



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:51 PM EDT

PDB ID : 6N0M / pdb_00006n0m
Title : CRYSTAL STRUCTURE OF SESTRIN2 IN COMPLEX WITH NV-0005138
Authors : O'Neill, D.
Deposited on : 2018-11-07
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

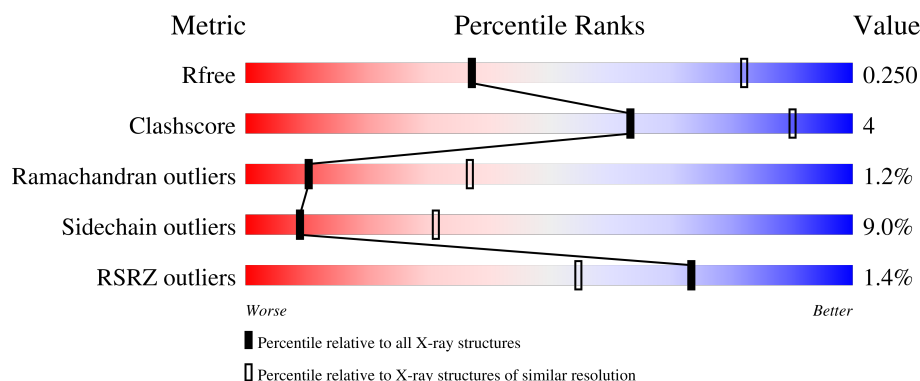
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	415	0.2% 75% 12% 12%
1	B	415	0.2% 76% 11% 12%
1	C	415	2% 71% 14% 12%
1	D	415	0.2% 70% 15% 12%
1	E	415	0.2% 67% 18% 12%

2 Entry composition [i](#)

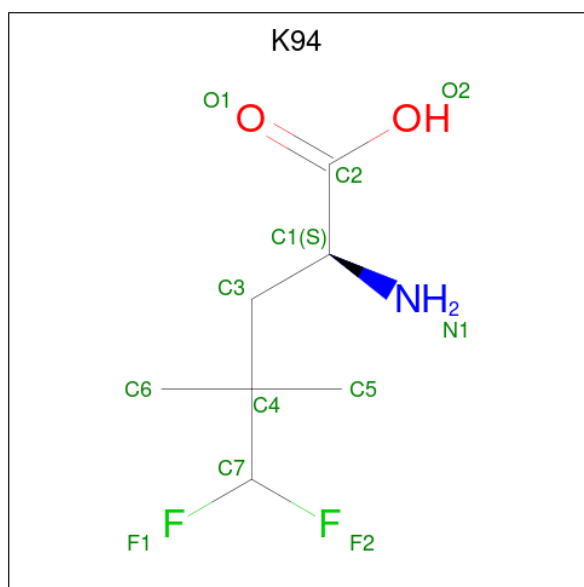
There are 2 unique types of molecules in this entry. The entry contains 14811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sestrin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2962	1897	513	534	18			
1	B	365	Total	C	N	O	S	0	0	0
			2936	1883	507	528	18			
1	C	364	Total	C	N	O	S	0	0	0
			2952	1892	511	531	18			
1	D	364	Total	C	N	O	S	0	0	0
			2945	1888	508	531	18			
1	E	365	Total	C	N	O	S	0	0	0
			2956	1894	512	532	18			

- Molecule 2 is 4-(difluoromethyl)-L-leucine (CCD ID: K94) (formula: $C_7H_{13}F_2NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			12	7	2	1	2		

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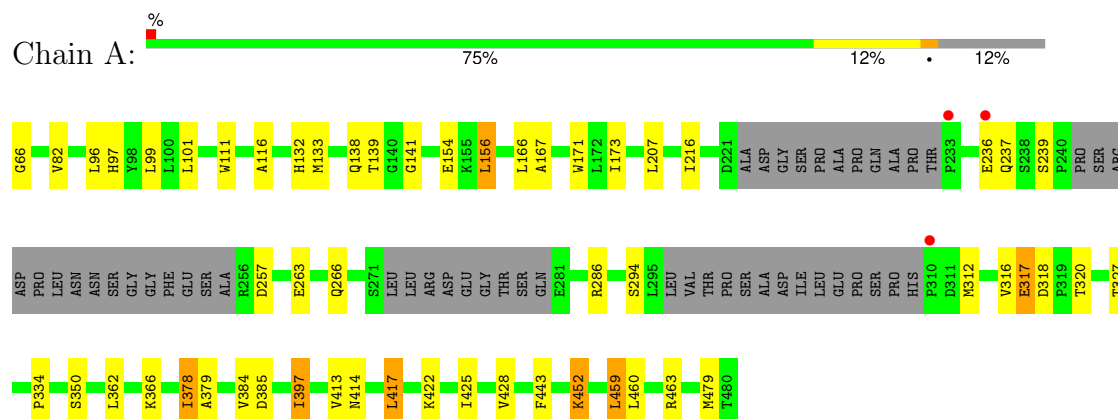
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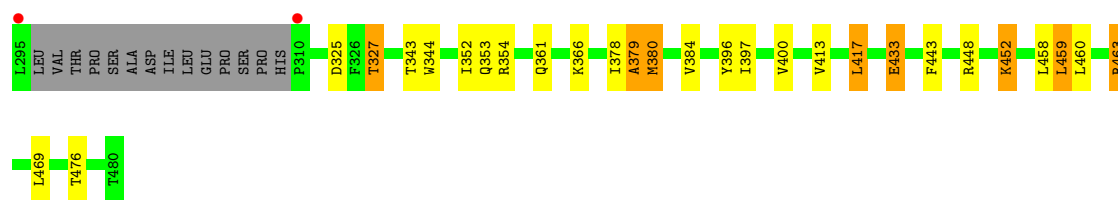
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			12	7	2	1	2		
2	C	1	Total	C	F	N	O	0	0
			12	7	2	1	2		
2	D	1	Total	C	F	N	O	0	0
			12	7	2	1	2		
2	E	1	Total	C	F	N	O	0	0
			12	7	2	1	2		

3 Residue-property plots [i](#)

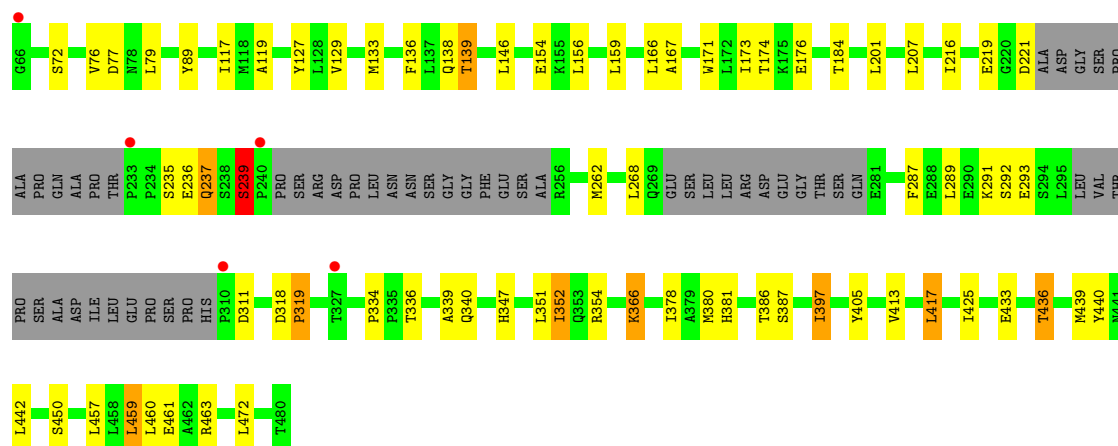
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sestrin-2

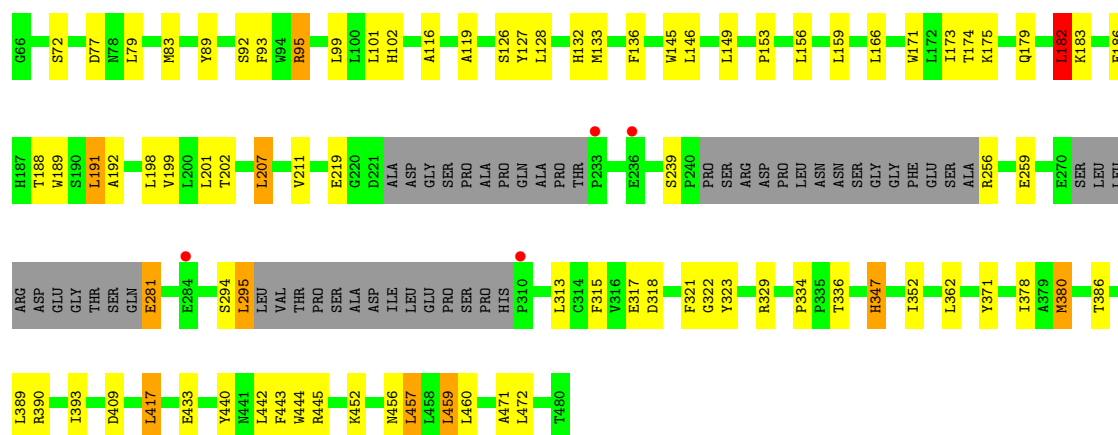




• Molecule 1: Sestrin-2



• Molecule 1: Sestrin-2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	290.41Å 290.41Å 290.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 3.30 48.40 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.40-3.30) 99.9 (48.40-3.30)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.184 , 0.250 0.187 , 0.250	Depositor DCC
R_{free} test set	3048 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	112.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 88.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14811	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K94

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	0.82	1/3039 (0.0%)	1.08	4/4115 (0.1%)
1	B	0.81	0/3013	1.09	5/4083 (0.1%)
1	C	0.78	1/3029 (0.0%)	1.05	3/4101 (0.1%)
1	D	0.80	1/3022 (0.0%)	1.07	1/4093 (0.0%)
1	E	0.75	0/3033	1.07	6/4107 (0.1%)
All	All	0.79	3/15136 (0.0%)	1.07	19/20499 (0.1%)

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
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	239	SER	CA-C	8.48	1.63	1.52
1	D	239	SER	CA-C	6.95	1.61	1.52
1	A	66	GLY	N-CA	5.21	1.53	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	186	GLU	N-CA-C	-7.61	102.68	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	HIS	N-CA-C	6.99	118.82	110.44
1	D	352	ILE	N-CA-C	-6.71	104.11	110.42
1	E	323	TYR	N-CA-C	-5.96	104.87	111.36
1	A	316	VAL	N-CA-C	5.91	117.22	108.65
1	E	456	ASN	N-CA-C	5.81	118.36	111.33
1	A	141	GLY	N-CA-C	-5.65	104.45	112.37
1	C	284	GLU	N-CA-C	5.63	119.67	112.34
1	E	182	LEU	N-CA-C	-5.56	102.25	110.48
1	E	183	LYS	N-CA-C	5.52	119.20	111.74
1	C	259	GLU	N-CA-C	-5.40	105.08	110.97
1	B	152	ALA	CA-C-N	5.27	126.43	119.84
1	B	152	ALA	C-N-CA	5.27	126.43	119.84
1	E	199	VAL	N-CA-C	-5.23	105.51	110.42
1	C	78	ASN	N-CA-C	5.18	118.38	111.75
1	A	138	GLN	CA-CB-CG	5.09	124.28	114.10
1	B	169	ARG	CA-C-N	5.09	124.70	119.05
1	B	169	ARG	C-N-CA	5.09	124.70	119.05
1	A	384	VAL	N-CA-C	5.05	115.85	108.53

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	233	PRO	Peptide
1	C	239	SER	Peptide
1	D	239	SER	Peptide
1	D	268	LEU	Peptide
1	E	322	GLY	Peptide

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	2962	0	2875	19	0
1	B	2936	0	2839	13	0
1	C	2952	0	2870	23	0
1	D	2945	0	2857	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2956	0	2870	32	0
2	A	12	0	0	0	0
2	B	12	0	0	1	0
2	C	12	0	0	0	0
2	D	12	0	0	0	0
2	E	12	0	0	0	0
All	All	14811	0	14311	115	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 4.

All (115) 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:B:116:ALA:HB1	1:B:132:HIS:CD2	2.18	0.79
1:E:378:ILE:HD11	1:E:386:THR:HG22	1.77	0.67
1:A:116:ALA:HB1	1:A:132:HIS:CD2	2.32	0.65
1:E:116:ALA:HB1	1:E:132:HIS:CD2	2.35	0.62
1:E:179:GLN:O	1:E:182:LEU:O	2.18	0.62
1:D:262:MET:SD	1:D:381:HIS:ND1	2.73	0.59
1:E:128:LEU:HD11	1:E:207:LEU:HB3	1.86	0.58
1:B:181:LEU:HD13	1:B:194:LEU:HD11	1.85	0.57
1:E:459:LEU:C	1:E:459:LEU:HD12	2.30	0.56
1:E:99:LEU:HD22	1:E:362:LEU:HD12	1.88	0.56
1:C:117:ILE:HG23	1:C:129:VAL:HG13	1.89	0.55
1:A:479:MET:HA	1:A:479:MET:HE2	1.90	0.54
1:C:379:ALA:O	1:C:448:ARG:HD3	2.09	0.53
1:D:166:LEU:HG	1:D:173:ILE:HD11	1.91	0.52
1:C:459:LEU:HD12	1:C:459:LEU:C	2.35	0.52
1:E:352:ILE:CD1	1:E:472:LEU:HD21	2.39	0.52
1:A:167:ALA:O	1:A:463:ARG:NH2	2.44	0.51
1:C:167:ALA:O	1:C:463:ARG:NH2	2.42	0.51
1:A:317:GLU:O	1:A:318:ASP:C	2.53	0.50
1:D:171:TRP:CE2	1:D:334:PRO:HB3	2.47	0.50
1:E:191:LEU:O	1:E:192:ALA:C	2.54	0.50
1:D:89:TYR:CD2	1:D:457:LEU:HD22	2.47	0.50
1:C:215:GLY:O	1:C:216:ILE:C	2.55	0.49
1:D:397:ILE:HD11	1:D:425:ILE:HG23	1.94	0.49
1:B:198:LEU:CD1	1:B:471:ALA:HB1	2.42	0.49
1:D:136:PHE:CD2	1:D:146:LEU:HD21	2.47	0.49
1:B:451:GLU:HG2	2:B:900:K94:N1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:TYR:CD2	1:E:457:LEU:HD22	2.48	0.49
1:E:77:ASP:HB2	1:E:127:TYR:OH	2.13	0.49
1:C:87:PRO:HA	1:C:90:PHE:HB3	1.94	0.49
1:C:413:VAL:HG13	1:C:417:LEU:HD22	1.94	0.49
1:E:145:TRP:CE2	1:E:153:PRO:HD3	2.47	0.49
1:A:378:ILE:HG23	1:A:378:ILE:O	2.13	0.48
1:B:396:TYR:O	1:B:399:CYS:HB3	2.12	0.48
1:D:79:LEU:HA	1:D:216:ILE:HD13	1.95	0.48
1:D:171:TRP:CD2	1:D:334:PRO:HB3	2.49	0.48
1:E:149:LEU:HB2	1:E:315:PHE:HA	1.95	0.47
1:E:171:TRP:CE2	1:E:334:PRO:HB3	2.49	0.47
1:A:99:LEU:HD22	1:A:362:LEU:HD12	1.96	0.47
1:D:318:ASP:N	1:D:319:PRO:CD	2.78	0.47
1:B:86:HIS:O	1:B:87:PRO:C	2.57	0.47
1:C:159:LEU:HD13	1:C:189:TRP:CZ2	2.50	0.47
1:C:378:ILE:O	1:C:380:MET:N	2.48	0.47
1:D:352:ILE:CD1	1:D:472:LEU:HD21	2.45	0.47
1:C:136:PHE:CD2	1:C:146:LEU:HD21	2.50	0.47
1:E:281:GLU:OE1	1:E:281:GLU:N	2.47	0.47
1:D:339:ALA:CB	1:D:405:TYR:CD1	2.98	0.46
1:E:378:ILE:CD1	1:E:386:THR:HG22	2.44	0.46
1:A:171:TRP:CE2	1:A:334:PRO:HB3	2.50	0.46
1:A:263:GLU:O	1:A:266:GLN:HB2	2.15	0.46
1:B:123:HIS:O	1:B:124:GLN:C	2.58	0.46
1:D:413:VAL:HG13	1:D:417:LEU:HD22	1.97	0.46
1:D:351:LEU:HD23	1:D:472:LEU:CD2	2.45	0.46
1:A:111:TRP:CE3	1:A:156:LEU:HD13	2.50	0.46
1:D:167:ALA:O	1:D:463:ARG:NH2	2.49	0.46
1:D:436:THR:HG23	1:D:439:MET:HE3	1.96	0.46
1:D:339:ALA:HB1	1:D:405:TYR:CE1	2.51	0.45
1:A:428:VAL:HG12	1:A:459:LEU:HD11	1.99	0.45
1:A:413:VAL:HG13	1:A:417:LEU:HD22	1.99	0.45
1:E:207:LEU:O	1:E:211:VAL:HG23	2.17	0.45
1:C:238:SER:O	1:C:239:SER:OG	2.35	0.44
1:A:443:PHE:CZ	1:A:452:LYS:HG3	2.51	0.44
1:E:101:LEU:HB2	1:E:102:HIS:CD2	2.53	0.44
1:E:443:PHE:O	1:E:452:LYS:NZ	2.42	0.44
1:A:414:ASN:OD1	1:A:422:LYS:NZ	2.50	0.44
1:D:351:LEU:HD23	1:D:472:LEU:HD22	2.00	0.44
1:B:344:TRP:HA	1:B:469:LEU:HD21	1.99	0.44
1:C:380:MET:N	1:C:380:MET:SD	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LEU:HD13	1:B:471:ALA:HB1	1.99	0.43
1:E:119:ALA:HB2	1:E:201:LEU:HD23	2.01	0.43
1:E:166:LEU:HD21	1:E:471:ALA:HB2	2.01	0.43
1:E:294:SER:C	1:E:295:LEU:HG	2.43	0.43
1:E:371:TYR:O	1:E:390:ARG:NH1	2.52	0.43
1:A:82:VAL:HG21	1:A:216:ILE:CD1	2.49	0.43
1:D:77:ASP:HB2	1:D:127:TYR:OH	2.18	0.43
1:C:79:LEU:HD12	1:C:211:VAL:HG22	2.01	0.43
1:D:291:LYS:NZ	1:D:336:THR:OG1	2.48	0.43
1:E:256:ARG:NH1	1:E:380:MET:HE3	2.34	0.43
1:D:117:ILE:HG23	1:D:129:VAL:HG13	2.00	0.43
1:B:385:ASP:OD1	1:B:385:ASP:C	2.62	0.43
1:D:397:ILE:HD13	1:D:459:LEU:HB2	2.00	0.43
1:D:136:PHE:O	1:D:139:THR:HG22	2.19	0.42
1:E:83:MET:HG3	1:E:93:PHE:CE2	2.54	0.42
1:E:166:LEU:HG	1:E:173:ILE:HD11	2.01	0.42
1:C:469:LEU:HD23	1:C:469:LEU:HA	1.89	0.42
1:E:317:GLU:O	1:E:318:ASP:C	2.63	0.42
1:A:96:LEU:HD22	1:A:366:LYS:HE2	2.00	0.42
1:C:262:MET:O	1:C:266:GLN:HG2	2.19	0.42
1:D:366:LYS:HD2	1:D:461:GLU:OE2	2.20	0.42
1:C:344:TRP:HA	1:C:469:LEU:HD21	2.02	0.42
1:A:166:LEU:HG	1:A:173:ILE:HD11	2.01	0.41
1:C:325:ASP:OD1	1:C:327:THR:HG22	2.20	0.41
1:A:385:ASP:C	1:A:385:ASP:OD1	2.64	0.41
1:B:459:LEU:C	1:B:459:LEU:HD12	2.46	0.41
1:E:136:PHE:CD2	1:E:146:LEU:HD21	2.55	0.41
1:C:185:GLY:O	1:C:186:GLU:C	2.63	0.41
1:D:287:PHE:CE2	1:D:336:THR:HG23	2.55	0.41
1:E:444:TRP:O	1:E:445:ARG:C	2.64	0.41
1:B:133:MET:HG2	1:B:146:LEU:HD22	2.01	0.41
1:C:149:LEU:O	1:C:151:ARG:N	2.53	0.41
1:E:159:LEU:HD13	1:E:189:TRP:CZ2	2.56	0.41
1:A:236:GLU:C	1:A:237:GLN:HG3	2.46	0.41
1:C:396:TYR:O	1:C:400:VAL:HG23	2.20	0.41
1:D:378:ILE:HD11	1:D:386:THR:HG22	2.02	0.41
1:E:440:TYR:CZ	1:E:452:LYS:HD3	2.55	0.41
1:A:397:ILE:HD11	1:A:425:ILE:HG23	2.02	0.41
1:E:393:ILE:HG13	1:E:417:LEU:HD11	2.03	0.41
1:D:119:ALA:HB2	1:D:201:LEU:HD23	2.02	0.40
1:D:237:GLN:HG2	1:D:440:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:LEU:C	1:D:459:LEU:HD12	2.47	0.40
1:C:195:ILE:HD12	1:C:352:ILE:HD13	2.03	0.40
1:E:95:ARG:HB3	1:E:362:LEU:HD22	2.02	0.40
1:B:268:LEU:HD13	1:B:416:LEU:HD11	2.03	0.40
1:C:238:SER:C	1:C:239:SER:OG	2.64	0.40
1:C:443:PHE:O	1:C:452:LYS:NZ	2.55	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	356/415 (86%)	332 (93%)	21 (6%)	3 (1%)	16	45
1	B	355/415 (86%)	328 (92%)	24 (7%)	3 (1%)	16	45
1	C	354/415 (85%)	325 (92%)	24 (7%)	5 (1%)	9	33
1	D	354/415 (85%)	327 (92%)	21 (6%)	6 (2%)	7	30
1	E	355/415 (86%)	328 (92%)	22 (6%)	5 (1%)	9	33
All	All	1774/2075 (86%)	1640 (92%)	112 (6%)	22 (1%)	10	37

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	A	379	ALA
1	C	239	SER
1	C	379	ALA
1	C	433	GLU
1	E	175	LYS
1	E	433	GLU
1	A	312	MET

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Mol	Chain	Res	Type
1	B	186	GLU
1	C	150	HIS
1	D	347	HIS
1	E	321	PHE
1	E	347	HIS
1	D	293	GLU
1	B	234	PRO
1	D	433	GLU
1	E	409	ASP
1	C	235	SER
1	D	184	THR
1	B	122	ARG
1	D	239	SER
1	D	319	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	313/359 (87%)	293 (94%)	20 (6%)	16	44
1	B	308/359 (86%)	286 (93%)	22 (7%)	13	40
1	C	312/359 (87%)	276 (88%)	36 (12%)	5	21
1	D	311/359 (87%)	279 (90%)	32 (10%)	7	25
1	E	312/359 (87%)	282 (90%)	30 (10%)	8	29
All	All	1556/1795 (87%)	1416 (91%)	140 (9%)	9	31

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	101	LEU
1	A	133	MET
1	A	139	THR
1	A	154	GLU

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Mol	Chain	Res	Type
1	A	156	LEU
1	A	207	LEU
1	A	239	SER
1	A	286	ARG
1	A	294	SER
1	A	317	GLU
1	A	320	THR
1	A	327	THR
1	A	350	SER
1	A	378	ILE
1	A	397	ILE
1	A	417	LEU
1	A	452	LYS
1	A	459	LEU
1	A	460	LEU
1	B	72	SER
1	B	76	VAL
1	B	139	THR
1	B	156	LEU
1	B	159	LEU
1	B	174	THR
1	B	188	THR
1	B	198	LEU
1	B	216	ILE
1	B	219	GLU
1	B	239	SER
1	B	311	ASP
1	B	327	THR
1	B	366	LYS
1	B	380	MET
1	B	417	LEU
1	B	433	GLU
1	B	458	LEU
1	B	459	LEU
1	B	460	LEU
1	B	463	ARG
1	B	479	MET
1	C	72	SER
1	C	139	THR
1	C	154	GLU
1	C	156	LEU
1	C	160	SER

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Mol	Chain	Res	Type
1	C	174	THR
1	C	175	LYS
1	C	179	GLN
1	C	183	LYS
1	C	188	THR
1	C	195	ILE
1	C	198	LEU
1	C	207	LEU
1	C	219	GLU
1	C	235	SER
1	C	236	GLU
1	C	239	SER
1	C	283	MET
1	C	294	SER
1	C	327	THR
1	C	343	THR
1	C	353	GLN
1	C	354	ARG
1	C	361	GLN
1	C	366	LYS
1	C	380	MET
1	C	384	VAL
1	C	397	ILE
1	C	417	LEU
1	C	433	GLU
1	C	452	LYS
1	C	458	LEU
1	C	459	LEU
1	C	460	LEU
1	C	463	ARG
1	C	476	THR
1	D	72	SER
1	D	76	VAL
1	D	133	MET
1	D	138	GLN
1	D	139	THR
1	D	154	GLU
1	D	156	LEU
1	D	159	LEU
1	D	174	THR
1	D	176	GLU
1	D	207	LEU

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Mol	Chain	Res	Type
1	D	219	GLU
1	D	221	ASP
1	D	235	SER
1	D	236	GLU
1	D	237	GLN
1	D	239	SER
1	D	289	LEU
1	D	292	SER
1	D	311	ASP
1	D	340	GLN
1	D	354	ARG
1	D	366	LYS
1	D	380	MET
1	D	387	SER
1	D	397	ILE
1	D	417	LEU
1	D	436	THR
1	D	442	LEU
1	D	450	SER
1	D	459	LEU
1	D	460	LEU
1	E	72	SER
1	E	79	LEU
1	E	92	SER
1	E	95	ARG
1	E	126	SER
1	E	133	MET
1	E	156	LEU
1	E	174	THR
1	E	182	LEU
1	E	188	THR
1	E	191	LEU
1	E	198	LEU
1	E	202	THR
1	E	207	LEU
1	E	219	GLU
1	E	239	SER
1	E	259	GLU
1	E	281	GLU
1	E	295	LEU
1	E	313	LEU
1	E	329	ARG

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Mol	Chain	Res	Type
1	E	336	THR
1	E	347	HIS
1	E	380	MET
1	E	389	LEU
1	E	417	LEU
1	E	442	LEU
1	E	457	LEU
1	E	459	LEU
1	E	460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	132	HIS
1	A	347	HIS
1	A	353	GLN
1	A	446	HIS
1	B	132	HIS
1	B	237	GLN
1	B	415	GLN
1	C	150	HIS
1	C	376	ASN
1	C	381	HIS
1	E	97	HIS
1	E	102	HIS
1	E	124	GLN
1	E	132	HIS
1	E	150	HIS
1	E	187	HIS
1	E	237	GLN
1	E	332	GLN
1	E	340	GLN
1	E	353	GLN
1	E	376	ASN
1	E	441	ASN

5.3.3 RNA ⓘ

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	$\# Z > 2$
2	K94	A	900	-	10,11,11	0.70	0	8,16,16	1.70	2 (25%)
2	K94	C	900	-	10,11,11	0.67	0	8,16,16	2.10	2 (25%)
2	K94	D	900	-	10,11,11	0.79	0	8,16,16	1.94	2 (25%)
2	K94	B	900	-	10,11,11	0.89	0	8,16,16	1.58	2 (25%)
2	K94	E	900	-	10,11,11	0.50	0	8,16,16	2.20	2 (25%)

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
2	K94	A	900	-	-	7/13/15/15	-
2	K94	C	900	-	-	6/13/15/15	-
2	K94	D	900	-	-	4/13/15/15	-
2	K94	B	900	-	-	4/13/15/15	-
2	K94	E	900	-	-	1/13/15/15	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	900	K94	O2-C2-O1	-4.45	113.98	124.08
2	C	900	K94	C3-C4-C7	-4.42	102.03	108.21
2	E	900	K94	C3-C4-C7	-3.98	102.64	108.21
2	D	900	K94	C3-C4-C7	-3.89	102.78	108.21
2	D	900	K94	O2-C2-O1	-3.45	116.25	124.08
2	A	900	K94	C3-C4-C7	-3.45	103.39	108.21
2	C	900	K94	O2-C2-O1	-3.42	116.33	124.08
2	B	900	K94	O2-C2-O1	-2.76	117.81	124.08
2	B	900	K94	C5-C4-C6	2.41	114.00	109.20
2	A	900	K94	O2-C2-O1	-2.28	118.90	124.08

There are no chirality outliers.

All (22) torsion outliers are listed below:

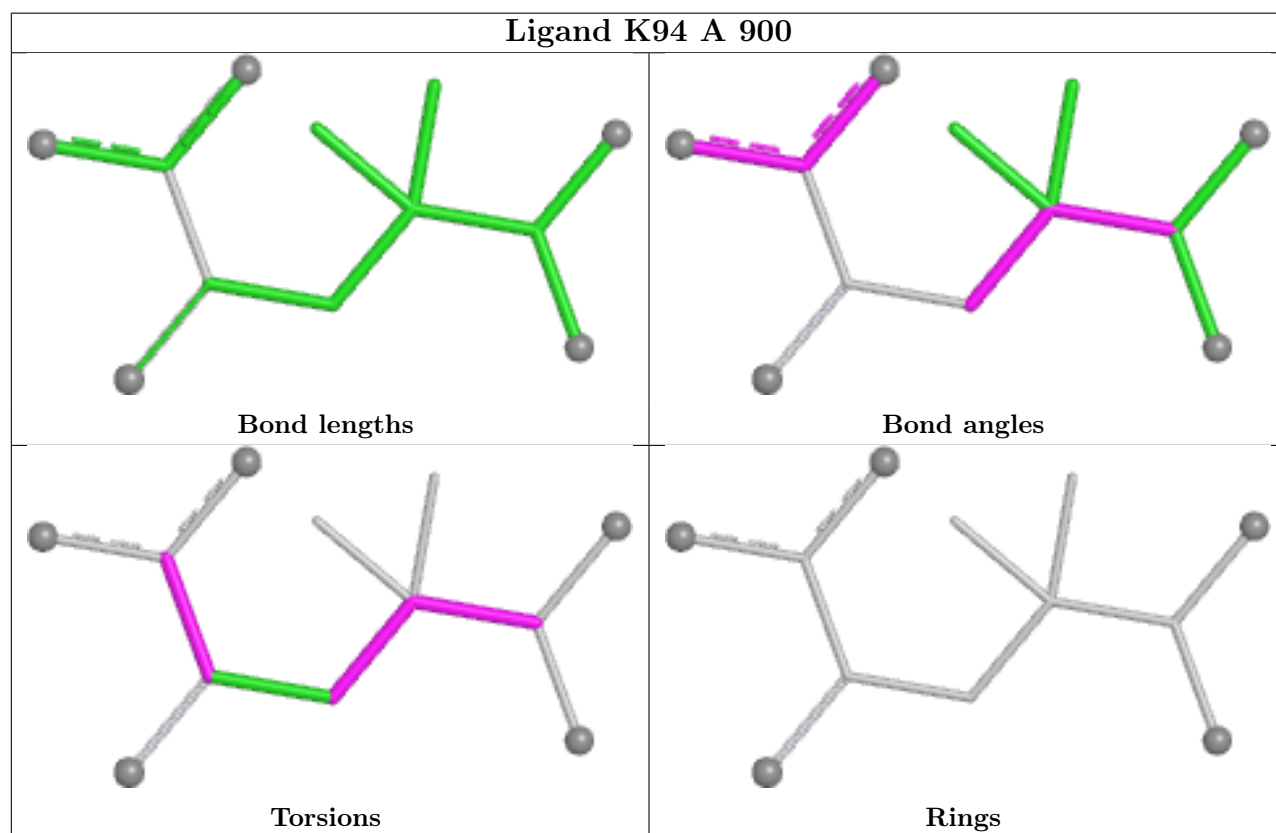
Mol	Chain	Res	Type	Atoms
2	A	900	K94	C6-C4-C7-F2
2	A	900	K94	C6-C4-C7-F1
2	A	900	K94	C5-C4-C7-F1
2	B	900	K94	N1-C1-C3-C4
2	C	900	K94	N1-C1-C3-C4
2	C	900	K94	C6-C4-C7-F2
2	C	900	K94	C6-C4-C7-F1
2	C	900	K94	C5-C4-C7-F2
2	C	900	K94	C5-C4-C7-F1
2	D	900	K94	N1-C1-C3-C4
2	E	900	K94	N1-C1-C3-C4
2	A	900	K94	C3-C1-C2-O2
2	B	900	K94	C2-C1-C3-C4
2	C	900	K94	C2-C1-C3-C4
2	D	900	K94	C2-C1-C3-C4
2	A	900	K94	C3-C1-C2-O1
2	D	900	K94	C3-C1-C2-O2
2	B	900	K94	C3-C1-C2-O2
2	A	900	K94	C1-C3-C4-C6
2	A	900	K94	C1-C3-C4-C5
2	D	900	K94	C3-C1-C2-O1
2	B	900	K94	C3-C1-C2-O1

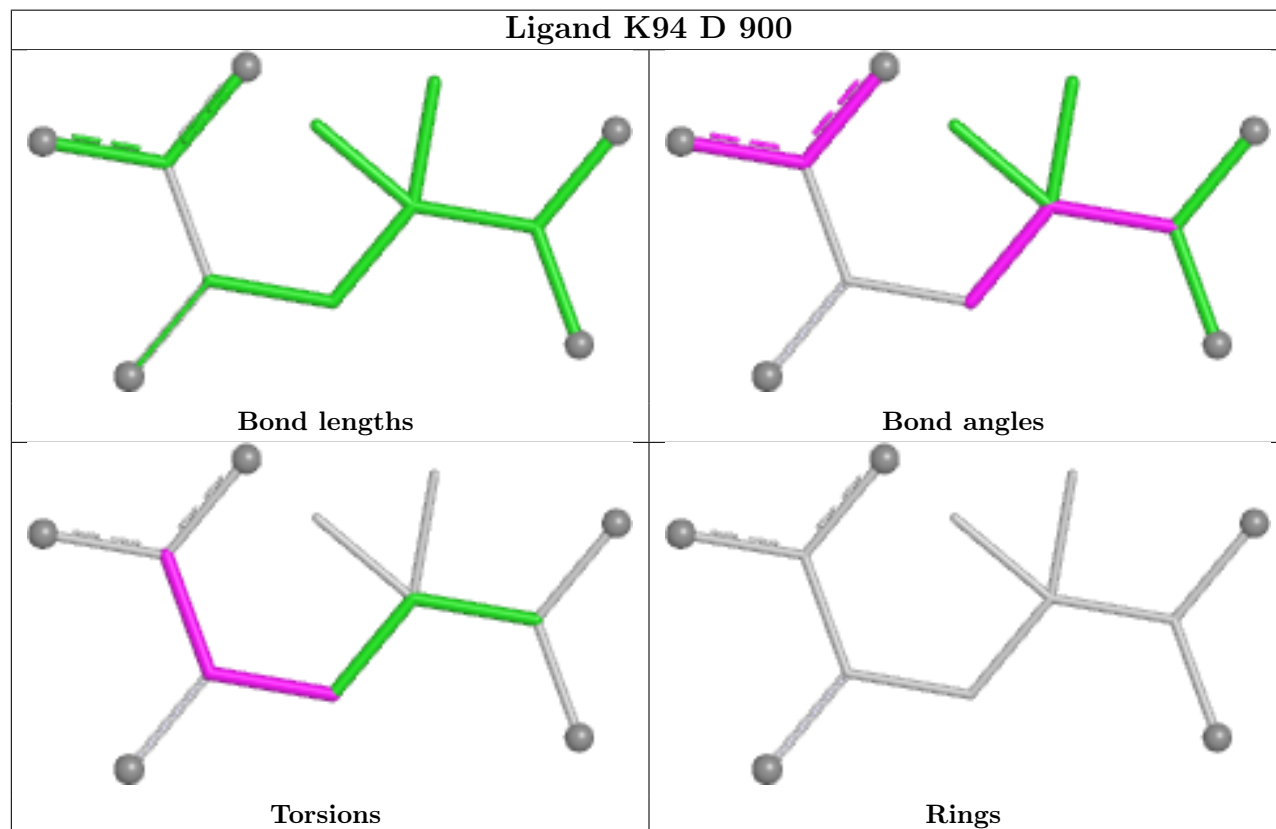
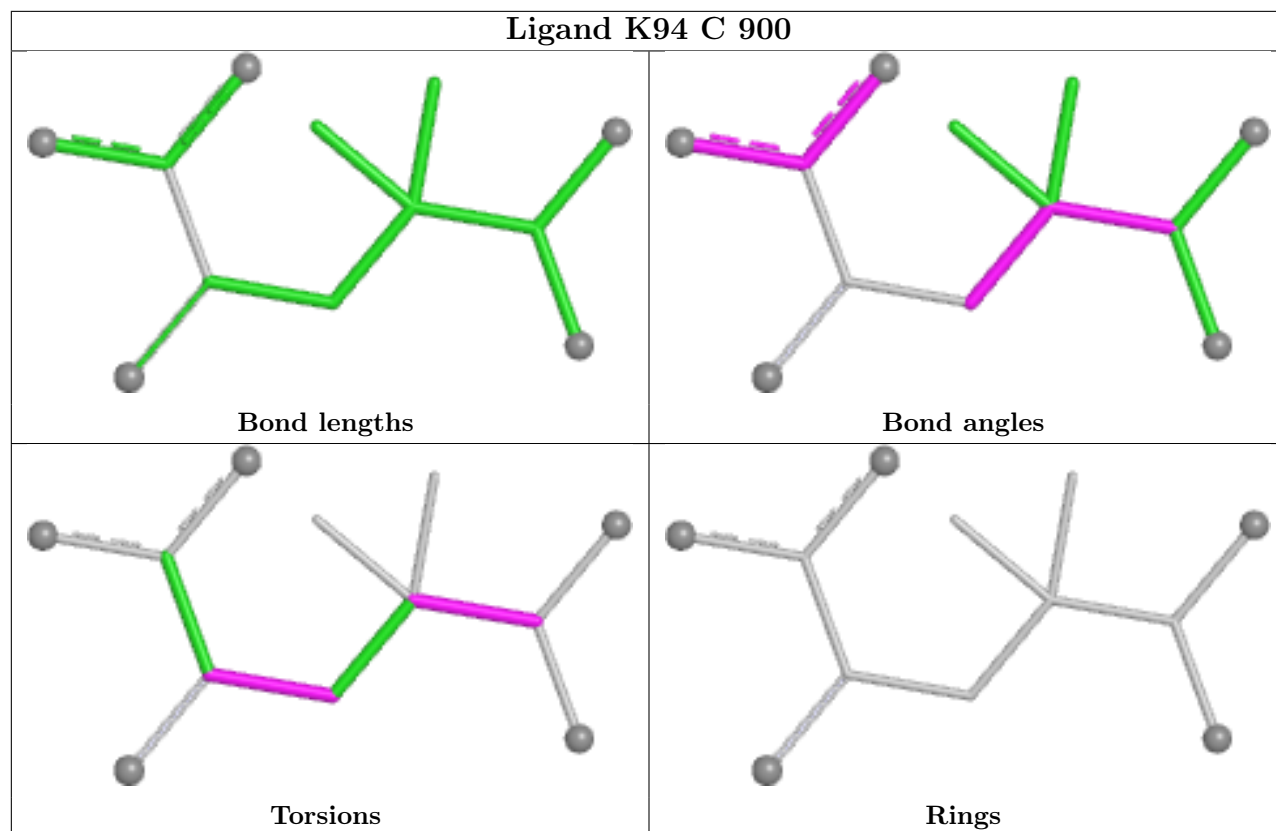
There are no ring outliers.

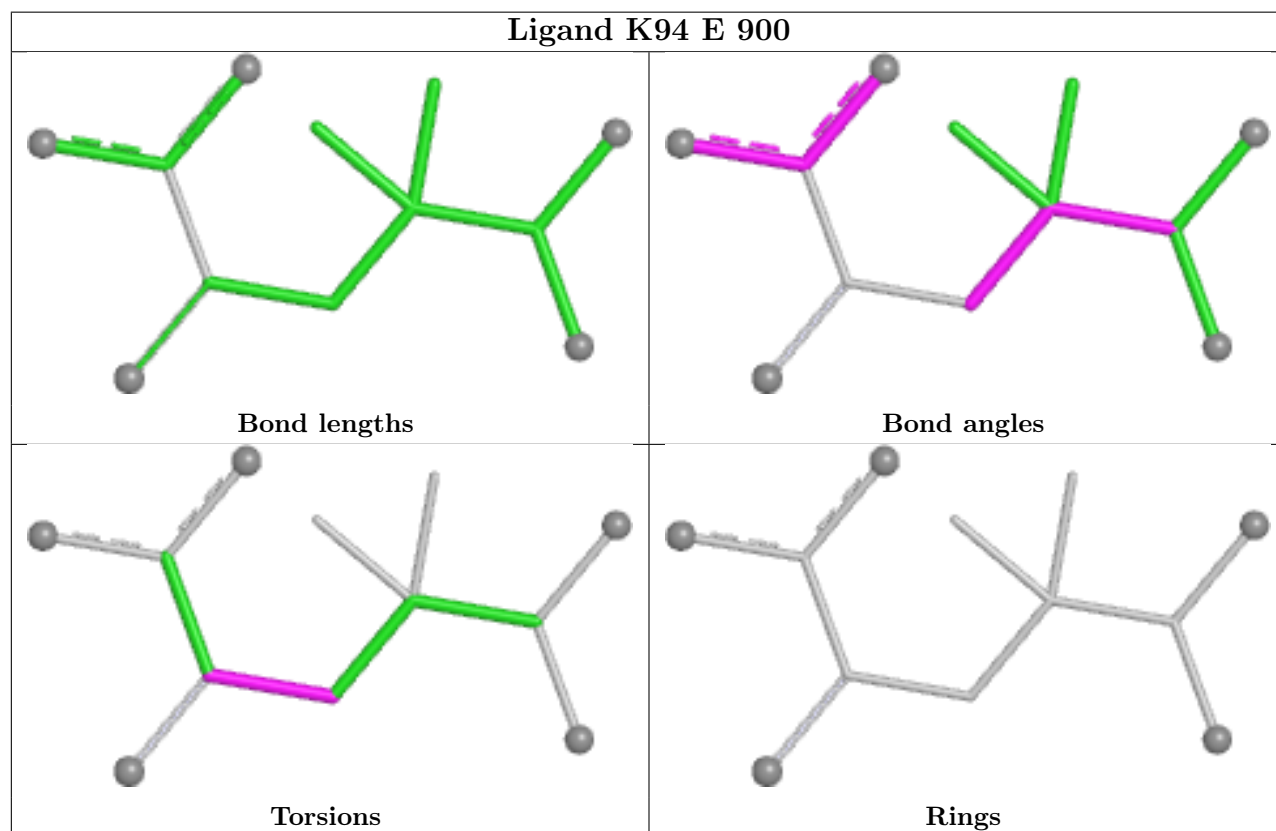
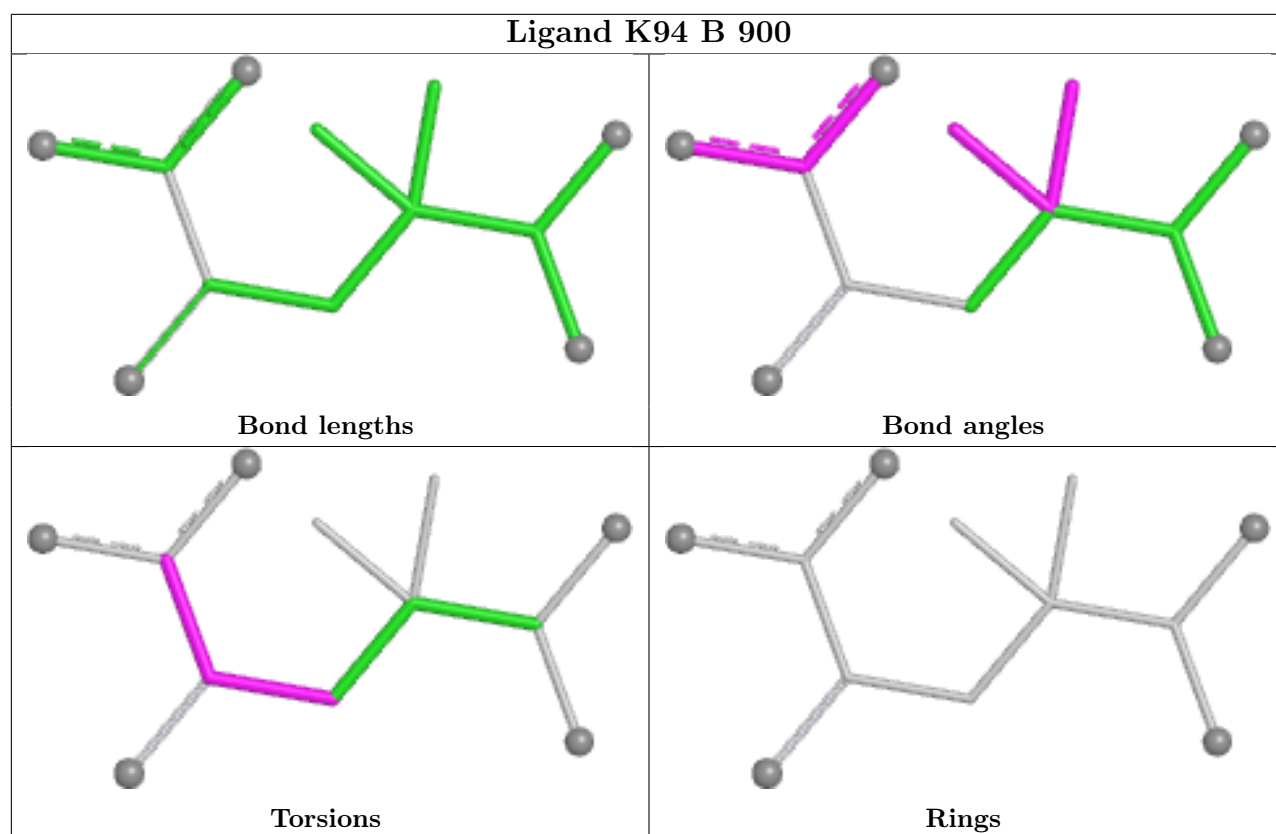
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	K94	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	366/415 (88%)	-0.53	3 (0%) 82 68	70, 95, 141, 171	0
1	B	365/415 (87%)	-0.50	6 (1%) 70 52	70, 95, 142, 170	0
1	C	364/415 (87%)	-0.42	7 (1%) 66 48	83, 112, 149, 189	0
1	D	364/415 (87%)	-0.40	5 (1%) 73 55	83, 111, 150, 184	0
1	E	365/415 (87%)	-0.46	4 (1%) 78 60	81, 109, 147, 166	0
All	All	1824/2075 (87%)	-0.46	25 (1%) 73 55	70, 105, 148, 189	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	240	PRO	4.9
1	A	310	PRO	4.6
1	B	479	MET	3.7
1	D	310	PRO	3.4
1	C	310	PRO	3.4
1	D	240	PRO	3.2
1	E	236	GLU	3.2
1	B	233	PRO	3.1
1	C	270	GLU	2.9
1	B	310	PRO	2.8
1	C	233	PRO	2.8
1	E	310	PRO	2.8
1	E	233	PRO	2.6
1	C	295	LEU	2.5
1	D	66	GLY	2.4
1	A	233	PRO	2.4
1	C	66	GLY	2.4
1	C	236	GLU	2.4
1	D	233	PRO	2.3
1	B	236	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	284	GLU	2.2
1	B	295	LEU	2.2
1	B	256	ARG	2.2
1	D	327	THR	2.2
1	A	236	GLU	2.1

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](#)

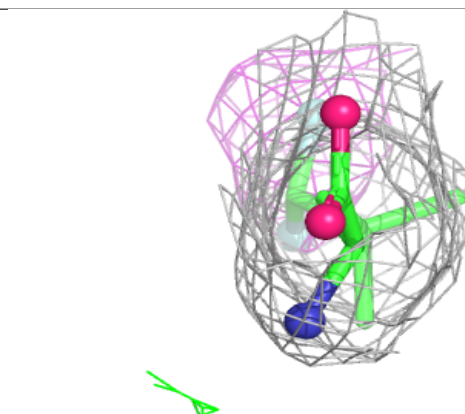
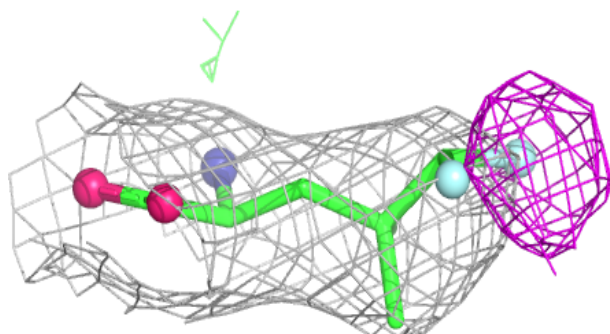
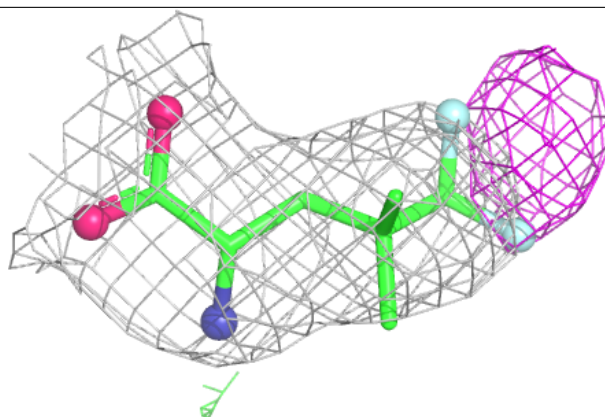
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	K94	A	900	12/12	0.94	0.14	88,93,101,111	0
2	K94	D	900	12/12	0.94	0.14	77,107,124,127	0
2	K94	C	900	12/12	0.95	0.13	86,103,117,123	0
2	K94	E	900	12/12	0.95	0.13	84,102,112,116	0
2	K94	B	900	12/12	0.97	0.11	79,93,114,120	0

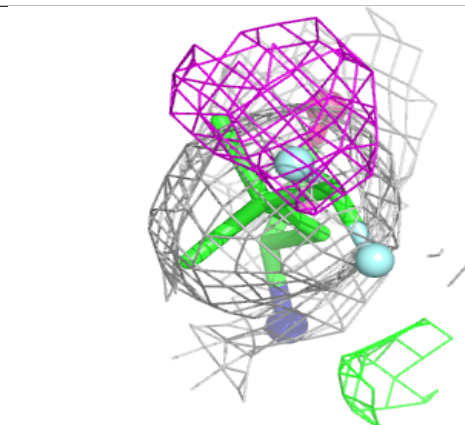
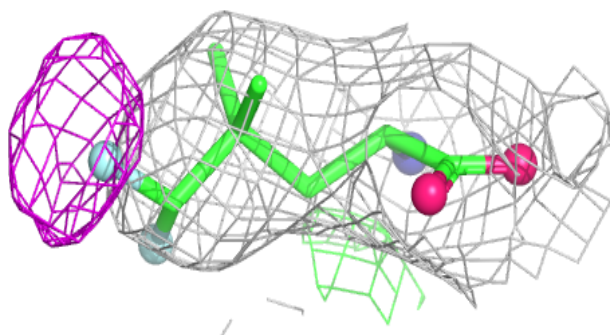
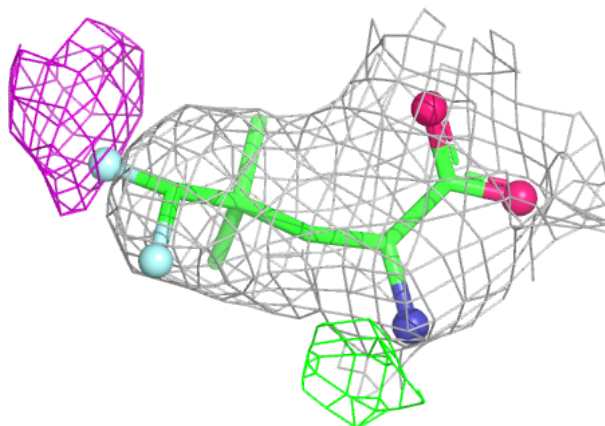
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K94 A 900:

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

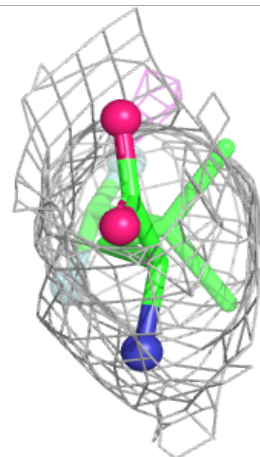
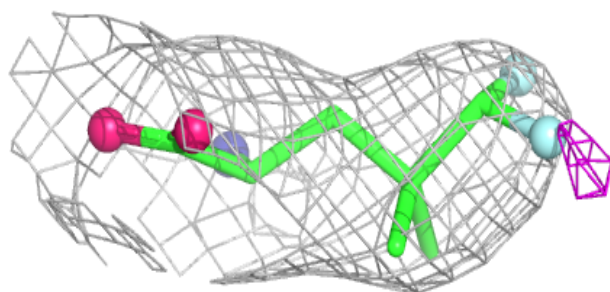
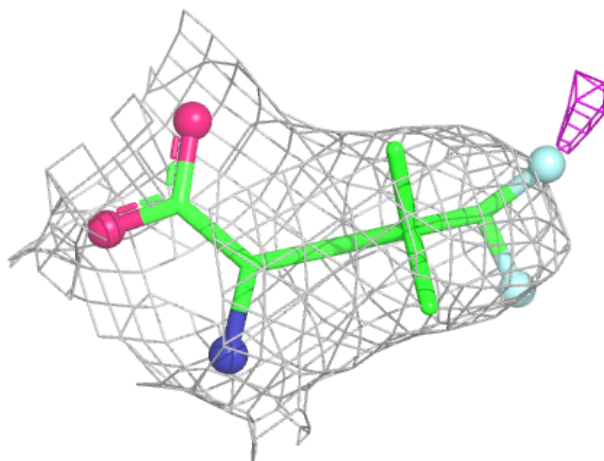
**Electron density around K94 D 900:**

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



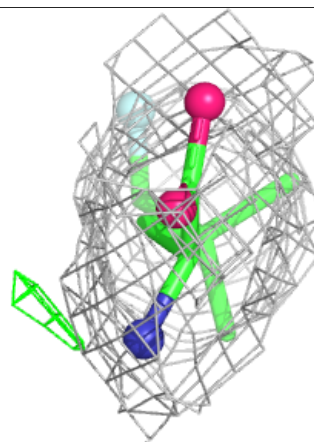
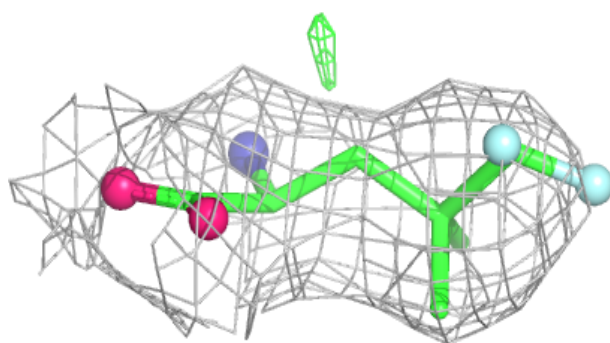
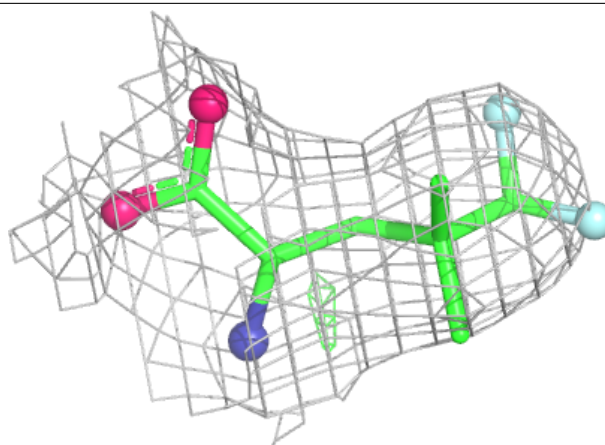
Electron density around K94 C 900:

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



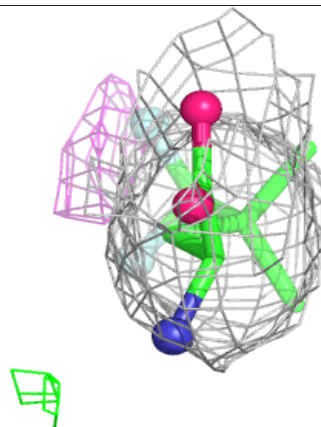
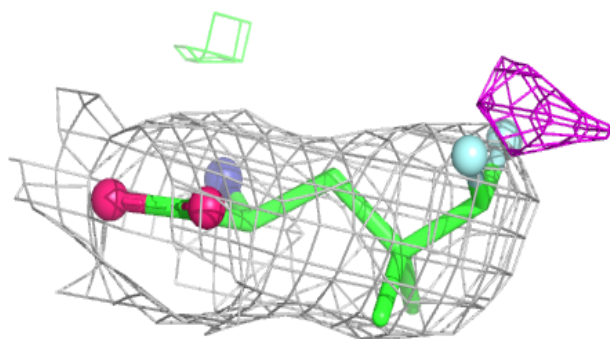
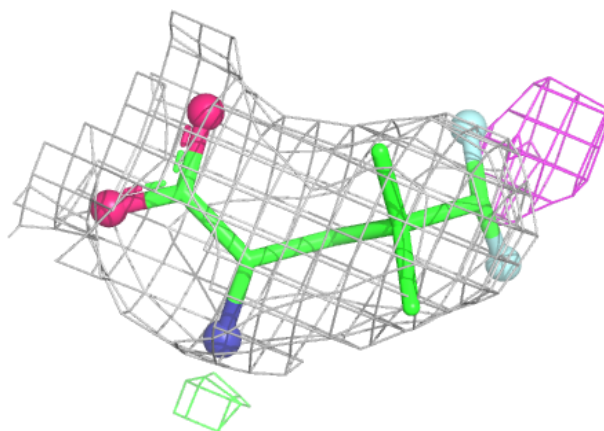
Electron density around K94 E 900:

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



Electron density around K94 B 900:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.