,39,39	1.23	4 (10%)
5	UCK	C	1206	-	28,28,28	2.56	8 (28%)	39,39,39	1.41	8 (20%)
4	ACT	B	1113	-	3,3,3	1.32	1 (33%)	3,3,3	0.98	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
5	UCK	I	1206	-	-	2/17/29/29	0/3/3/3
5	UCK	F	1206	-	-	0/17/29/29	0/3/3/3
5	UCK	C	1206	-	-	0/17/29/29	0/3/3/3
5	UCK	L	1206	-	-	0/17/29/29	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1206	UCK	C17-N16	7.73	1.52	1.34
5	C	1206	UCK	C17-N16	7.70	1.52	1.34
5	C	1206	UCK	C05-N06	7.33	1.50	1.33
5	I	1206	UCK	C05-N06	7.15	1.50	1.33
5	L	1206	UCK	C17-N16	7.12	1.51	1.34
5	F	1206	UCK	C17-N16	7.05	1.50	1.34
5	F	1206	UCK	C05-N06	7.04	1.50	1.33
5	L	1206	UCK	C05-N06	6.54	1.48	1.33
5	I	1206	UCK	C18-C19	4.08	1.45	1.39
5	F	1206	UCK	C26-C02	-3.97	1.47	1.52
5	L	1206	UCK	C26-C02	-3.86	1.47	1.52
5	I	1206	UCK	C26-C02	-3.76	1.47	1.52
5	C	1206	UCK	C26-C02	-3.63	1.47	1.52
5	C	1206	UCK	C18-C19	3.30	1.44	1.39
5	F	1206	UCK	C18-C19	3.17	1.43	1.39
5	C	1206	UCK	C09-C08	2.87	1.44	1.38
5	L	1206	UCK	C18-C19	2.82	1.43	1.39
5	F	1206	UCK	C13-C11	2.69	1.43	1.38
5	C	1206	UCK	C13-C11	2.64	1.42	1.38
5	F	1206	UCK	C09-C08	2.61	1.44	1.38
5	L	1206	UCK	C09-C08	2.45	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1206	UCK	C04-C05	2.36	1.58	1.52
5	I	1206	UCK	C04-C05	2.34	1.58	1.52
5	I	1206	UCK	C13-C11	2.31	1.42	1.38
5	C	1206	UCK	C04-C05	2.23	1.58	1.52
5	L	1206	UCK	C13-C11	2.22	1.42	1.38
5	F	1206	UCK	C04-C05	2.16	1.58	1.52
5	L	1206	UCK	C26-N16	-2.13	1.44	1.47
5	I	1206	UCK	C09-C08	2.10	1.43	1.38
5	C	1206	UCK	C10-C11	2.10	1.41	1.38
5	I	1206	UCK	C18-C17	2.08	1.53	1.50
5	L	1206	UCK	C03-C04	-2.06	1.50	1.53
4	B	1113	ACT	CH3-C	2.02	1.57	1.49

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1206	UCK	C26-N16-C04	-3.60	107.06	111.83
5	C	1206	UCK	C26-N16-C04	-3.41	107.31	111.83
5	C	1206	UCK	C07-N06-C05	3.08	126.52	122.29
5	I	1206	UCK	C05-C04-N16	3.05	120.81	112.50
5	I	1206	UCK	C07-N06-C05	2.77	126.09	122.29
5	F	1206	UCK	C24-C18-C19	2.69	120.93	117.79
5	L	1206	UCK	C24-C18-C19	2.68	120.93	117.79
5	C	1206	UCK	C24-C18-C19	2.64	120.87	117.79
5	C	1206	UCK	C10-C11-CL1	2.53	123.10	119.36
5	F	1206	UCK	C08-C07-N06	2.46	118.25	113.07
5	F	1206	UCK	C13-C11-C10	-2.34	118.34	121.24
5	C	1206	UCK	C02-C26-N16	2.33	105.24	103.00
5	I	1206	UCK	C03-C04-N16	2.28	105.89	103.17
5	C	1206	UCK	C03-C04-N16	2.25	105.85	103.17
5	F	1206	UCK	C14-C13-C11	2.23	121.48	119.24
5	L	1206	UCK	C26-N16-C04	-2.13	109.01	111.83
5	F	1206	UCK	C10-C11-CL1	2.05	122.39	119.36
5	L	1206	UCK	C05-C04-N16	2.05	118.08	112.50
5	L	1206	UCK	C03-C04-N16	2.04	105.60	103.17
5	C	1206	UCK	C18-C17-N16	2.03	120.64	117.85
5	L	1206	UCK	C10-C11-CL1	2.03	122.35	119.36
5	C	1206	UCK	C21-C19-C18	-2.00	119.14	121.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1206	UCK	C03-C04-C05-O15
5	I	1206	UCK	C03-C04-C05-N06

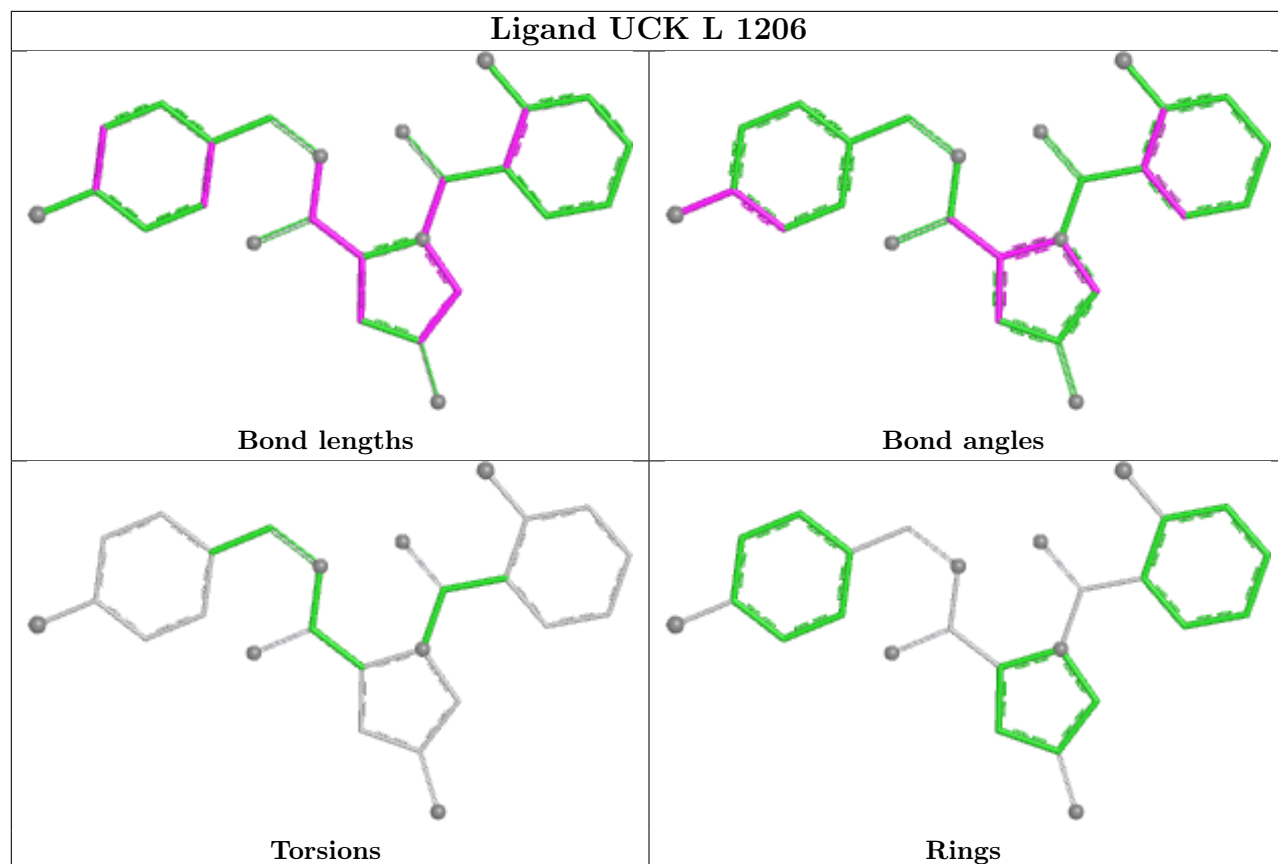
There are no ring outliers.

3 monomers are involved in 6 short contacts:

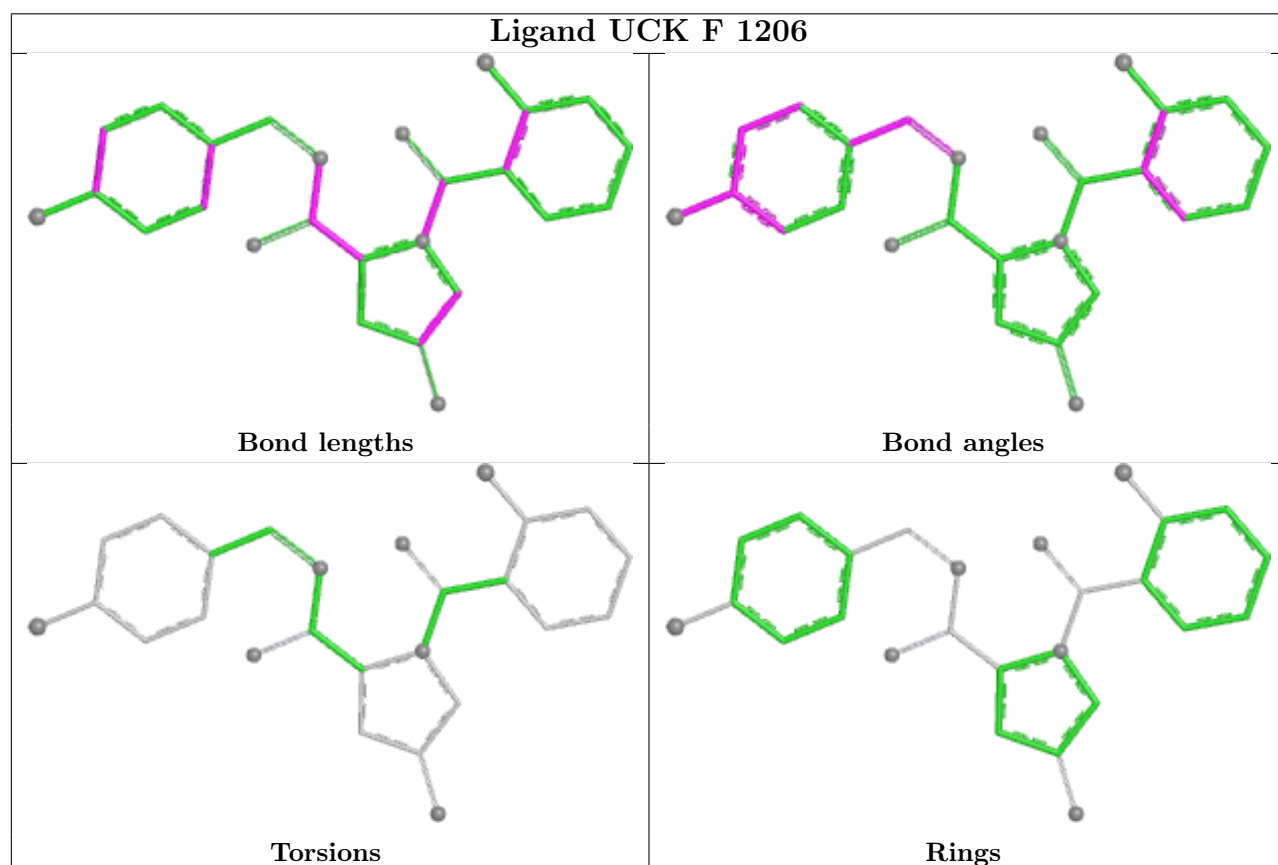
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1206	UCK	1	0
5	F	1206	UCK	2	0
5	C	1206	UCK	3	0

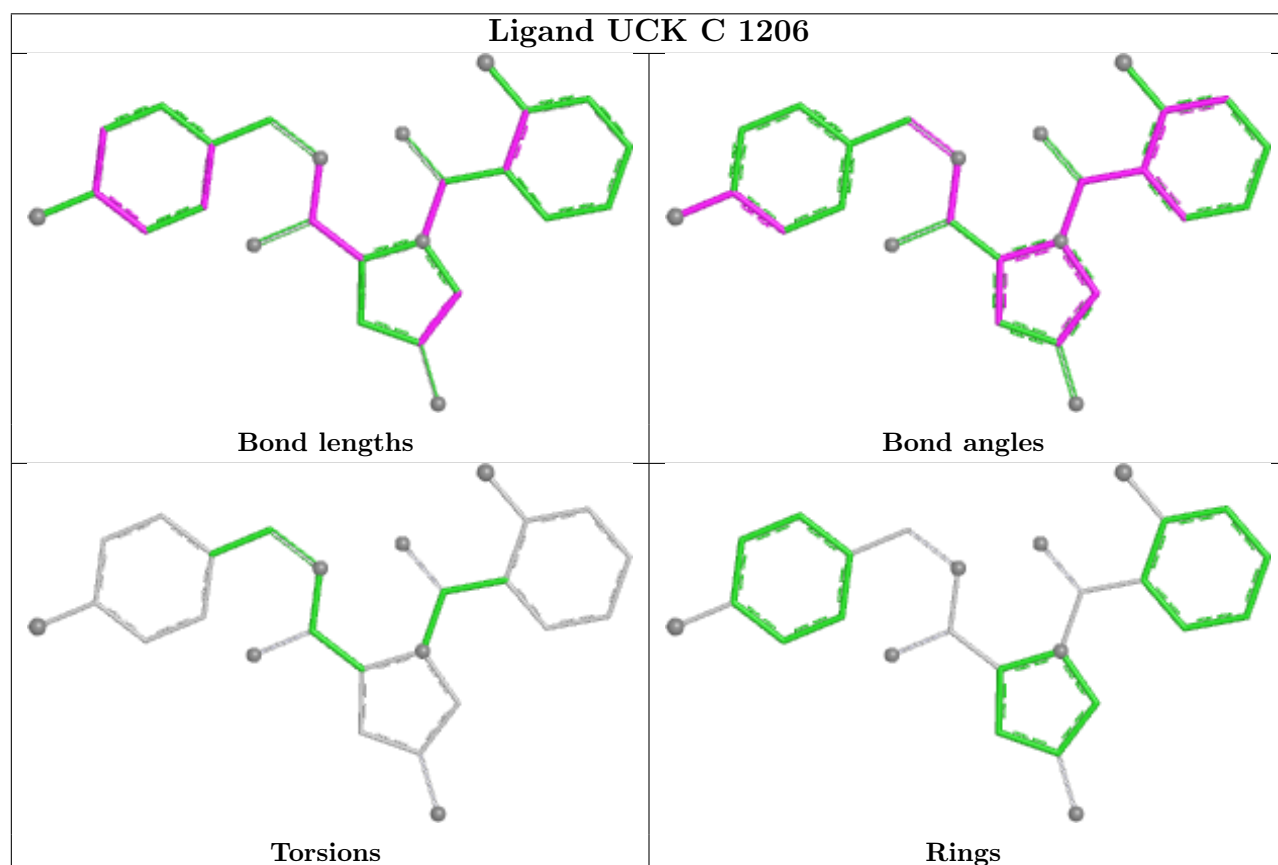
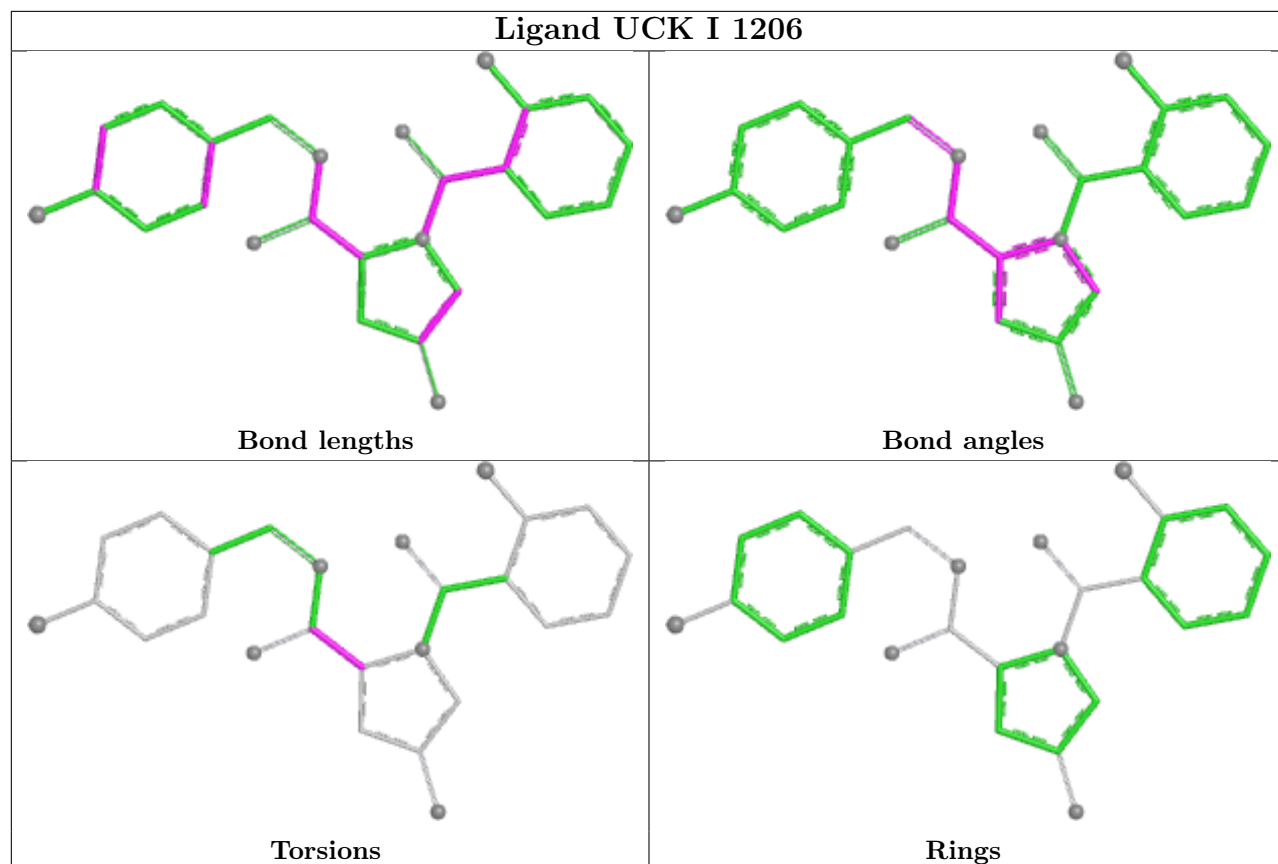
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand UCK L 1206



Ligand UCK F 1206





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/118 (88%)	-0.28	1 (0%) 79 72	33, 51, 95, 129	0
1	D	95/118 (80%)	-0.09	2 (2%) 63 54	42, 59, 87, 95	0
1	G	103/118 (87%)	-0.09	0 100 100	43, 64, 87, 99	0
1	J	102/118 (86%)	-0.25	3 (2%) 53 43	34, 53, 83, 99	0
2	B	87/97 (89%)	-0.32	0 100 100	22, 51, 81, 92	1 (1%)
2	E	87/97 (89%)	-0.29	0 100 100	35, 55, 83, 99	0
2	H	87/97 (89%)	-0.17	1 (1%) 78 70	39, 56, 90, 114	0
2	K	86/97 (88%)	-0.27	1 (1%) 76 68	34, 48, 81, 104	0
3	C	134/162 (82%)	-0.20	0 100 100	35, 56, 84, 99	0
3	F	139/162 (85%)	-0.21	2 (1%) 73 64	34, 57, 91, 121	0
3	I	144/162 (88%)	-0.25	0 100 100	38, 59, 80, 94	0
3	L	140/162 (86%)	-0.21	2 (1%) 73 64	17, 51, 82, 102	1 (0%)
All	All	1309/1508 (86%)	-0.22	12 (0%) 81 74	17, 56, 87, 129	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	78	ALA	2.7
1	J	81	ALA	2.7
1	J	83	ASP	2.6
1	J	101	ASP	2.6
3	L	147	ILE	2.3
3	F	143	ASP	2.2
2	K	46	LEU	2.2
1	D	86	GLU	2.2
2	H	17	MET	2.2
3	F	139	SER	2.1
1	A	103	MET	2.0

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Mol	Chain	Res	Type	RSRZ
3	L	205	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

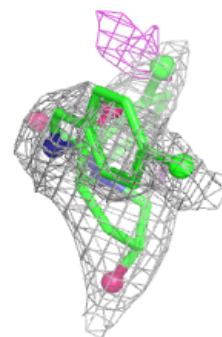
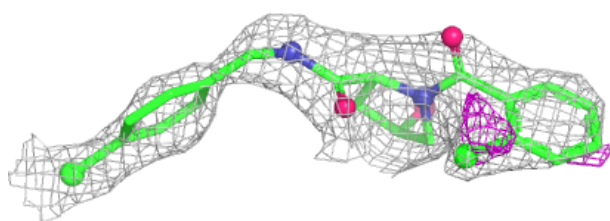
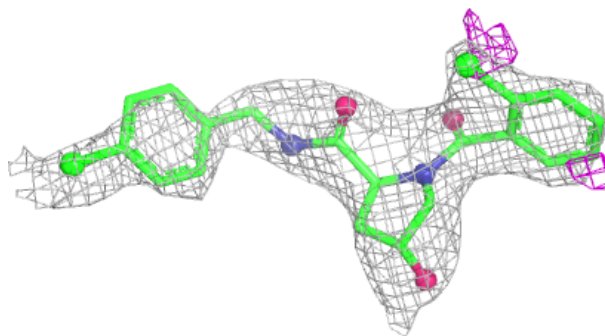
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	B	1113	4/4	0.82	0.18	56,57,59,66	0
5	UCK	F	1206	26/26	0.85	0.13	70,82,90,92	0
5	UCK	I	1206	26/26	0.88	0.11	60,65,73,83	0
5	UCK	C	1206	26/26	0.91	0.10	52,59,63,65	0
5	UCK	L	1206	26/26	0.91	0.09	45,52,57,63	0

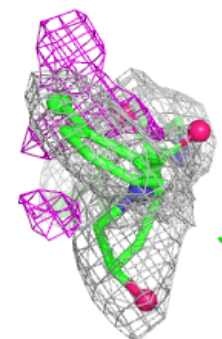
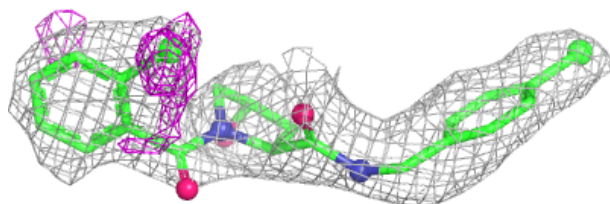
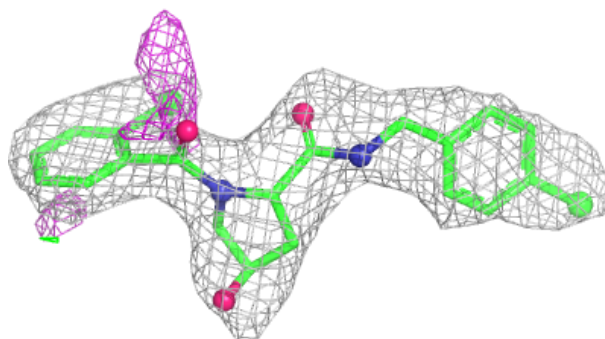
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UCK F 1206:

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

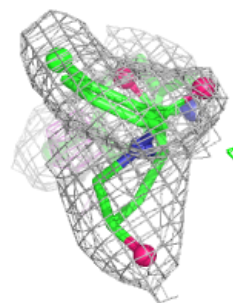
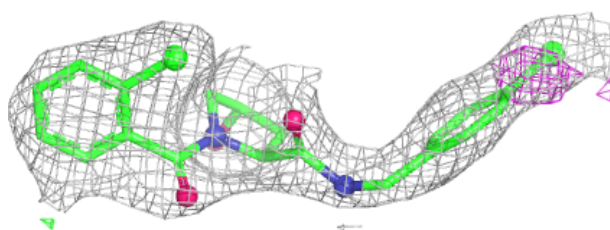
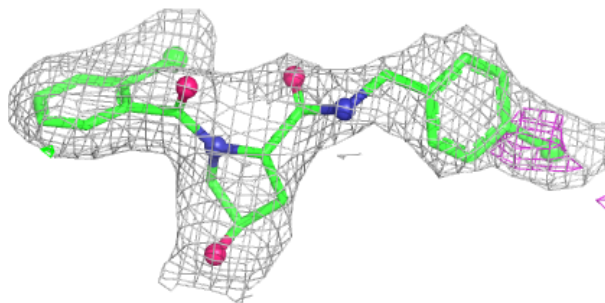
**Electron density around UCK I 1206:**

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

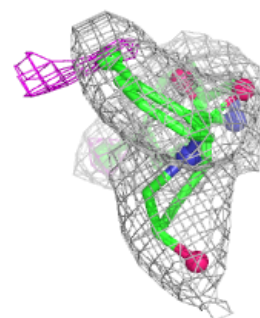
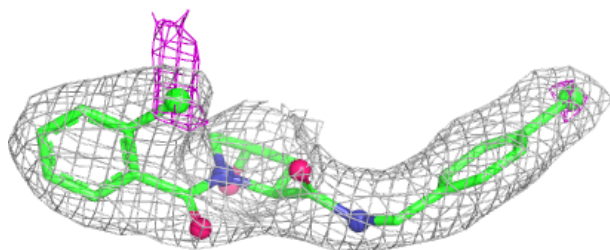
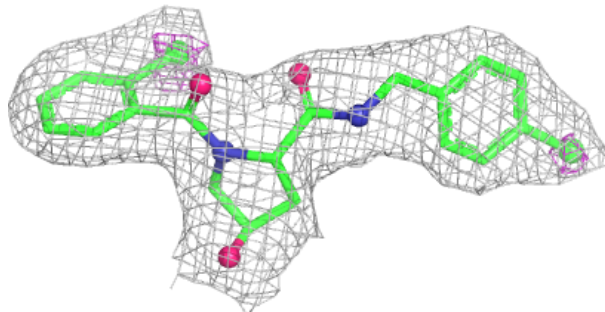


Electron density around UCK C 1206:

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

**Electron density around UCK L 1206:**

$2mF_o-DF_c$ (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.