



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:05 am BST

PDB ID : 6N0M
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 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

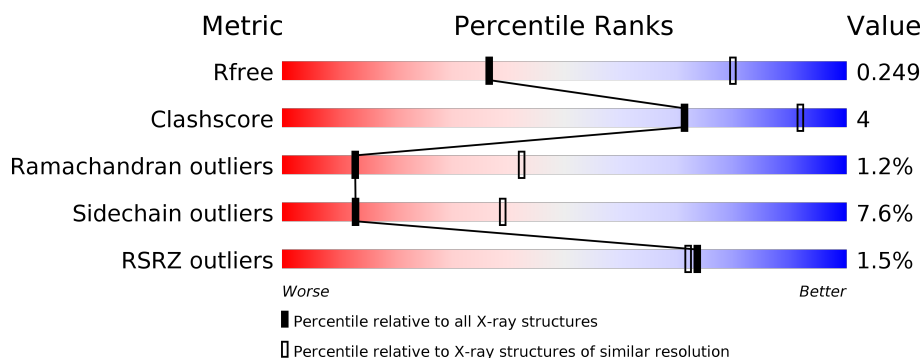
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 10%, yellow 12%, green 77%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 77% 10% 12% </div> </div>
1	B	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 10%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 78% 10% 12% </div> </div>
1	C	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 10%, yellow 13%, green 73%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 73% 13% 12% </div> </div>
1	D	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 10%, yellow 15%, green 71%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 71% 15% 12% </div> </div>
1	E	415	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 10%, yellow 16%, green 70%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 70% 16% 12% </div> </div>

2 Entry composition [i](#)

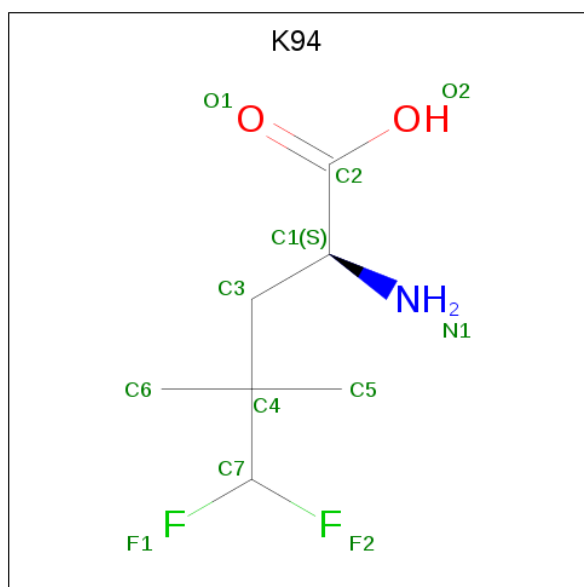
There are 2 unique types of molecules in this entry. The entry contains 14811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: K94) (formula: $C_7H_{13}F_2NO_2$) (labeled as "Ligand of Interest" by author).



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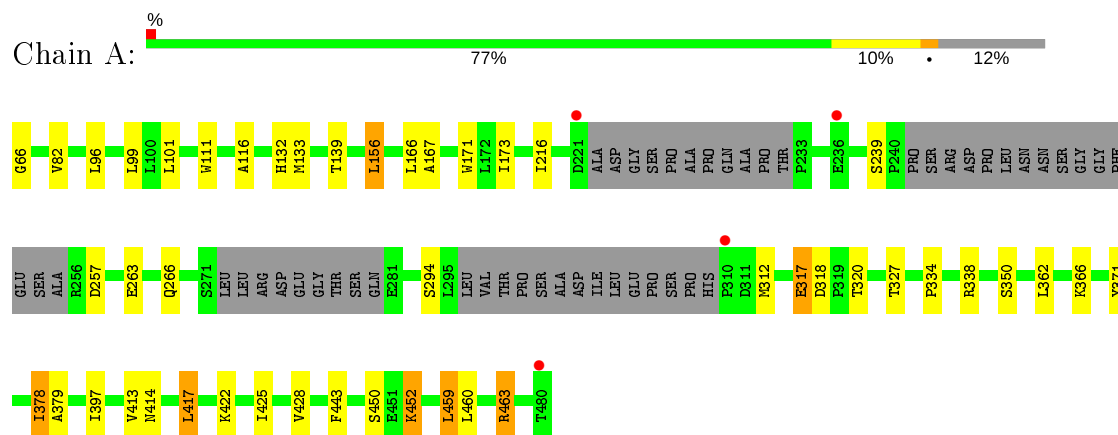
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			12	7	2	1	2		
2	C	1	Total	C	F	N	O	0	0
			12	7	2	1	2		
2	D	1	Total	C	F	N	O	0	0
			12	7	2	1	2		
2	E	1	Total	C	F	N	O	0	0
			12	7	2	1	2		

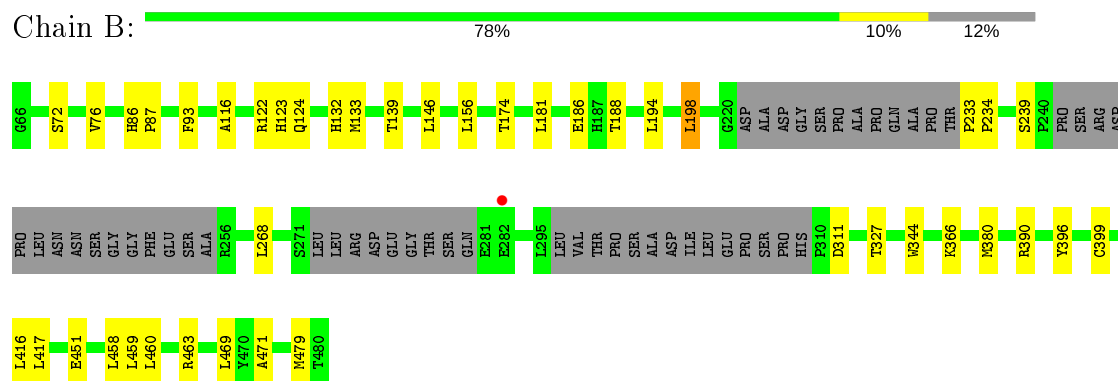
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

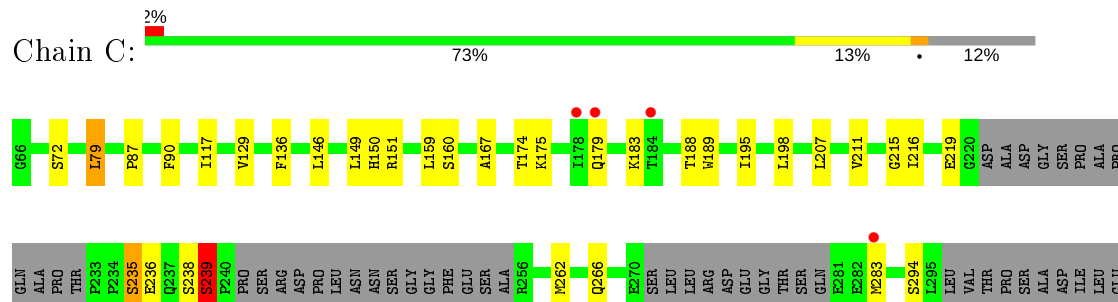
• Molecule 1: Sestrin-2



• Molecule 1: Sestrin-2

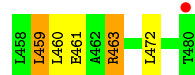
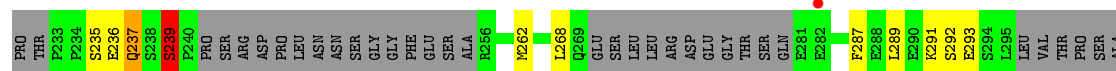


• Molecule 1: Sestrin-2

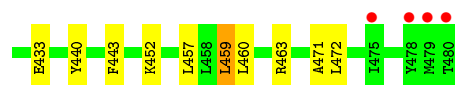
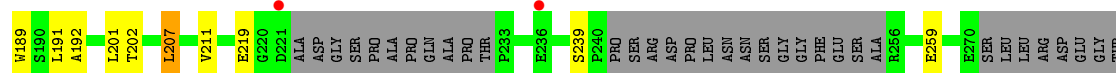




• Molecule 1: Sestrin-2



• 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 , 0.249	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)	0.34 , 80.0	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	0.95	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	0.61	1/3039 (0.0%)	0.84	2/4115 (0.0%)
1	B	0.59	0/3013	0.85	3/4083 (0.1%)
1	C	0.59	0/3029	0.79	1/4101 (0.0%)
1	D	0.60	0/3022	0.84	3/4093 (0.1%)
1	E	0.57	0/3033	0.83	1/4107 (0.0%)
All	All	0.59	1/15136 (0.0%)	0.83	10/20499 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GLY	N-CA	5.22	1.53	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	463	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	B	463	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	463	ARG	NE-CZ-NH2	-7.79	116.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	463	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	E	463	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	463	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	463	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	463	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	390	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	391	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	16	0
1	B	2936	0	2839	11	0
1	C	2952	0	2870	22	0
1	D	2945	0	2857	26	0
1	E	2956	0	2870	28	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	103	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 (103) 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: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: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:E:459:LEU:C	1:E:459:LEU:HD12	2.30	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:D:171:TRP:CE2	1:D:334:PRO:HB3	2.47	0.50
1:D:89:TYR:CD2	1:D:457:LEU:HD22	2.47	0.50
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
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:413:VAL:HG13	1:C:417:LEU:HD22	1.94	0.49
1:C:87:PRO:HA	1:C:90:PHE:HB3	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: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:C:459:LEU:C	1:C:459:LEU:HD12	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:263:GLU:O	1:A:266:GLN:HB2	2.15	0.46
1:A:171:TRP:CE2	1:A:334:PRO:HB3	2.50	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:A:317:GLU:O	1:A:318:ASP:C	2.53	0.46
1:D:167:ALA:O	1:D:463:ARG:NH2	2.49	0.46
1:D:339:ALA:HB1	1:D:405:TYR:CE1	2.51	0.45
1:E:191:LEU:O	1:E:192:ALA:C	2.54	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:C:215:GLY:O	1:C:216:ILE:C	2.55	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
1:B:198:LEU:HD13	1:B:471:ALA:HB1	1.99	0.43
1:E:166:LEU:HD21	1:E:471:ALA:HB2	2.01	0.43
1:E:119:ALA:HB2	1:E:201:LEU:HD23	2.01	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:D:117:ILE:HG23	1:D:129:VAL:HG13	2.00	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:B:86:HIS:O	1:B:87:PRO:C	2.57	0.42
1:C:469:LEU:HD23	1:C:469:LEU:HA	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:136:PHE:CD2	1:E:146:LEU:HD21	2.55	0.41
1:B:123:HIS:O	1:B:124:GLN:C	2.58	0.41
1:D:287:PHE:CE2	1:D:336:THR:HG23	2.55	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: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:C:342:TYR:HH	1:C:476:THR:HG1	1.68	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
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: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%)	19	51
1	B	355/415 (86%)	328 (92%)	24 (7%)	3 (1%)	19	51
1	C	354/415 (85%)	325 (92%)	24 (7%)	5 (1%)	11	38
1	D	354/415 (85%)	327 (92%)	21 (6%)	6 (2%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	355/415 (86%)	328 (92%)	22 (6%)	5 (1%)	11	38
All	All	1774/2075 (86%)	1640 (92%)	112 (6%)	22 (1%)	13	42

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
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%)	295 (94%)	18 (6%)	20	50
1	B	308/359 (86%)	290 (94%)	18 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	312/359 (87%)	283 (91%)	29 (9%)	9	30
1	D	311/359 (87%)	284 (91%)	27 (9%)	10	34
1	E	312/359 (87%)	286 (92%)	26 (8%)	11	36
All	All	1556/1795 (87%)	1438 (92%)	118 (8%)	13	39

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	133	MET
1	A	139	THR
1	A	156	LEU
1	A	239	SER
1	A	294	SER
1	A	317	GLU
1	A	320	THR
1	A	327	THR
1	A	338	ARG
1	A	350	SER
1	A	371	TYR
1	A	378	ILE
1	A	417	LEU
1	A	450	SER
1	A	452	LYS
1	A	459	LEU
1	A	460	LEU
1	B	72	SER
1	B	76	VAL
1	B	93	PHE
1	B	139	THR
1	B	156	LEU
1	B	174	THR
1	B	188	THR
1	B	198	LEU
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	458	LEU

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Mol	Chain	Res	Type
1	B	459	LEU
1	B	460	LEU
1	B	479	MET
1	C	72	SER
1	C	79	LEU
1	C	160	SER
1	C	174	THR
1	C	175	LYS
1	C	179	GLN
1	C	183	LYS
1	C	188	THR
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	354	ARG
1	C	361	GLN
1	C	366	LYS
1	C	380	MET
1	C	399	CYS
1	C	417	LEU
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	138	GLN
1	D	139	THR
1	D	156	LEU
1	D	159	LEU
1	D	174	THR
1	D	207	LEU
1	D	219	GLU
1	D	221	ASP

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Mol	Chain	Res	Type
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	371	TYR
1	D	380	MET
1	D	417	LEU
1	D	436	THR
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	133	MET
1	E	151	ARG
1	E	156	LEU
1	E	174	THR
1	E	182	LEU
1	E	188	THR
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
1	E	347	HIS
1	E	380	MET
1	E	389	LEU
1	E	417	LEU
1	E	420	ASN
1	E	459	LEU

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Mol	Chain	Res	Type
1	E	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	132	HIS
1	A	269	GLN
1	A	353	GLN
1	A	441	ASN
1	B	132	HIS
1	C	150	HIS
1	E	97	HIS
1	E	102	HIS
1	E	132	HIS
1	E	150	HIS
1	E	187	HIS
1	E	353	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	-	8,11,11	0.82	0	7,16,16	1.55	1 (14%)
2	K94	B	900	-	8,11,11	0.89	0	7,16,16	1.31	1 (14%)
2	K94	C	900	-	8,11,11	0.71	0	7,16,16	1.79	1 (14%)
2	K94	D	900	-	8,11,11	0.83	0	7,16,16	1.56	1 (14%)
2	K94	E	900	-	8,11,11	0.59	0	7,16,16	1.58	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	K94	A	900	-	-	5/9/15/15	-
2	K94	B	900	-	-	2/9/15/15	-
2	K94	C	900	-	-	5/9/15/15	-
2	K94	D	900	-	-	2/9/15/15	-
2	K94	E	900	-	-	1/9/15/15	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	K94	C3-C4-C7	-4.26	102.03	108.18
2	E	900	K94	C3-C4-C7	-3.84	102.64	108.18
2	D	900	K94	C3-C4-C7	-3.74	102.78	108.18
2	A	900	K94	C3-C4-C7	-3.32	103.39	108.18
2	B	900	K94	C5-C4-C6	2.37	114.00	109.17

There are no chirality outliers.

All (15) 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

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Mol	Chain	Res	Type	Atoms
2	B	900	K94	C2-C1-C3-C4
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	C2-C1-C3-C4
2	D	900	K94	N1-C1-C3-C4
2	E	900	K94	N1-C1-C3-C4
2	A	900	K94	C1-C3-C4-C6
2	A	900	K94	C1-C3-C4-C5

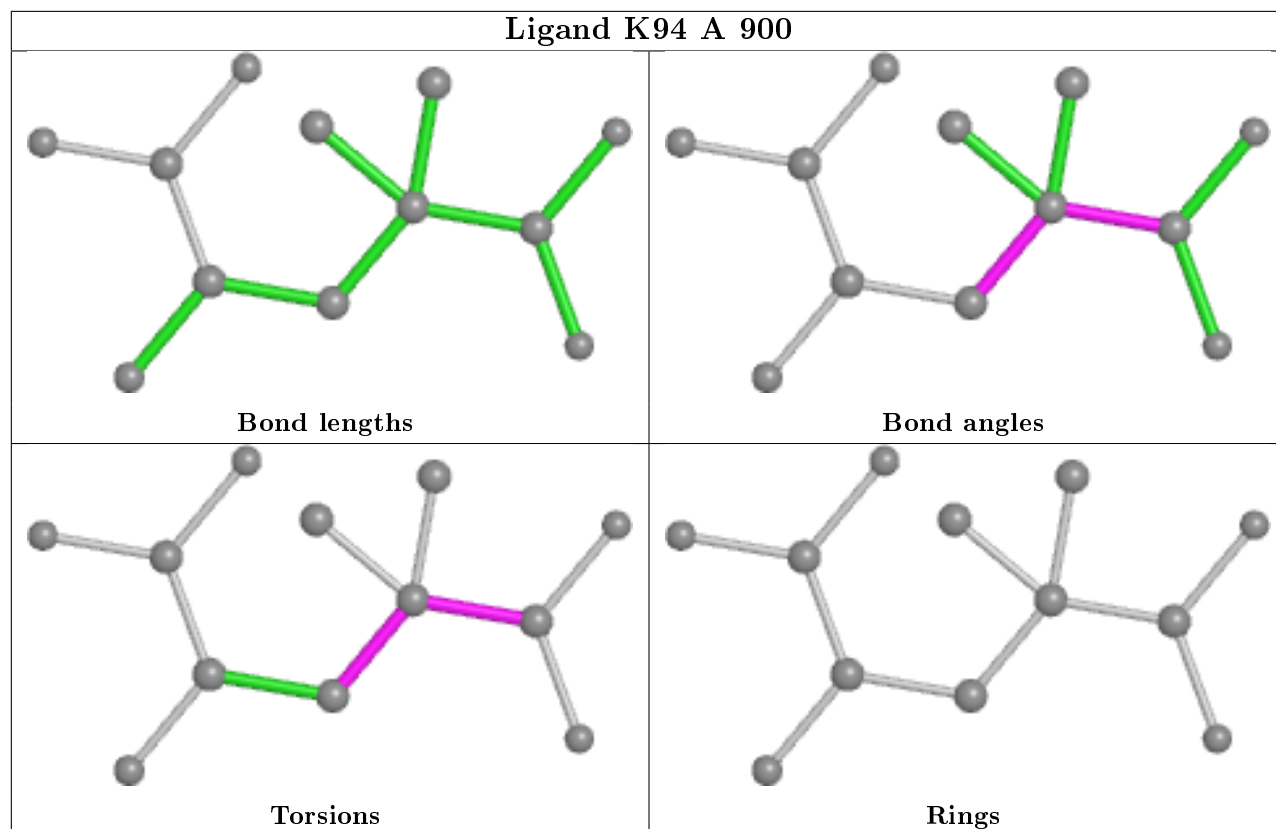
There are no ring outliers.

1 monomer is involved in 1 short contact:

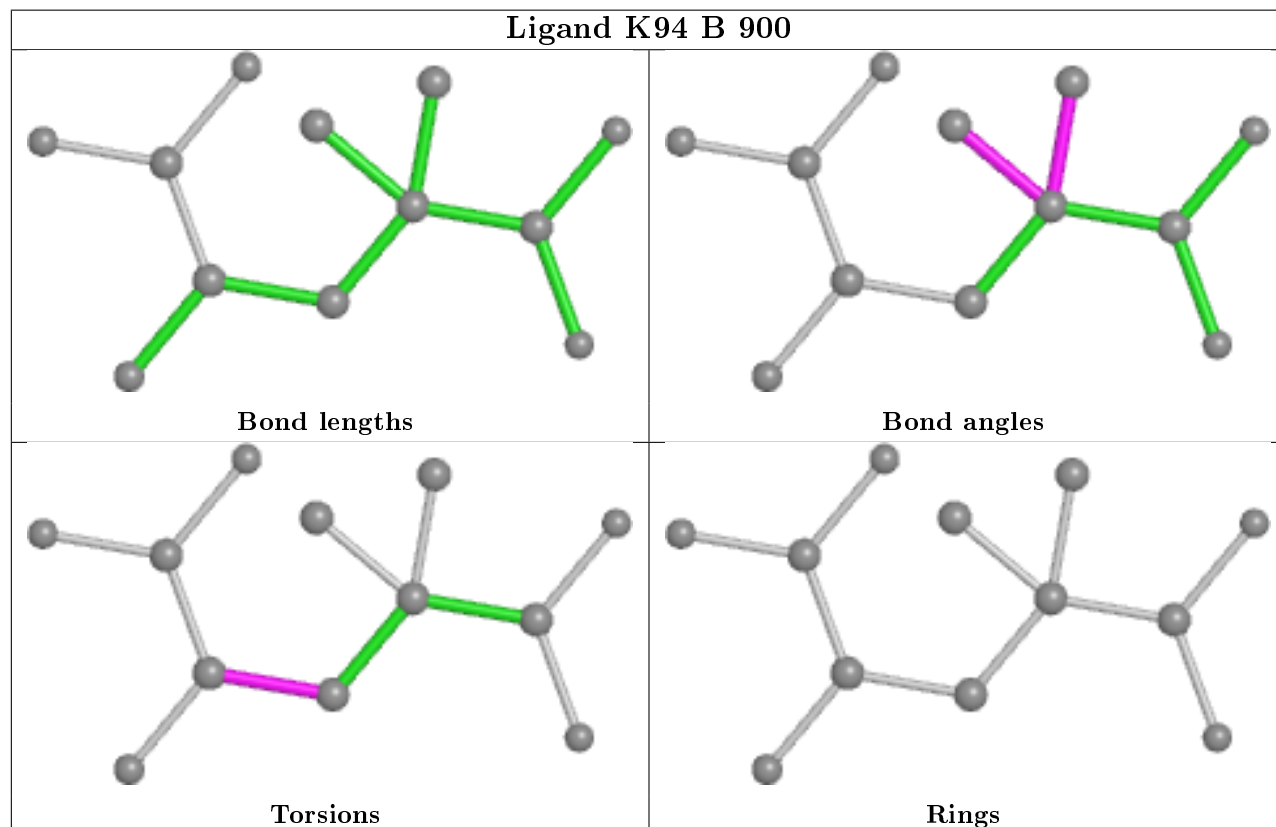
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	K94	1	0

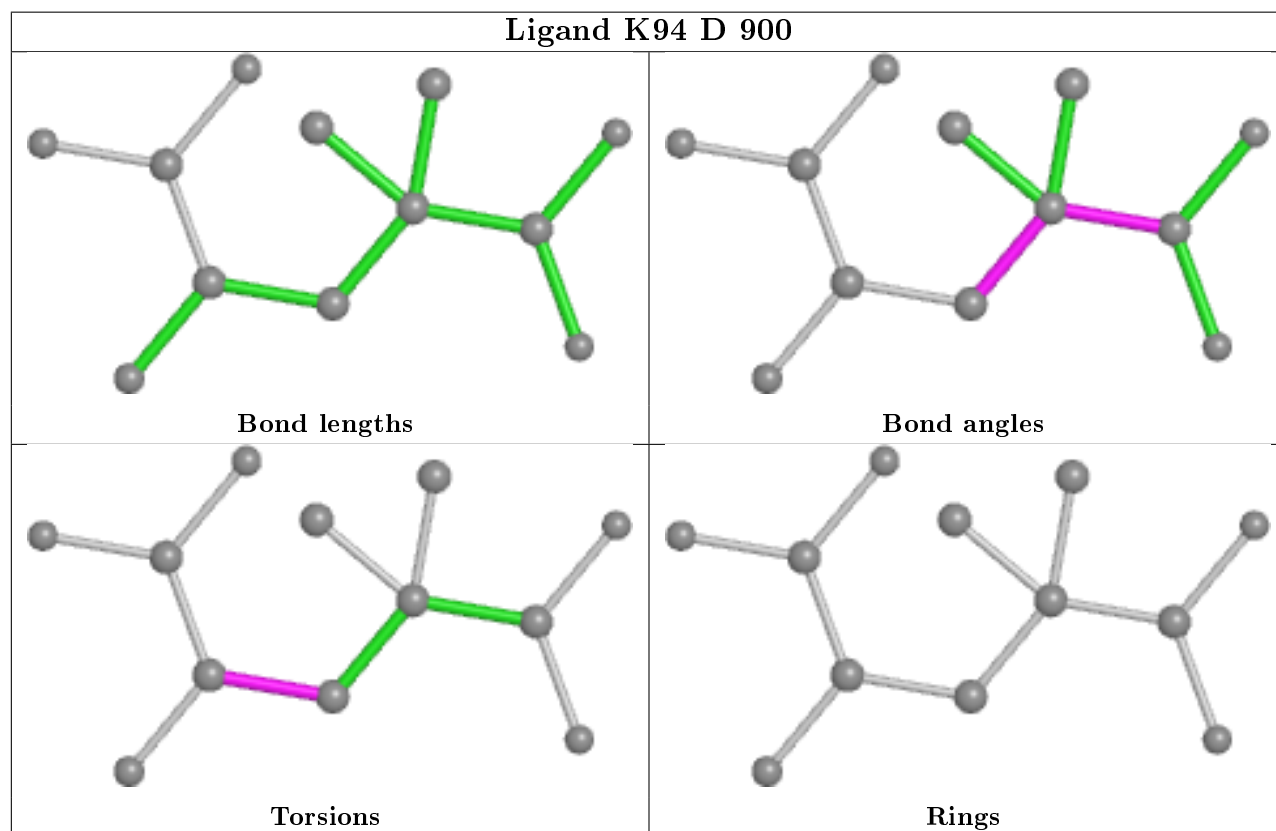
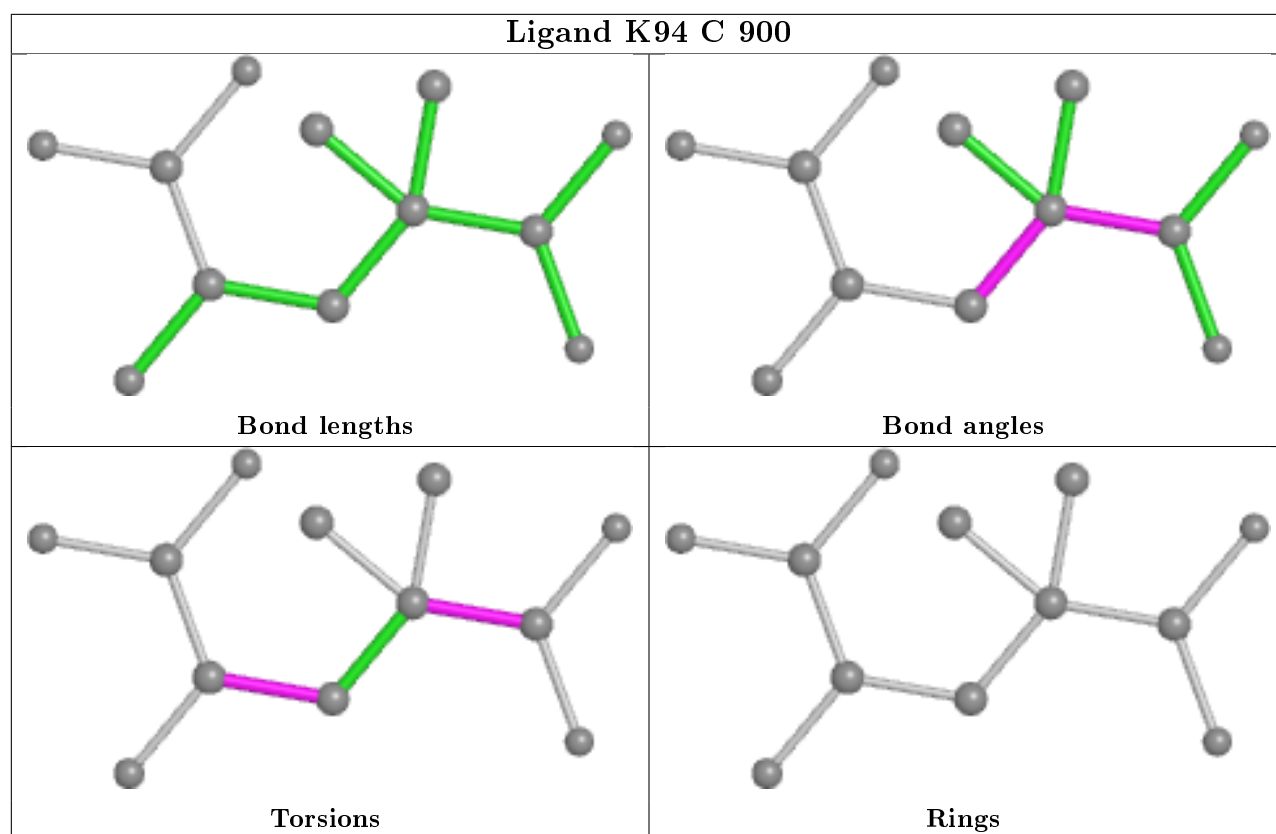
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

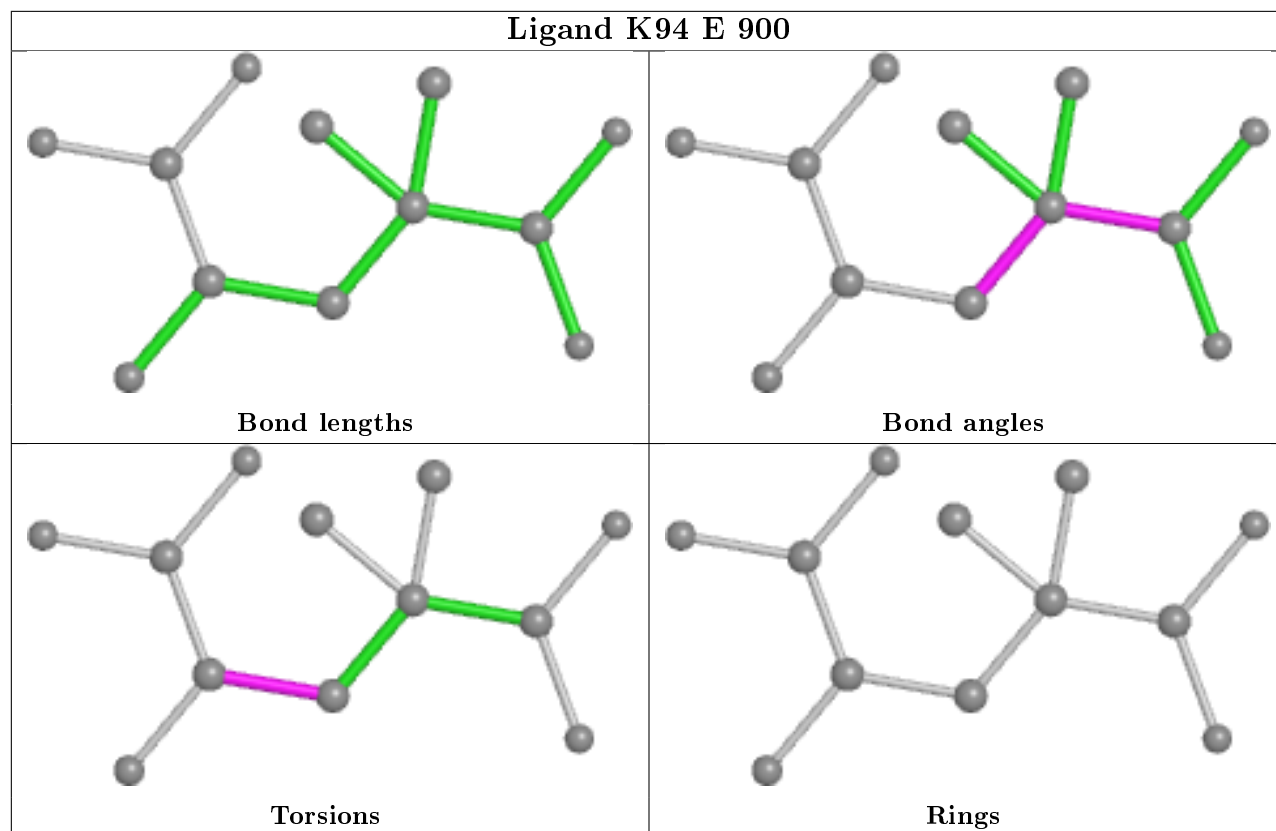
Ligand K94 A 900



Ligand K94 B 900







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%)	-0.01	4 (1%) 80 81	70, 95, 141, 171	0
1	B	365/415 (87%)	-0.02	1 (0%) 94 94	70, 95, 142, 170	0
1	C	364/415 (87%)	0.19	8 (2%) 62 60	83, 112, 149, 189	0
1	D	364/415 (87%)	0.15	5 (1%) 75 75	83, 111, 150, 184	0
1	E	365/415 (87%)	0.09	10 (2%) 54 52	81, 109, 147, 166	0
All	All	1824/2075 (87%)	0.08	28 (1%) 73 72	70, 105, 148, 189	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	480	THR	4.7
1	C	355	LEU	3.8
1	D	282	GLU	3.3
1	C	480	THR	3.1
1	E	342	TYR	3.1
1	E	310	PRO	2.9
1	A	310	PRO	2.9
1	D	66	GLY	2.8
1	E	236	GLU	2.7
1	A	221	ASP	2.6
1	E	475	ILE	2.5
1	C	184	THR	2.5
1	E	479	MET	2.5
1	D	184	THR	2.4
1	C	310	PRO	2.4
1	A	480	THR	2.3
1	D	106	PRO	2.3
1	C	283	MET	2.3
1	E	66	GLY	2.3
1	E	355	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	178	ILE	2.2
1	A	236	GLU	2.2
1	C	354	ARG	2.2
1	C	179	GLN	2.2
1	E	221	ASP	2.2
1	D	480	THR	2.1
1	E	478	TYR	2.1
1	B	282	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

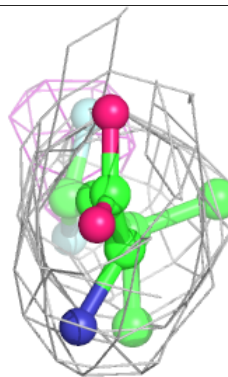
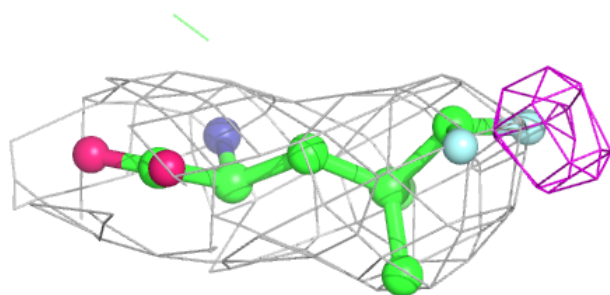
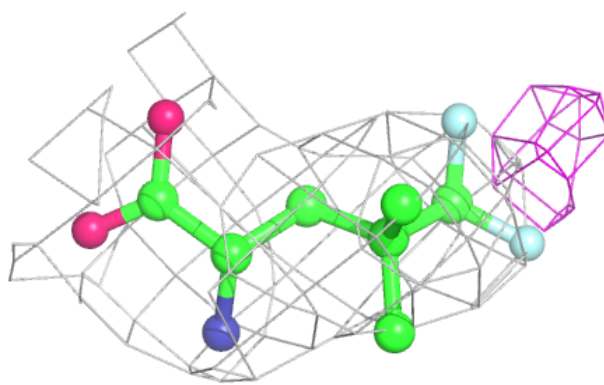
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	K94	A	900	12/12	0.91	0.34	88,93,101,111	0
2	K94	D	900	12/12	0.92	0.37	77,107,124,127	0
2	K94	C	900	12/12	0.95	0.43	86,103,117,123	0
2	K94	E	900	12/12	0.95	0.32	84,102,112,116	0
2	K94	B	900	12/12	0.98	0.43	79,93,114,120	0

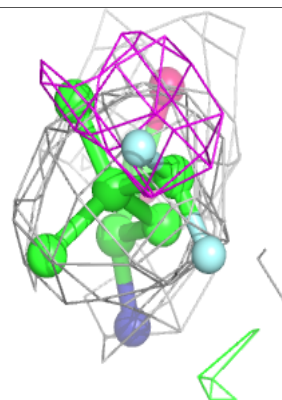
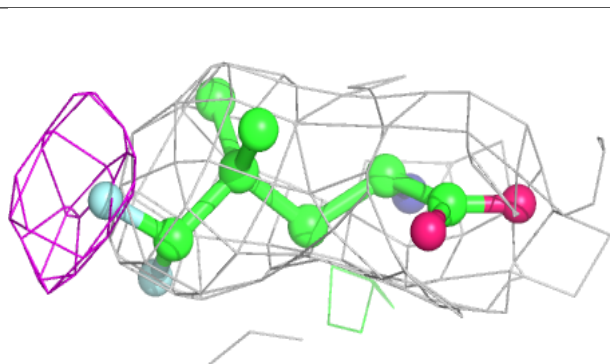
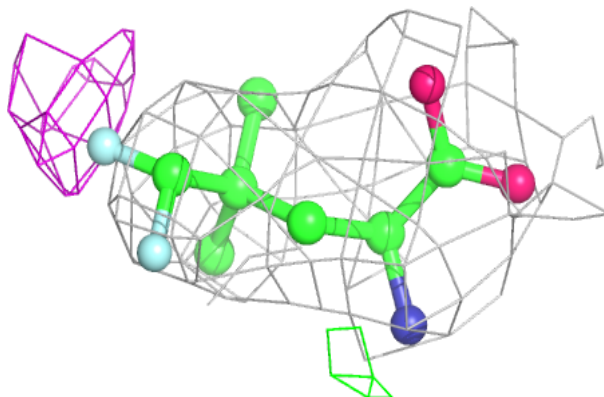
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

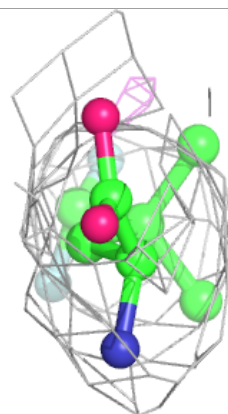
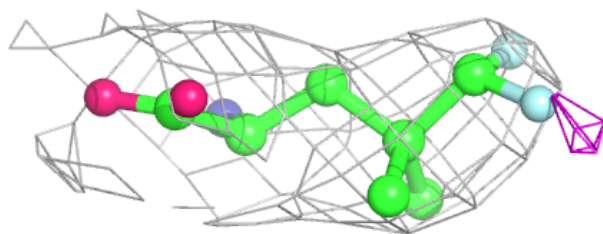
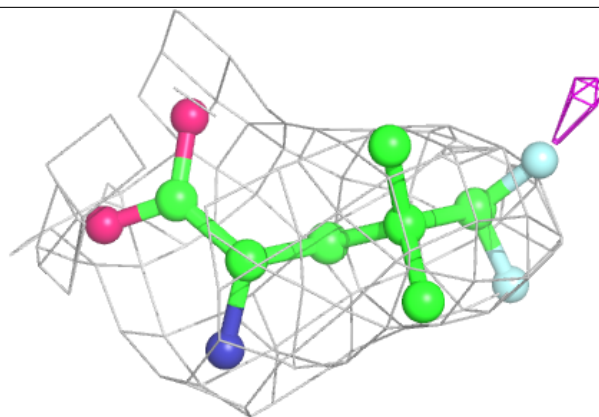
**Electron density around K94 D 900:**

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

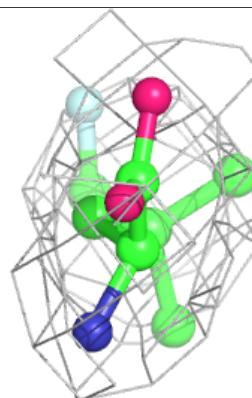
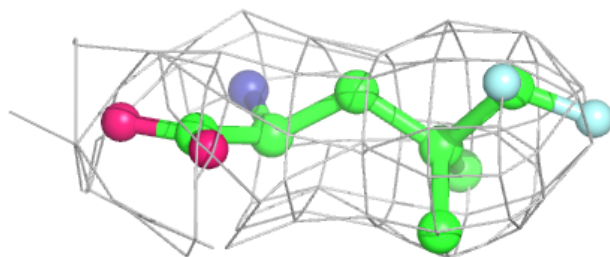
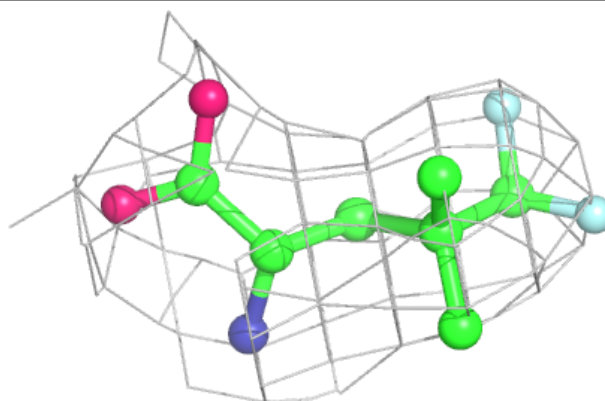


Electron density around K94 C 900:

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

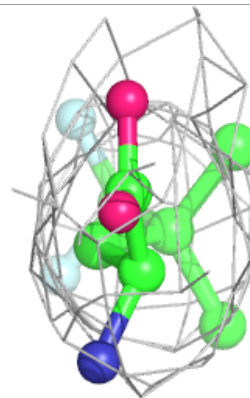
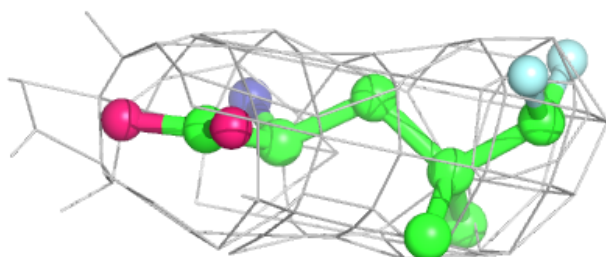
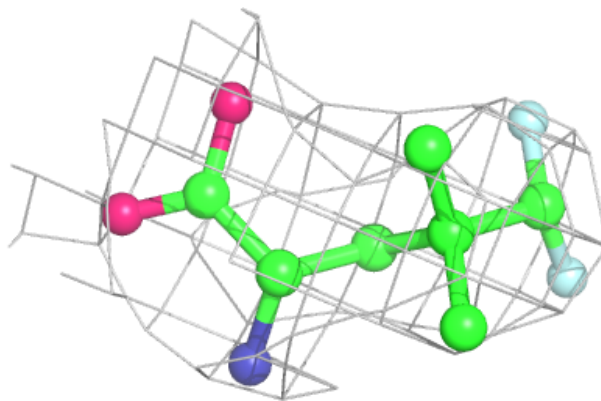
**Electron density around K94 E 900:**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.