



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:01 AM UTC

PDB ID : 2OAX / pdb_00002oax
Title : Crystal structure of the S810L mutant mineralocorticoid receptor associated with SC9420
Authors : Huyet, J.; Pinon, G.M.; Fay, M.R.; Rafestin-Oblin, M.E.; Fagart, J.
Deposited on : 2006-12-18
Resolution : 2.29 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

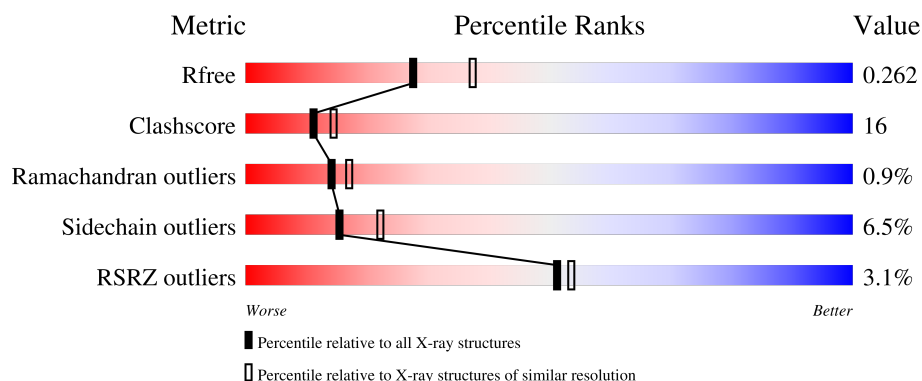
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	256	2% 60% 27% • 9%
1	B	256	% 60% 26% 5% 9%
1	C	256	% 65% 24% • 9%
1	D	256	3% 63% 25% • 9%
1	E	256	7% 49% 39% • 9%

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Mol	Chain	Length	Quality of chain
1	F	256	3% 62% 29% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12016 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 Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1903	1242	303	344	14			
1	B	233	Total	C	N	O	S	0	0	0
			1916	1248	307	347	14			
1	C	233	Total	C	N	O	S	0	0	0
			1913	1246	306	347	14			
1	D	234	Total	C	N	O	S	0	0	0
			1919	1250	308	347	14			
1	E	234	Total	C	N	O	S	0	0	0
			1912	1244	307	347	14			
1	F	238	Total	C	N	O	S	0	0	0
			1940	1261	311	354	14			

There are 24 discrepancies between the modelled and reference sequences:

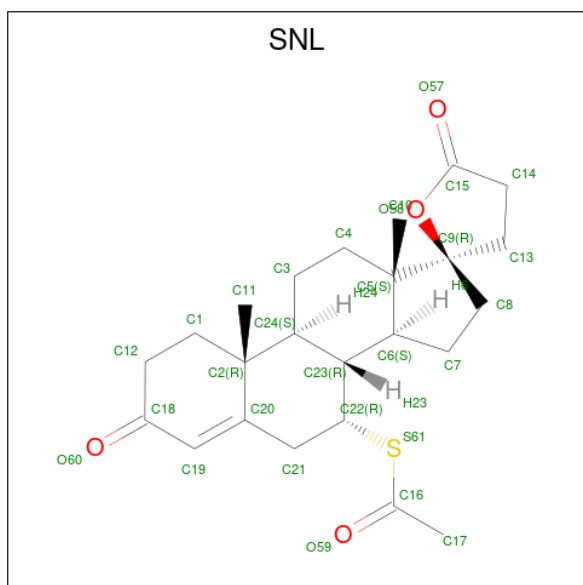
Chain	Residue	Modelled	Actual	Comment	Reference
A	729	GLY	-	expression tag	UNP P08235
A	730	SER	-	expression tag	UNP P08235
A	810	LEU	SER	engineered mutation	UNP P08235
A	910	ALA	CYS	engineered mutation	UNP P08235
B	729	GLY	-	expression tag	UNP P08235
B	730	SER	-	expression tag	UNP P08235
B	810	LEU	SER	engineered mutation	UNP P08235
B	910	ALA	CYS	engineered mutation	UNP P08235
C	729	GLY	-	expression tag	UNP P08235
C	730	SER	-	expression tag	UNP P08235
C	810	LEU	SER	engineered mutation	UNP P08235
C	910	ALA	CYS	engineered mutation	UNP P08235
D	729	GLY	-	expression tag	UNP P08235
D	730	SER	-	expression tag	UNP P08235
D	810	LEU	SER	engineered mutation	UNP P08235
D	910	ALA	CYS	engineered mutation	UNP P08235
E	729	GLY	-	expression tag	UNP P08235

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Chain	Residue	Modelled	Actual	Comment	Reference
E	730	SER	-	expression tag	UNP P08235
E	810	LEU	SER	engineered mutation	UNP P08235
E	910	ALA	CYS	engineered mutation	UNP P08235
F	729	GLY	-	expression tag	UNP P08235
F	730	SER	-	expression tag	UNP P08235
F	810	LEU	SER	engineered mutation	UNP P08235
F	910	ALA	CYS	engineered mutation	UNP P08235

- Molecule 2 is SPIRONOLACTONE (CCD ID: SNL) (formula: $C_{24}H_{32}O_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			29	24	4	1		
2	B	1	Total	C	O	S	0	0
			29	24	4	1		
2	C	1	Total	C	O	S	0	0
			29	24	4	1		
2	D	1	Total	C	O	S	0	0
			29	24	4	1		
2	E	1	Total	C	O	S	0	0
			29	24	4	1		
2	F	1	Total	C	O	S	0	0
			29	24	4	1		

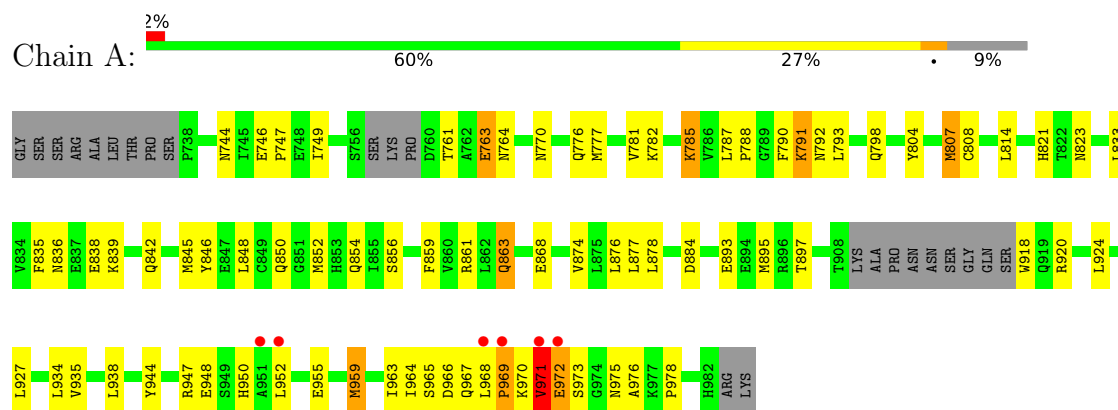
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total 54	O 54	0	0
3	B	53	Total 53	O 53	0	0
3	C	72	Total 72	O 72	0	0
3	D	66	Total 66	O 66	0	0
3	E	34	Total 34	O 34	0	0
3	F	60	Total 60	O 60	0	0

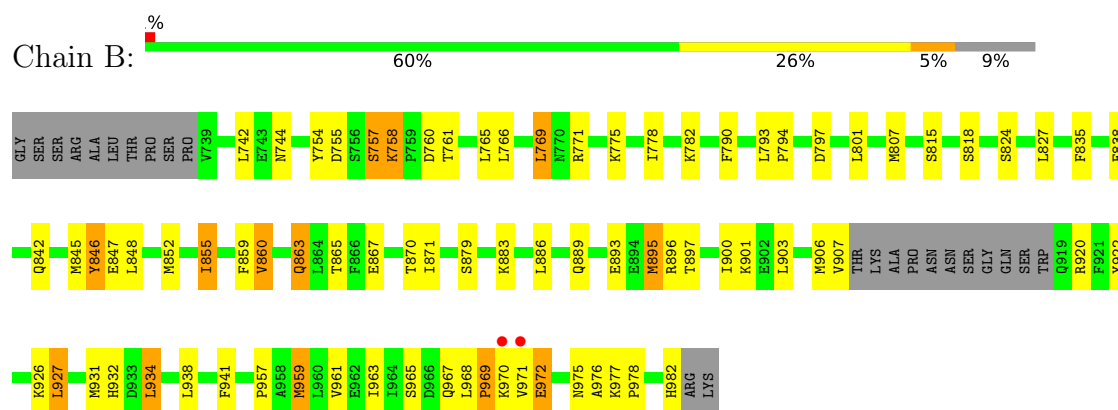
3 Residue-property plots

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

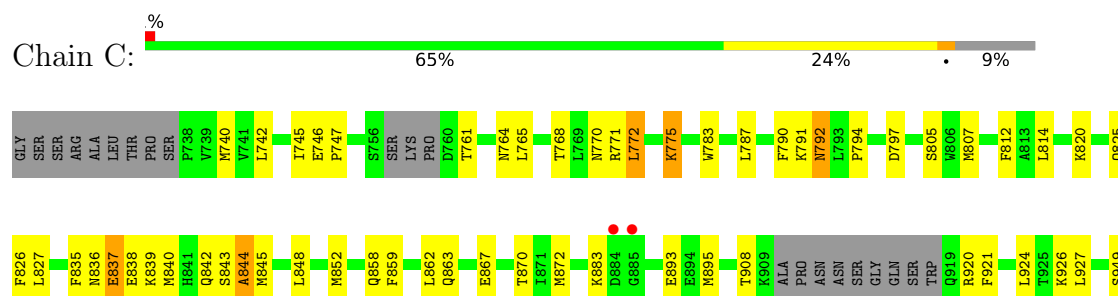
• Molecule 1: Mineralocorticoid receptor



• Molecule 1: Mineralocorticoid receptor

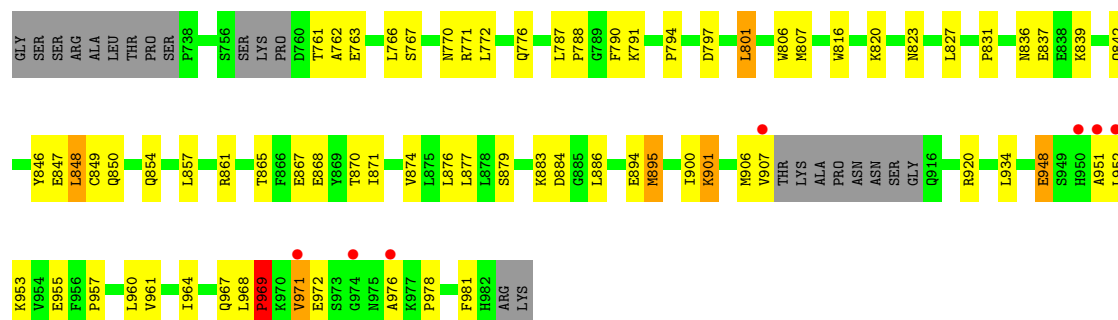


• Molecule 1: Mineralocorticoid receptor

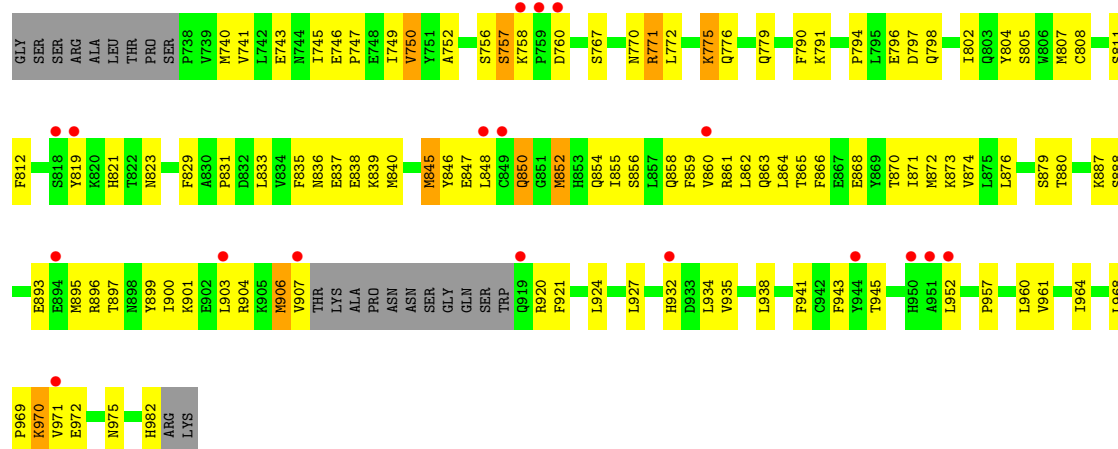




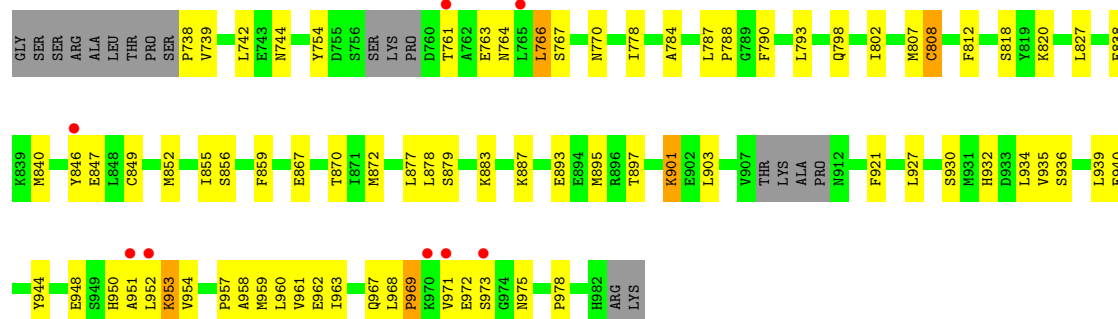
• Molecule 1: Mineralocorticoid receptor



• Molecule 1: Mineralocorticoid receptor



• Molecule 1: Mineralocorticoid receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	122.20Å 122.20Å 91.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.92 – 2.29 14.92 – 2.29	Depositor EDS
% Data completeness (in resolution range)	91.2 (14.92-2.29) 91.2 (14.92-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.263 0.239 , 0.262	Depositor DCC
R_{free} test set	3220 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.034 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12016	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.32 % 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 8.1530e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/1948	0.90	4/2636 (0.2%)
1	B	0.46	0/1960	0.89	6/2647 (0.2%)
1	C	0.48	0/1956	0.92	3/2641 (0.1%)
1	D	0.46	0/1963	0.95	4/2651 (0.2%)
1	E	0.47	2/1956 (0.1%)	0.93	3/2643 (0.1%)
1	F	0.42	0/1984	0.88	4/2680 (0.1%)
All	All	0.45	2/11767 (0.0%)	0.91	24/15898 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	758	LYS	CA-C	-6.54	1.45	1.53
1	E	757	SER	N-CA	5.63	1.53	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	837	GLU	N-CA-C	-9.27	101.39	112.89
1	A	846	TYR	N-CA-C	8.94	121.92	111.02
1	D	972	GLU	N-CA-C	-7.16	102.50	112.45
1	A	821	HIS	N-CA-C	6.70	119.94	111.69
1	B	972	GLU	N-CA-C	-6.66	104.78	113.17
1	B	941	PHE	N-CA-C	-6.18	104.46	111.07
1	B	846	TYR	N-CA-C	-6.11	102.90	110.41
1	B	855	ILE	N-CA-C	-5.93	104.73	110.72
1	E	805	SER	N-CA-C	5.88	119.76	112.59
1	F	778	ILE	N-CA-C	-5.88	104.78	110.72
1	D	971	VAL	CB-CA-C	-5.69	101.95	111.29
1	C	921	PHE	N-CA-C	-5.62	105.30	111.82
1	D	971	VAL	CA-C-N	-5.58	109.74	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	971	VAL	C-N-CA	-5.58	109.74	121.64
1	B	778	ILE	N-CA-C	-5.49	105.15	110.42
1	B	927	LEU	N-CA-C	-5.47	105.34	112.23
1	E	771	ARG	N-CA-C	-5.28	105.42	111.07
1	C	844	ALA	N-CA-C	-5.20	106.88	113.23
1	F	808	CYS	N-CA-C	-5.13	105.60	111.14
1	A	868	GLU	N-CA-C	-5.11	105.41	111.69
1	A	972	GLU	N-CA-C	-5.03	104.80	112.04
1	F	793	LEU	CA-C-N	-5.02	114.78	119.85
1	F	793	LEU	C-N-CA	-5.02	114.78	119.85
1	E	756	SER	N-CA-C	5.00	120.27	113.37

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	1903	0	1887	65	0
1	B	1916	0	1929	71	0
1	C	1913	0	1920	42	0
1	D	1919	0	1921	57	0
1	E	1912	0	1919	80	0
1	F	1940	0	1932	59	0
2	A	29	0	32	4	0
2	B	29	0	32	2	0
2	C	29	0	32	6	0
2	D	29	0	32	5	0
2	E	29	0	32	5	0
2	F	29	0	32	11	0
3	A	54	0	0	3	0
3	B	53	0	0	1	0
3	C	72	0	0	1	0
3	D	66	0	0	2	0
3	E	34	0	0	3	0
3	F	60	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12016	0	11700	382	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 16.

All (382) 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:F:6001:SNL:C23	2:F:6001:SNL:C24	1.74	1.65
2:F:6001:SNL:S61	2:F:6001:SNL:C22	2.04	1.44
2:C:3001:SNL:S61	2:C:3001:SNL:C22	2.08	1.39
1:A:852:MET:HE2	1:A:934:LEU:CD2	1.52	1.37
1:A:852:MET:CE	1:A:934:LEU:HD23	1.58	1.31
1:F:761:THR:H	1:F:764:ASN:ND2	1.49	1.09
1:F:878:LEU:HD11	1:F:895:MET:HE2	1.29	1.07
1:F:761:THR:N	1:F:764:ASN:HD22	1.54	1.05
1:A:852:MET:HE2	1:A:934:LEU:HD21	1.34	1.03
1:A:852:MET:CE	1:A:934:LEU:CD2	2.22	1.02
1:A:852:MET:HE1	1:A:934:LEU:HD23	1.41	1.00
1:B:926:LYS:HD2	1:B:982:HIS:ND1	1.78	0.98
1:B:758:LYS:HD2	1:B:758:LYS:N	1.80	0.97
1:F:812:PHE:HZ	1:F:872:MET:HE2	1.34	0.93
1:E:807:MET:HE1	2:E:5001:SNL:H23	1.55	0.88
1:B:758:LYS:N	1:B:758:LYS:CD	2.38	0.87
1:E:772:LEU:HD23	2:E:5001:SNL:H121	1.56	0.86
1:B:794:PRO:HG2	1:B:797:ASP:OD2	1.76	0.85
1:E:767:SER:HB3	1:E:771:ARG:HH12	1.40	0.85
1:D:831:PRO:HG3	3:D:7319:HOH:O	1.79	0.82
1:B:926:LYS:HD2	1:B:982:HIS:CE1	2.15	0.81
1:F:932:HIS:CE1	1:F:978:PRO:HB3	2.15	0.81
1:A:965:SER:O	1:A:969:PRO:HG3	1.83	0.78
1:E:852:MET:HE3	1:E:855:ILE:HG13	1.66	0.76
1:C:839:LYS:HA	1:C:842:GLN:HE21	1.49	0.75
1:A:749:ILE:HD12	1:A:749:ILE:H	1.51	0.75
1:C:790:PHE:HA	1:C:895:MET:HE2	1.68	0.74
1:A:808:CYS:HB3	1:A:876:LEU:HD22	1.70	0.74
1:F:878:LEU:CD1	1:F:895:MET:HE2	2.14	0.73
1:D:790:PHE:HA	1:D:895:MET:HE2	1.68	0.73
1:A:848:LEU:HG	1:A:938:LEU:HD23	1.71	0.72
1:C:761:THR:HG23	1:C:764:ASN:H	1.53	0.72
1:D:976:ALA:O	1:D:978:PRO:HD3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:957:PRO:O	1:D:961:VAL:HG23	1.90	0.72
1:A:948:GLU:O	1:A:952:LEU:HG	1.89	0.71
2:F:6001:SNL:C24	2:F:6001:SNL:C6	2.67	0.71
1:F:878:LEU:HD11	1:F:895:MET:CE	2.13	0.71
1:C:839:LYS:HD3	1:C:842:GLN:NE2	2.06	0.70
1:B:758:LYS:CD	1:B:758:LYS:H	2.02	0.70
1:C:920:ARG:O	1:C:924:LEU:HG	1.90	0.70
1:B:927:LEU:HD23	1:B:927:LEU:O	1.91	0.70
1:E:837:GLU:HA	1:E:840:MET:HE2	1.73	0.70
1:C:794:PRO:HG2	1:C:797:ASP:OD2	1.93	0.69
1:F:761:THR:HG22	1:F:764:ASN:ND2	2.07	0.69
1:D:836:ASN:H	1:D:839:LYS:HB2	1.58	0.69
1:B:967:GLN:O	1:B:971:VAL:HB	1.93	0.69
1:D:960:LEU:HD22	1:D:964:ILE:HD11	1.74	0.69
1:D:787:LEU:HD21	1:D:874:VAL:HG13	1.74	0.68
1:A:968:LEU:N	1:A:969:PRO:HD2	2.08	0.68
1:C:836:ASN:H	1:C:839:LYS:HB2	1.58	0.68
1:E:866:PHE:O	1:E:870:THR:HG23	1.94	0.68
1:E:767:SER:HB3	1:E:771:ARG:NH1	2.08	0.67
1:F:968:LEU:N	1:F:969:PRO:HD2	2.09	0.67
1:A:863:GLN:NE2	1:A:863:GLN:HA	2.08	0.67
1:F:840:MET:HE2	1:F:849:CYS:HB3	1.77	0.66
1:A:959:MET:SD	1:A:963:ILE:HD11	2.36	0.66
1:B:846:TYR:O	1:B:847:GLU:HB2	1.94	0.66
1:C:825:GLN:HG2	1:C:826:PHE:CE1	2.30	0.66
2:F:6001:SNL:C24	2:F:6001:SNL:C22	2.70	0.65
1:E:750:VAL:HG23	3:E:7012:HOH:O	1.98	0.64
1:F:959:MET:O	1:F:963:ILE:HG13	1.99	0.63
1:A:776:GLN:OE1	3:A:7021:HOH:O	2.15	0.63
1:F:761:THR:H	1:F:764:ASN:HD22	0.73	0.63
1:A:804:TYR:CE2	1:A:971:VAL:HG11	2.34	0.63
1:E:798:GLN:O	1:E:802:ILE:HG12	1.99	0.63
1:E:945:THR:HG23	1:E:952:LEU:HD22	1.80	0.63
1:B:927:LEU:HD23	1:B:927:LEU:C	2.24	0.62
1:E:752:ALA:HB2	1:E:772:LEU:HD13	1.81	0.62
1:C:807:MET:HE1	2:C:3001:SNL:H101	1.81	0.62
1:B:797:ASP:OD1	1:B:886:LEU:HB3	1.99	0.62
1:F:738:PRO:N	3:F:7175:HOH:O	2.32	0.62
1:B:968:LEU:N	1:B:969:PRO:HD2	2.13	0.62
1:A:838:GLU:O	1:A:842:GLN:HG2	2.00	0.62
1:A:976:ALA:O	1:A:978:PRO:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:790:PHE:CA	1:D:895:MET:HE2	2.30	0.61
1:F:808:CYS:SG	1:F:935:VAL:HG21	2.41	0.61
1:C:764:ASN:O	1:C:768:THR:HG23	2.00	0.61
1:A:746:GLU:CD	1:A:747:PRO:HD2	2.25	0.61
1:E:794:PRO:HG2	1:E:797:ASP:OD2	2.00	0.61
1:B:758:LYS:H	1:B:758:LYS:HD3	1.66	0.61
1:B:897:THR:HG22	1:B:901:LYS:HE3	1.83	0.61
1:E:772:LEU:CD2	2:E:5001:SNL:H121	2.30	0.60
1:F:807:MET:HE1	2:F:6001:SNL:H101	1.83	0.60
1:A:807:MET:HE1	2:A:1001:SNL:H23	1.83	0.60
1:E:876:LEU:HA	1:E:879:SER:OG	2.02	0.60
1:A:947:ARG:NH2	1:A:968:LEU:HD11	2.17	0.59
1:A:968:LEU:O	1:A:972:GLU:HB2	2.03	0.59
1:B:848:LEU:HG	1:B:938:LEU:HD23	1.83	0.59
1:B:865:THR:OG1	1:B:867:GLU:HG2	2.02	0.59
1:E:845:MET:HE3	1:E:848:LEU:HD23	1.84	0.59
1:A:790:PHE:CE2	1:A:798:GLN:HG2	2.38	0.59
1:C:772:LEU:HA	1:C:775:LYS:HE2	1.85	0.59
1:A:833:LEU:HD11	1:A:835:PHE:HE1	1.68	0.59
1:C:970:LYS:O	1:C:975:ASN:HB2	2.03	0.59
1:D:787:LEU:HD11	1:D:874:VAL:HG22	1.85	0.59
1:F:766:LEU:HG	2:F:6001:SNL:H142	1.85	0.58
1:B:957:PRO:O	1:B:961:VAL:HG23	2.04	0.58
1:B:807:MET:HE1	2:B:2001:SNL:H101	1.84	0.58
1:B:907:VAL:HG13	1:B:920:ARG:HD3	1.85	0.58
1:E:741:VAL:O	1:E:745:ILE:HG12	2.04	0.58
1:C:790:PHE:CA	1:C:895:MET:HE2	2.33	0.58
1:D:807:MET:HE1	2:D:4001:SNL:H101	1.84	0.58
1:F:742:LEU:HB3	1:F:870:THR:OG1	2.03	0.58
1:A:782:LYS:O	1:A:785:LYS:HG2	2.04	0.58
1:A:807:MET:HE1	2:A:1001:SNL:H111	1.85	0.58
1:B:838:GLU:O	1:B:842:GLN:HG3	2.05	0.57
1:B:967:GLN:HE21	1:B:967:GLN:HA	1.68	0.57
1:C:742:LEU:HB3	1:C:870:THR:OG1	2.04	0.57
1:A:823:ASN:HB2	1:E:887:LYS:HG2	1.85	0.57
1:D:850:GLN:O	1:D:854:GLN:HG2	2.04	0.57
1:E:771:ARG:HG3	1:E:771:ARG:HH11	1.69	0.57
1:B:969:PRO:C	1:B:971:VAL:H	2.12	0.57
1:E:879:SER:HB3	1:E:932:HIS:CE1	2.40	0.57
1:D:766:LEU:HD22	2:D:4001:SNL:H142	1.85	0.57
1:C:839:LYS:HD3	1:C:842:GLN:HE21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:845:MET:HG2	1:E:848:LEU:HD23	1.86	0.56
1:E:901:LYS:HE3	1:E:904:ARG:HH22	1.69	0.56
1:C:867:GLU:O	1:C:870:THR:HG22	2.06	0.56
1:F:812:PHE:CZ	1:F:872:MET:HE2	2.26	0.56
1:B:961:VAL:O	1:B:965:SER:HB3	2.05	0.56
1:E:856:SER:O	1:E:860:VAL:HG23	2.05	0.56
1:B:867:GLU:HB3	3:B:7013:HOH:O	2.06	0.56
1:B:815:SER:OG	1:B:859:PHE:CE2	2.56	0.56
1:E:861:ARG:HH11	1:E:862:LEU:HD21	1.71	0.55
1:B:883:LYS:HG2	1:B:975:ASN:OD1	2.07	0.55
1:D:951:ALA:O	1:D:953:LYS:HG3	2.06	0.55
1:C:845:MET:HG2	1:C:848:LEU:HB2	1.87	0.55
1:E:807:MET:HB3	1:E:935:VAL:HG13	1.88	0.55
1:E:903:LEU:O	1:E:907:VAL:HG23	2.06	0.55
1:A:893:GLU:O	1:A:897:THR:HG23	2.06	0.55
1:E:790:PHE:HA	1:E:895:MET:HE2	1.87	0.55
2:F:6001:SNL:C23	2:F:6001:SNL:C2	2.78	0.55
1:F:897:THR:O	1:F:901:LYS:HD2	2.07	0.55
1:F:968:LEU:O	1:F:972:GLU:HB2	2.07	0.54
1:F:763:GLU:OE1	1:F:953:LYS:HB3	2.07	0.54
1:E:907:VAL:HG11	1:E:921:PHE:N	2.23	0.54
1:A:804:TYR:OH	1:A:971:VAL:HG21	2.07	0.54
1:F:770:ASN:O	1:F:957:PRO:HG2	2.08	0.54
1:C:805:SER:HB3	3:C:7287:HOH:O	2.08	0.54
2:F:6001:SNL:C23	2:F:6001:SNL:C3	2.79	0.54
1:E:907:VAL:HG13	1:E:920:ARG:HD3	1.90	0.53
1:A:948:GLU:HB2	1:A:952:LEU:HD11	1.89	0.53
1:F:838:GLU:H	1:F:838:GLU:CD	2.16	0.53
1:B:897:THR:O	1:B:901:LYS:HG3	2.09	0.53
1:C:883:LYS:HB2	1:C:975:ASN:CG	2.33	0.53
1:D:846:TYR:O	1:D:847:GLU:HB3	2.08	0.52
1:E:861:ARG:NH1	1:E:862:LEU:HD21	2.24	0.52
1:D:770:ASN:OD1	2:D:4001:SNL:H42	2.10	0.52
2:F:6001:SNL:S61	2:F:6001:SNL:C21	2.92	0.52
1:D:971:VAL:O	1:D:971:VAL:HG12	2.10	0.52
1:F:932:HIS:ND1	1:F:978:PRO:HB3	2.25	0.52
1:F:958:ALA:O	1:F:962:GLU:HG2	2.10	0.52
1:C:814:LEU:HD23	1:C:852:MET:HG2	1.92	0.52
1:E:897:THR:HG23	1:E:901:LYS:NZ	2.24	0.52
1:B:968:LEU:O	1:B:972:GLU:HB2	2.09	0.52
1:E:872:MET:CE	1:E:927:LEU:HD22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:GLN:HG3	3:A:7267:HOH:O	2.09	0.51
1:B:742:LEU:HB3	1:B:870:THR:OG1	2.10	0.51
1:A:856:SER:O	1:A:859:PHE:HB2	2.10	0.51
1:D:772:LEU:O	1:D:776:GLN:HG3	2.10	0.51
1:E:872:MET:HE1	1:E:927:LEU:HD22	1.91	0.51
1:F:807:MET:HE2	1:F:939:LEU:HD23	1.93	0.51
1:E:771:ARG:NH1	1:E:771:ARG:HG3	2.25	0.51
1:F:739:VAL:HG21	1:F:867:GLU:HG3	1.92	0.51
1:B:967:GLN:HA	1:B:967:GLN:NE2	2.25	0.51
1:E:771:ARG:HB3	1:E:775:LYS:HE2	1.92	0.51
1:B:860:VAL:O	1:B:863:GLN:NE2	2.43	0.51
1:F:867:GLU:O	1:F:870:THR:HG22	2.10	0.51
1:D:766:LEU:HD22	2:D:4001:SNL:C14	2.41	0.51
1:E:968:LEU:O	1:E:972:GLU:HB2	2.11	0.51
1:F:856:SER:O	1:F:859:PHE:HB2	2.10	0.51
1:F:957:PRO:O	1:F:961:VAL:HG23	2.12	0.50
2:F:6001:SNL:C23	2:F:6001:SNL:S61	2.95	0.50
1:A:845:MET:HE3	2:A:1001:SNL:H171	1.94	0.50
1:D:900:ILE:HD13	1:D:981:PHE:HE1	1.76	0.50
1:A:971:VAL:HA	1:A:975:ASN:HB2	1.93	0.50
1:C:812:PHE:HZ	1:C:872:MET:HE2	1.76	0.50
1:D:761:THR:HG23	1:D:763:GLU:HB2	1.93	0.50
1:E:982:HIS:HB3	1:F:940:GLU:OE1	2.11	0.50
1:F:967:GLN:HG3	3:F:7249:HOH:O	2.12	0.50
1:C:836:ASN:N	1:C:839:LYS:HB2	2.25	0.50
1:D:767:SER:OG	1:D:955:GLU:HG2	2.12	0.49
1:D:816:TRP:CZ2	1:D:820:LYS:HD2	2.46	0.49
1:A:790:PHE:C	1:A:792:ASN:H	2.19	0.49
2:C:3001:SNL:S61	2:C:3001:SNL:C23	2.96	0.49
1:D:876:LEU:O	1:D:879:SER:HB2	2.12	0.49
1:D:907:VAL:HG13	1:D:920:ARG:HD3	1.92	0.49
1:F:798:GLN:O	1:F:802:ILE:HG12	2.12	0.49
1:B:846:TYR:O	1:B:847:GLU:CB	2.61	0.49
1:C:771:ARG:HA	1:C:957:PRO:HG2	1.94	0.49
1:A:944:TYR:CE1	1:A:948:GLU:HG3	2.47	0.49
1:A:770:ASN:OD1	2:A:1001:SNL:H42	2.13	0.49
1:B:871:ILE:HG21	1:B:903:LEU:HB2	1.95	0.49
1:D:788:PRO:HA	1:D:791:LYS:NZ	2.28	0.49
1:B:893:GLU:HA	1:B:893:GLU:OE1	2.12	0.48
1:F:761:THR:HG23	1:F:763:GLU:H	1.79	0.48
1:F:784:ALA:HB1	1:F:790:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:846:TYR:O	1:F:847:GLU:HB2	2.13	0.48
1:F:770:ASN:HB3	1:F:957:PRO:HD3	1.95	0.48
1:B:755:ASP:HB3	1:B:758:LYS:NZ	2.29	0.48
1:B:793:LEU:HD11	1:B:895:MET:HE2	1.95	0.48
1:B:794:PRO:CG	1:B:797:ASP:OD2	2.55	0.48
1:D:794:PRO:HG2	1:D:797:ASP:OD2	2.13	0.48
1:E:846:TYR:HD1	1:E:847:GLU:HG2	1.78	0.48
1:D:797:ASP:CG	1:D:886:LEU:HB3	2.39	0.48
1:E:794:PRO:HG3	1:E:888:SER:OG	2.13	0.48
1:D:968:LEU:HB3	1:D:969:PRO:HD3	1.94	0.48
1:A:878:LEU:HD22	1:A:895:MET:HE3	1.96	0.48
1:B:976:ALA:O	1:B:978:PRO:HD3	2.14	0.48
1:A:964:ILE:C	1:A:966:ASP:H	2.21	0.48
1:E:804:TYR:HB3	1:E:880:THR:HB	1.96	0.47
1:F:930:SER:O	1:F:934:LEU:HD13	2.14	0.47
1:F:968:LEU:O	1:F:969:PRO:O	2.32	0.47
1:C:770:ASN:OD1	2:C:3001:SNL:H42	2.14	0.47
1:D:797:ASP:OD1	1:D:886:LEU:HB3	2.15	0.47
1:E:796:GLU:HB2	1:E:887:LYS:HD3	1.97	0.47
1:B:867:GLU:HG3	1:B:906:MET:SD	2.55	0.47
1:D:790:PHE:CE1	1:D:877:LEU:HD21	2.48	0.47
1:A:761:THR:HG23	1:A:764:ASN:H	1.80	0.47
1:C:783:TRP:CZ2	1:C:787:LEU:HD11	2.49	0.47
1:D:967:GLN:C	1:D:971:VAL:HG23	2.40	0.47
1:F:738:PRO:O	1:F:742:LEU:HG	2.15	0.47
1:D:854:GLN:NE2	1:D:857:LEU:HD12	2.29	0.47
1:F:903:LEU:HD23	1:F:921:PHE:CE1	2.50	0.47
1:E:868:GLU:OE1	1:E:906:MET:HE2	2.15	0.47
1:A:787:LEU:HD21	1:A:874:VAL:HG13	1.97	0.46
1:A:848:LEU:HG	1:A:938:LEU:CD2	2.42	0.46
1:D:790:PHE:CE1	1:D:801:LEU:HD23	2.50	0.46
1:A:791:LYS:HA	1:A:798:GLN:NE2	2.30	0.46
1:B:793:LEU:HD11	1:B:895:MET:CE	2.44	0.46
1:E:836:ASN:HD22	1:E:837:GLU:H	1.62	0.46
1:D:861:ARG:HE	1:D:861:ARG:HB2	1.42	0.46
1:E:836:ASN:C	1:E:838:GLU:N	2.73	0.46
1:B:855:ILE:HD11	1:B:934:LEU:HD21	1.97	0.46
1:B:757:SER:C	1:B:758:LYS:HD2	2.40	0.46
1:C:977:LYS:N	1:C:978:PRO:HD3	2.31	0.46
1:C:812:PHE:CZ	1:C:872:MET:HE2	2.51	0.46
1:A:807:MET:HE2	1:A:807:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:VAL:HG13	1:A:975:ASN:HB2	1.98	0.46
1:D:790:PHE:HD1	1:D:895:MET:HE1	1.81	0.46
1:E:750:VAL:HG21	1:E:776:GLN:HG2	1.97	0.46
1:B:959:MET:HE1	1:B:963:ILE:HD11	1.97	0.45
1:E:840:MET:HE3	1:E:846:TYR:CE2	2.51	0.45
1:B:932:HIS:CE1	1:B:978:PRO:HB3	2.51	0.45
1:F:787:LEU:HD12	1:F:788:PRO:HD2	1.97	0.45
1:B:755:ASP:CB	1:B:758:LYS:NZ	2.79	0.45
1:E:935:VAL:HA	1:E:938:LEU:HD12	1.99	0.45
1:C:825:GLN:HG2	1:C:826:PHE:CD1	2.51	0.45
1:A:761:THR:HG22	1:A:764:ASN:OD1	2.16	0.45
1:B:969:PRO:O	1:B:971:VAL:N	2.48	0.45
1:B:824:SER:HB2	1:B:860:VAL:HG21	1.99	0.45
1:D:901:LYS:HE3	1:D:901:LYS:HA	1.98	0.45
1:F:952:LEU:C	1:F:954:VAL:H	2.25	0.45
1:B:867:GLU:O	1:B:870:THR:HG22	2.16	0.45
1:D:967:GLN:O	1:D:971:VAL:HG23	2.17	0.45
1:E:969:PRO:HG2	1:E:970:LYS:H	1.81	0.45
1:D:865:THR:OG1	1:D:868:GLU:HG3	2.17	0.45
1:D:772:LEU:CD2	2:D:4001:SNL:H121	2.47	0.44
1:E:941:PHE:HE2	2:E:5001:SNL:H142	1.82	0.44
1:F:744:ASN:C	1:F:744:ASN:ND2	2.75	0.44
1:B:766:LEU:HD22	2:B:2001:SNL:H142	1.99	0.44
1:B:852:MET:HE1	1:B:931:MET:HE1	2.00	0.44
1:B:967:GLN:HE21	1:B:967:GLN:CA	2.26	0.44
1:D:806:TRP:CH2	1:D:960:LEU:HD21	2.52	0.44
1:E:819:TYR:O	1:E:823:ASN:HA	2.18	0.44
1:A:920:ARG:O	1:A:924:LEU:HG	2.17	0.44
1:E:846:TYR:CD1	1:E:847:GLU:HG2	2.53	0.44
1:C:859:PHE:HE1	1:C:927:LEU:HD21	1.83	0.44
1:E:811:SER:HB2	1:E:852:MET:SD	2.57	0.44
1:E:943:PHE:CE2	1:E:964:ILE:HG23	2.52	0.44
1:B:845:MET:O	1:B:845:MET:HG2	2.18	0.44
1:C:960:LEU:HA	1:C:960:LEU:HD23	1.74	0.44
1:B:922:TYR:O	1:B:926:LYS:HB2	2.17	0.44
1:F:967:GLN:O	1:F:971:VAL:HB	2.18	0.44
1:C:746:GLU:CD	1:C:747:PRO:HD2	2.43	0.44
1:E:858:GLN:O	1:E:862:LEU:HG	2.18	0.44
1:F:770:ASN:OD1	2:F:6001:SNL:H42	2.17	0.44
1:F:883:LYS:N	1:F:975:ASN:O	2.51	0.44
1:A:787:LEU:HD12	1:A:788:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:MET:HB3	1:A:935:VAL:HG13	1.99	0.43
1:D:870:THR:CG2	1:D:871:ILE:N	2.81	0.43
1:E:743:GLU:HG2	1:E:866:PHE:CE2	2.53	0.43
1:E:859:PHE:CD1	1:E:864:LEU:HD22	2.53	0.43
1:E:897:THR:O	1:E:900:ILE:HB	2.18	0.43
1:B:757:SER:OG	1:B:758:LYS:HD2	2.17	0.43
1:D:883:LYS:HG3	1:D:884:ASP:N	2.33	0.43
1:E:957:PRO:O	1:E:961:VAL:HG23	2.18	0.43
1:A:948:GLU:C	1:A:950:HIS:N	2.75	0.43
1:E:747:PRO:HB3	1:E:779:GLN:HB3	2.00	0.43
1:F:971:VAL:HG12	1:F:971:VAL:O	2.18	0.43
1:A:850:GLN:O	1:A:854:GLN:HG2	2.19	0.43
1:C:761:THR:HG22	1:C:764:ASN:HB2	2.00	0.43
1:D:968:LEU:N	1:D:969:PRO:HD2	2.33	0.43
1:E:821:HIS:HE1	3:E:7042:HOH:O	2.02	0.43
1:A:814:LEU:HD12	1:A:814:LEU:O	2.19	0.43
1:A:874:VAL:O	1:A:877:LEU:HB3	2.18	0.43
1:B:815:SER:HG	1:B:859:PHE:HE2	1.54	0.43
1:A:746:GLU:CG	1:A:747:PRO:HD2	2.48	0.43
1:B:769:LEU:CD2	1:B:845:MET:HE1	2.49	0.43
1:E:746:GLU:OE1	1:E:747:PRO:HD2	2.19	0.43
1:E:840:MET:HE3	1:E:846:TYR:HE2	1.83	0.43
1:A:782:LYS:HA	1:A:785:LYS:HD3	2.00	0.42
1:C:839:LYS:HA	1:C:842:GLN:NE2	2.26	0.42
1:E:836:ASN:ND2	1:E:837:GLU:H	2.16	0.42
1:E:872:MET:SD	1:E:924:LEU:HD22	2.59	0.42
1:E:897:THR:HG23	1:E:901:LYS:HZ3	1.83	0.42
1:A:790:PHE:C	1:A:792:ASN:N	2.77	0.42
1:D:900:ILE:CD1	1:D:981:PHE:HE1	2.31	0.42
1:F:818:SER:OG	1:F:827:LEU:HA	2.19	0.42
1:C:745:ILE:HD11	1:C:787:LEU:HD23	2.02	0.42
1:C:836:ASN:O	1:C:840:MET:HG3	2.19	0.42
1:F:790:PHE:CE1	1:F:877:LEU:HD21	2.54	0.42
1:F:855:ILE:HD11	1:F:934:LEU:HD21	2.01	0.42
1:F:883:LYS:HB2	1:F:975:ASN:HA	2.01	0.42
1:B:969:PRO:C	1:B:971:VAL:N	2.77	0.42
1:A:761:THR:HG21	1:A:763:GLU:OE1	2.19	0.42
1:D:957:PRO:HG2	3:D:7247:HOH:O	2.18	0.42
1:F:968:LEU:N	1:F:969:PRO:CD	2.79	0.42
1:A:777:MET:O	1:A:781:VAL:HG23	2.19	0.42
1:A:969:PRO:HG2	1:A:970:LYS:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:968:LEU:CB	1:D:969:PRO:HD3	2.48	0.42
1:F:827:LEU:HD11	1:F:849:CYS:O	2.19	0.42
1:D:948:GLU:O	1:D:952:LEU:HG	2.20	0.42
1:E:749:ILE:CG2	1:E:831:PRO:HG2	2.50	0.42
1:E:906:MET:HE3	1:E:906:MET:O	2.20	0.42
1:F:927:LEU:O	1:F:927:LEU:HD23	2.19	0.42
1:A:763:GLU:CD	3:A:7186:HOH:O	2.62	0.42
1:C:893:GLU:OE1	1:C:893:GLU:HA	2.19	0.42
1:D:761:THR:OG1	1:D:762:ALA:N	2.52	0.42
1:E:808:CYS:O	1:E:812:PHE:HB2	2.20	0.42
1:F:820:LYS:HE2	3:F:7238:HOH:O	2.19	0.42
1:B:754:TYR:OH	1:B:760:ASP:OD1	2.36	0.41
1:E:861:ARG:HD2	1:E:862:LEU:HD23	2.01	0.41
1:B:896:ARG:O	1:B:900:ILE:HG13	2.20	0.41
1:D:867:GLU:O	1:D:870:THR:HG22	2.20	0.41
1:A:971:VAL:HG13	1:A:975:ASN:CB	2.50	0.41
1:B:827:LEU:HB2	1:B:835:PHE:HB2	2.01	0.41
1:E:873:LYS:HB3	3:E:7058:HOH:O	2.20	0.41
1:B:889:GLN:O	1:B:893:GLU:HG2	2.20	0.41
2:C:3001:SNL:S61	2:C:3001:SNL:H6	2.61	0.41
1:D:968:LEU:CB	1:D:969:PRO:CD	2.99	0.41
1:A:948:GLU:C	1:A:950:HIS:H	2.28	0.41
1:B:971:VAL:HG12	1:B:971:VAL:O	2.20	0.41
1:C:838:GLU:O	1:C:842:GLN:HG2	2.20	0.41
2:C:3001:SNL:S61	2:C:3001:SNL:C21	3.00	0.41
1:E:829:PHE:HB2	1:E:833:LEU:HD23	2.03	0.41
1:A:790:PHE:HD1	1:A:895:MET:HE1	1.85	0.41
1:B:755:ASP:HB3	1:B:758:LYS:HZ2	1.84	0.41
1:B:965:SER:O	1:B:969:PRO:HG3	2.20	0.41
1:F:950:HIS:ND1	1:F:951:ALA:N	2.68	0.41
1:A:927:LEU:C	1:A:927:LEU:HD23	2.45	0.41
1:B:855:ILE:HD11	1:B:934:LEU:CD2	2.51	0.41
1:B:977:LYS:HA	1:B:978:PRO:HD3	1.89	0.41
1:C:858:GLN:O	1:C:862:LEU:HB2	2.21	0.41
1:E:874:VAL:HG11	1:E:899:TYR:CE1	2.56	0.41
1:E:921:PHE:HE2	1:F:944:TYR:HH	1.60	0.41
1:D:827:LEU:HD11	1:D:849:CYS:O	2.21	0.41
1:E:971:VAL:HG12	1:E:971:VAL:O	2.21	0.41
1:C:765:LEU:HD12	1:C:835:PHE:CZ	2.56	0.40
1:C:783:TRP:CH2	1:C:787:LEU:HD11	2.57	0.40
1:E:770:ASN:OD1	2:E:5001:SNL:H42	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:850:GLN:HE21	1:E:850:GLN:HB3	1.63	0.40
1:E:896:ARG:O	1:E:900:ILE:HG13	2.21	0.40
1:B:771:ARG:O	1:B:775:LYS:HD3	2.20	0.40
1:B:959:MET:CE	1:B:963:ILE:HD11	2.51	0.40
1:E:921:PHE:HD2	1:F:944:TYR:HH	1.62	0.40
1:A:836:ASN:H	1:A:839:LYS:HB2	1.87	0.40
1:B:790:PHE:HD1	1:B:895:MET:HE1	1.85	0.40
1:B:818:SER:OG	1:B:827:LEU:HA	2.21	0.40
1:C:792:ASN:HD22	1:C:792:ASN:C	2.29	0.40
1:D:790:PHE:HE1	1:D:801:LEU:HD23	1.86	0.40
1:D:846:TYR:O	1:D:847:GLU:CB	2.70	0.40
1:E:897:THR:HA	1:E:900:ILE:HD12	2.02	0.40
1:B:927:LEU:C	1:B:927:LEU:CD2	2.93	0.40
1:C:843:SER:O	1:C:844:ALA:HB3	2.22	0.40
1:D:787:LEU:HD11	1:D:874:VAL:CG2	2.50	0.40
1:D:836:ASN:N	1:D:839:LYS:HB2	2.30	0.40
1:D:968:LEU:HB3	1:D:969:PRO:CD	2.51	0.40
1:E:852:MET:CE	1:E:934:LEU:HD23	2.50	0.40
1:E:907:VAL:CG1	1:E:920:ARG:HB3	2.51	0.40
1:A:918:TRP:O	1:A:918:TRP:HE3	2.04	0.40
1:D:846:TYR:C	1:D:848:LEU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/256 (89%)	214 (94%)	9 (4%)	4 (2%)	6	6
1	B	229/256 (90%)	217 (95%)	10 (4%)	2 (1%)	14	17
1	C	227/256 (89%)	217 (96%)	9 (4%)	1 (0%)	30	38
1	D	228/256 (89%)	214 (94%)	13 (6%)	1 (0%)	30	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	230/256 (90%)	211 (92%)	18 (8%)	1 (0%)	30	38
1	F	232/256 (91%)	210 (90%)	19 (8%)	3 (1%)	9	10
All	All	1373/1536 (89%)	1283 (93%)	78 (6%)	12 (1%)	14	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	969	PRO
1	C	908	THR
1	F	969	PRO
1	F	973	SER
1	A	969	PRO
1	A	971	VAL
1	B	970	LYS
1	E	970	LYS
1	A	973	SER
1	D	969	PRO
1	A	791	LYS
1	F	754	TYR

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	210/234 (90%)	199 (95%)	11 (5%)	21	31
1	B	215/234 (92%)	201 (94%)	14 (6%)	15	22
1	C	214/234 (92%)	198 (92%)	16 (8%)	12	17
1	D	214/234 (92%)	201 (94%)	13 (6%)	17	24
1	E	214/234 (92%)	195 (91%)	19 (9%)	9	12
1	F	216/234 (92%)	205 (95%)	11 (5%)	21	32
All	All	1283/1404 (91%)	1199 (94%)	84 (6%)	15	22

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	ASN
1	A	763	GLU
1	A	785	LYS
1	A	793	LEU
1	A	807	MET
1	A	861	ARG
1	A	863	GLN
1	A	884	ASP
1	A	955	GLU
1	A	959	MET
1	A	971	VAL
1	B	744	ASN
1	B	757	SER
1	B	758	LYS
1	B	761	THR
1	B	765	LEU
1	B	769	LEU
1	B	782	LYS
1	B	801	LEU
1	B	860	VAL
1	B	863	GLN
1	B	879	SER
1	B	895	MET
1	B	934	LEU
1	B	959	MET
1	C	740	MET
1	C	772	LEU
1	C	775	LYS
1	C	791	LYS
1	C	792	ASN
1	C	820	LYS
1	C	827	LEU
1	C	837	GLU
1	C	863	GLN
1	C	926	LYS
1	C	949	SER
1	C	959	MET
1	C	962	GLU
1	C	970	LYS
1	C	972	GLU
1	C	973	SER
1	D	771	ARG
1	D	801	LEU

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Mol	Chain	Res	Type
1	D	823	ASN
1	D	837	GLU
1	D	842	GLN
1	D	848	LEU
1	D	894	GLU
1	D	895	MET
1	D	901	LYS
1	D	906	MET
1	D	934	LEU
1	D	948	GLU
1	D	969	PRO
1	E	740	MET
1	E	750	VAL
1	E	757	SER
1	E	760	ASP
1	E	775	LYS
1	E	791	LYS
1	E	835	PHE
1	E	839	LYS
1	E	845	MET
1	E	850	GLN
1	E	852	MET
1	E	854	GLN
1	E	863	GLN
1	E	865	THR
1	E	871	ILE
1	E	893	GLU
1	E	906	MET
1	E	960	LEU
1	E	975	ASN
1	F	766	LEU
1	F	767	SER
1	F	852	MET
1	F	879	SER
1	F	887	LYS
1	F	893	GLU
1	F	901	LYS
1	F	936	SER
1	F	948	GLU
1	F	953	LYS
1	F	960	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	764	ASN
1	A	779	GLN
1	A	841	HIS
1	A	854	GLN
1	A	950	HIS
1	B	764	ASN
1	B	803	GLN
1	B	821	HIS
1	B	842	GLN
1	B	950	HIS
1	B	967	GLN
1	C	779	GLN
1	C	792	ASN
1	C	803	GLN
1	C	825	GLN
1	C	842	GLN
1	C	853	HIS
1	C	854	GLN
1	D	779	GLN
1	D	803	GLN
1	D	825	GLN
1	D	842	GLN
1	D	850	GLN
1	D	853	HIS
1	D	854	GLN
1	D	975	ASN
1	E	779	GLN
1	E	798	GLN
1	E	803	GLN
1	E	821	HIS
1	E	836	ASN
1	E	850	GLN
1	E	854	GLN
1	E	863	GLN
1	E	919	GLN
1	E	923	GLN
1	F	764	ASN
1	F	803	GLN
1	F	823	ASN
1	F	842	GLN
1	F	850	GLN
1	F	853	HIS

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Mol	Chain	Res	Type
1	F	854	GLN
1	F	863	GLN
1	F	913	ASN
1	F	923	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	SNL	C	3001	-	33,33,33	5.87	26 (78%)	54,54,54	2.72	21 (38%)
2	SNL	E	5001	-	33,33,33	4.61	22 (66%)	54,54,54	2.68	16 (29%)
2	SNL	B	2001	-	33,33,33	5.16	22 (66%)	54,54,54	3.06	24 (44%)
2	SNL	F	6001	-	33,33,33	5.75	22 (66%)	54,54,54	2.11	20 (37%)
2	SNL	A	1001	-	33,33,33	4.21	18 (54%)	54,54,54	2.50	20 (37%)
2	SNL	D	4001	-	33,33,33	5.25	23 (69%)	54,54,54	2.84	21 (38%)

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	SNL	C	3001	-	-	0/4/80/80	0/5/5/5
2	SNL	E	5001	-	-	0/4/80/80	0/5/5/5
2	SNL	B	2001	-	-	0/4/80/80	0/5/5/5
2	SNL	F	6001	-	-	0/4/80/80	0/5/5/5
2	SNL	A	1001	-	-	0/4/80/80	0/5/5/5
2	SNL	D	4001	-	-	0/4/80/80	0/5/5/5

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	SNL	C22-S61	21.63	2.08	1.83
2	F	6001	SNL	C22-S61	17.95	2.04	1.83
2	E	5001	SNL	C22-S61	11.30	1.96	1.83
2	F	6001	SNL	C23-C24	10.93	1.74	1.53
2	A	1001	SNL	C22-S61	10.87	1.95	1.83
2	D	4001	SNL	C4-C5	10.65	1.72	1.54
2	D	4001	SNL	C23-C24	10.34	1.73	1.53
2	B	2001	SNL	C23-C24	9.65	1.72	1.53
2	F	6001	SNL	C1-C2	9.58	1.71	1.54
2	B	2001	SNL	C4-C5	9.56	1.71	1.54
2	C	3001	SNL	C2-C20	9.51	1.71	1.52
2	A	1001	SNL	C4-C5	9.47	1.70	1.54
2	B	2001	SNL	C22-S61	9.46	1.94	1.83
2	F	6001	SNL	C4-C5	9.26	1.70	1.54
2	B	2001	SNL	C1-C2	9.22	1.71	1.54
2	F	6001	SNL	C12-C18	9.00	1.68	1.50
2	F	6001	SNL	C10-C5	8.95	1.71	1.54
2	D	4001	SNL	C22-S61	8.82	1.93	1.83
2	E	5001	SNL	C4-C5	8.78	1.69	1.54
2	B	2001	SNL	C11-C2	8.74	1.68	1.54
2	C	3001	SNL	C23-C24	8.58	1.70	1.53
2	D	4001	SNL	C3-C24	8.55	1.67	1.53
2	A	1001	SNL	C23-C24	8.39	1.70	1.53
2	C	3001	SNL	C4-C5	8.30	1.68	1.54
2	B	2001	SNL	C2-C20	8.19	1.68	1.52
2	D	4001	SNL	C2-C20	8.08	1.68	1.52
2	B	2001	SNL	C10-C5	7.98	1.69	1.54
2	C	3001	SNL	C1-C2	7.87	1.68	1.54
2	E	5001	SNL	C12-C18	7.78	1.66	1.50
2	D	4001	SNL	C23-C22	7.64	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SNL	C1-C2	7.62	1.68	1.54
2	E	5001	SNL	C1-C2	7.62	1.68	1.54
2	D	4001	SNL	C9-C5	7.53	1.68	1.54
2	F	6001	SNL	C2-C20	7.49	1.67	1.52
2	F	6001	SNL	C19-C20	7.42	1.44	1.34
2	E	5001	SNL	C23-C24	7.26	1.67	1.53
2	B	2001	SNL	C13-C9	7.01	1.66	1.53
2	B	2001	SNL	C21-C22	-6.93	1.45	1.53
2	D	4001	SNL	C12-C18	6.92	1.64	1.50
2	D	4001	SNL	C1-C2	6.83	1.66	1.54
2	B	2001	SNL	O58-C15	6.63	1.46	1.35
2	C	3001	SNL	C19-C20	6.63	1.43	1.34
2	C	3001	SNL	C3-C24	6.60	1.64	1.53
2	E	5001	SNL	C10-C5	6.50	1.66	1.54
2	E	5001	SNL	C19-C20	6.48	1.43	1.34
2	B	2001	SNL	O58-C9	-6.12	1.38	1.47
2	D	4001	SNL	C21-C20	6.05	1.63	1.51
2	E	5001	SNL	O58-C9	6.05	1.55	1.47
2	D	4001	SNL	C21-C22	-5.98	1.46	1.53
2	C	3001	SNL	C13-C9	5.76	1.64	1.53
2	E	5001	SNL	C21-C20	5.61	1.62	1.51
2	D	4001	SNL	C19-C20	5.54	1.42	1.34
2	B	2001	SNL	C21-C20	5.52	1.62	1.51
2	B	2001	SNL	C23-C22	5.39	1.59	1.53
2	C	3001	SNL	C23-C22	5.39	1.59	1.53
2	F	6001	SNL	C13-C9	5.20	1.63	1.53
2	E	5001	SNL	C11-C2	5.18	1.63	1.54
2	D	4001	SNL	C5-C6	5.15	1.63	1.54
2	A	1001	SNL	C5-C6	5.10	1.63	1.54
2	A	1001	SNL	C12-C18	5.07	1.60	1.50
2	A	1001	SNL	C21-C20	4.96	1.61	1.51
2	A	1001	SNL	C10-C5	4.88	1.63	1.54
2	A	1001	SNL	C2-C20	4.84	1.62	1.52
2	E	5001	SNL	C2-C20	4.81	1.62	1.52
2	F	6001	SNL	C5-C6	4.78	1.63	1.54
2	D	4001	SNL	C7-C6	4.77	1.64	1.54
2	F	6001	SNL	C4-C3	-4.76	1.43	1.53
2	F	6001	SNL	O58-C9	4.72	1.53	1.47
2	C	3001	SNL	C10-C5	4.70	1.63	1.54
2	A	1001	SNL	C3-C24	4.58	1.61	1.53
2	C	3001	SNL	C21-C20	4.25	1.60	1.51
2	D	4001	SNL	C1-C12	4.15	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5001	SNL	C9-C5	4.11	1.62	1.54
2	C	3001	SNL	C13-C14	4.09	1.62	1.52
2	C	3001	SNL	C16-S61	4.09	1.84	1.77
2	A	1001	SNL	C16-S61	4.09	1.84	1.77
2	D	4001	SNL	C16-S61	4.08	1.84	1.77
2	F	6001	SNL	C16-S61	4.07	1.84	1.77
2	E	5001	SNL	C5-C6	4.00	1.61	1.54
2	D	4001	SNL	C19-C18	3.98	1.54	1.45
2	C	3001	SNL	C12-C18	3.91	1.58	1.50
2	D	4001	SNL	O58-C9	-3.88	1.41	1.47
2	A	1001	SNL	C19-C20	3.88	1.39	1.34
2	C	3001	SNL	O58-C9	-3.82	1.42	1.47
2	C	3001	SNL	O58-C15	3.81	1.41	1.35
2	A	1001	SNL	C11-C2	3.80	1.60	1.54
2	E	5001	SNL	C23-C6	3.73	1.61	1.53
2	C	3001	SNL	C8-C9	3.71	1.60	1.53
2	C	3001	SNL	C5-C6	3.71	1.61	1.54
2	F	6001	SNL	C19-C18	3.69	1.53	1.45
2	A	1001	SNL	O58-C15	3.54	1.41	1.35
2	E	5001	SNL	C13-C9	3.50	1.60	1.53
2	E	5001	SNL	C3-C24	3.44	1.59	1.53
2	B	2001	SNL	C8-C7	-3.44	1.43	1.54
2	D	4001	SNL	C4-C3	-3.43	1.46	1.53
2	C	3001	SNL	C21-C22	-3.39	1.49	1.53
2	F	6001	SNL	C9-C5	3.32	1.60	1.54
2	E	5001	SNL	C13-C14	3.27	1.60	1.52
2	F	6001	SNL	C8-C9	3.25	1.59	1.53
2	C	3001	SNL	C14-C15	3.24	1.56	1.50
2	F	6001	SNL	C13-C14	3.19	1.60	1.52
2	C	3001	SNL	C1-C12	3.18	1.59	1.53
2	C	3001	SNL	C23-C6	3.07	1.59	1.53
2	F	6001	SNL	C7-C6	3.05	1.60	1.54
2	E	5001	SNL	C14-C15	3.04	1.55	1.50
2	A	1001	SNL	C21-C22	3.01	1.56	1.53
2	C	3001	SNL	C2-C24	2.98	1.60	1.56
2	F	6001	SNL	C2-C24	2.81	1.60	1.56
2	B	2001	SNL	C3-C24	2.79	1.58	1.53
2	F	6001	SNL	C3-C24	2.78	1.58	1.53
2	E	5001	SNL	O58-C15	-2.74	1.31	1.35
2	B	2001	SNL	C9-C5	2.70	1.59	1.54
2	B	2001	SNL	C19-C18	2.69	1.51	1.45
2	D	4001	SNL	C11-C2	2.69	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SNL	C2-C24	2.64	1.60	1.56
2	B	2001	SNL	C5-C6	2.61	1.59	1.54
2	C	3001	SNL	C11-C2	2.58	1.58	1.54
2	A	1001	SNL	C13-C9	2.56	1.58	1.53
2	B	2001	SNL	C1-C12	2.51	1.58	1.53
2	C	3001	SNL	C4-C3	-2.49	1.48	1.53
2	C	3001	SNL	C19-C18	2.38	1.50	1.45
2	E	5001	SNL	O60-C18	2.38	1.26	1.23
2	B	2001	SNL	C14-C15	2.35	1.54	1.50
2	A	1001	SNL	C1-C12	2.34	1.58	1.53
2	B	2001	SNL	C12-C18	2.14	1.54	1.50
2	B	2001	SNL	C19-C20	2.13	1.37	1.34
2	D	4001	SNL	C8-C9	2.13	1.57	1.53
2	F	6001	SNL	O57-C15	-2.13	1.16	1.22
2	F	6001	SNL	C21-C20	2.11	1.55	1.51
2	D	4001	SNL	O60-C18	2.11	1.26	1.23
2	E	5001	SNL	C23-C22	2.09	1.56	1.53
2	E	5001	SNL	C2-C24	2.08	1.59	1.56
2	D	4001	SNL	C13-C9	2.01	1.57	1.53

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5001	SNL	C17-C16-S61	9.86	125.44	113.19
2	B	2001	SNL	C17-C16-S61	9.72	125.28	113.19
2	E	5001	SNL	C21-C22-C23	8.38	115.11	110.27
2	B	2001	SNL	C21-C22-C23	8.11	114.95	110.27
2	C	3001	SNL	C21-C22-C23	7.80	114.77	110.27
2	D	4001	SNL	C21-C22-C23	7.17	114.41	110.27
2	C	3001	SNL	C17-C16-S61	7.00	121.89	113.19
2	F	6001	SNL	C17-C16-S61	6.99	121.87	113.19
2	D	4001	SNL	C17-C16-S61	6.97	121.86	113.19
2	A	1001	SNL	C17-C16-S61	6.95	121.82	113.19
2	D	4001	SNL	O58-C9-C8	-6.93	101.65	109.42
2	E	5001	SNL	O59-C16-S61	-6.92	117.93	122.93
2	D	4001	SNL	O58-C9-C5	6.77	116.92	110.83
2	B	2001	SNL	O59-C16-S61	-6.51	118.22	122.93
2	B	2001	SNL	C22-S61-C16	6.17	107.94	100.68
2	C	3001	SNL	C23-C22-S61	-6.10	107.04	112.01
2	B	2001	SNL	O58-C15-O57	5.77	125.67	120.81
2	A	1001	SNL	C21-C22-C23	5.47	113.42	110.27
2	C	3001	SNL	O58-C15-O57	5.22	125.21	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5001	SNL	O58-C15-O57	5.21	125.20	120.81
2	A	1001	SNL	C6-C23-C22	5.05	116.13	112.94
2	E	5001	SNL	C22-S61-C16	4.82	106.35	100.68
2	B	2001	SNL	C7-C6-C23	4.68	124.78	118.36
2	A	1001	SNL	O58-C15-O57	4.68	124.75	120.81
2	D	4001	SNL	C9-C5-C6	-4.59	95.02	99.78
2	D	4001	SNL	C22-S61-C16	4.55	106.03	100.68
2	D	4001	SNL	C8-C9-C5	4.55	107.31	103.67
2	C	3001	SNL	C10-C5-C9	4.48	114.01	108.69
2	D	4001	SNL	C23-C22-S61	-4.41	108.42	112.01
2	C	3001	SNL	C7-C6-C23	4.30	124.26	118.36
2	B	2001	SNL	C7-C6-C5	4.29	109.21	103.70
2	F	6001	SNL	C21-C22-C23	4.25	112.72	110.27
2	D	4001	SNL	C7-C6-C5	4.20	109.10	103.70
2	C	3001	SNL	C7-C6-C5	4.18	109.07	103.70
2	C	3001	SNL	C4-C5-C9	-4.12	114.30	117.86
2	B	2001	SNL	C11-C2-C20	-4.12	102.10	108.38
2	B	2001	SNL	C8-C9-C5	4.11	106.96	103.67
2	B	2001	SNL	C7-C8-C9	4.09	112.23	105.42
2	C	3001	SNL	C12-C18-C19	4.06	122.91	116.73
2	A	1001	SNL	C8-C9-C5	4.01	106.88	103.67
2	A	1001	SNL	C22-S61-C16	3.99	105.37	100.68
2	C	3001	SNL	O59-C16-S61	-3.98	120.05	122.93
2	F	6001	SNL	O59-C16-S61	-3.97	120.06	122.93
2	D	4001	SNL	O59-C16-S61	-3.97	120.06	122.93
2	D	4001	SNL	O58-C15-O57	3.96	124.15	120.81
2	A	1001	SNL	O59-C16-S61	-3.96	120.07	122.93
2	B	2001	SNL	C23-C22-S61	-3.88	108.85	112.01
2	A	1001	SNL	C7-C6-C23	3.84	123.62	118.36
2	F	6001	SNL	O58-C15-O57	3.67	123.90	120.81
2	A	1001	SNL	C12-C18-C19	3.65	122.28	116.73
2	C	3001	SNL	C22-C21-C20	3.63	115.02	112.62
2	A	1001	SNL	C11-C2-C20	-3.52	103.00	108.38
2	B	2001	SNL	C10-C5-C9	3.46	112.80	108.69
2	C	3001	SNL	C21-C22-S61	3.45	113.30	110.43
2	D	4001	SNL	C7-C8-C9	3.44	111.16	105.42
2	C	3001	SNL	C1-C2-C24	3.39	113.22	108.74
2	E	5001	SNL	C11-C2-C20	-3.38	103.22	108.38
2	B	2001	SNL	C12-C18-C19	3.34	121.81	116.73
2	D	4001	SNL	C7-C6-C23	3.34	122.93	118.36
2	A	1001	SNL	C7-C8-C9	3.28	110.89	105.42
2	A	1001	SNL	C23-C22-S61	-3.26	109.35	112.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	SNL	C9-C5-C6	-3.25	96.41	99.78
2	B	2001	SNL	C1-C2-C24	3.11	112.86	108.74
2	F	6001	SNL	C6-C23-C22	3.09	114.90	112.94
2	F	6001	SNL	C4-C5-C9	-3.04	115.23	117.86
2	E	5001	SNL	C12-C18-C19	3.04	121.35	116.73
2	E	5001	SNL	C7-C8-C9	3.00	110.41	105.42
2	D	4001	SNL	C12-C18-C19	2.95	121.22	116.73
2	F	6001	SNL	C7-C8-C9	2.91	110.26	105.42
2	B	2001	SNL	C6-C23-C22	2.89	114.77	112.94
2	A	1001	SNL	O58-C9-C8	-2.88	106.19	109.42
2	C	3001	SNL	C8-C9-C5	2.86	105.96	103.67
2	E	5001	SNL	O58-C9-C5	2.85	113.39	110.83
2	A	1001	SNL	C10-C5-C9	2.83	112.05	108.69
2	D	4001	SNL	C11-C2-C20	-2.80	104.10	108.38
2	F	6001	SNL	C10-C5-C9	2.80	112.01	108.69
2	B	2001	SNL	C13-C9-C5	2.77	120.77	116.46
2	A	1001	SNL	C22-C21-C20	2.77	114.45	112.62
2	D	4001	SNL	C10-C5-C9	2.74	111.94	108.69
2	A	1001	SNL	C1-C2-C24	2.73	112.35	108.74
2	F	6001	SNL	C7-C6-C5	2.70	107.17	103.70
2	A	1001	SNL	C9-C5-C6	-2.67	97.00	99.78
2	C	3001	SNL	O60-C18-C12	-2.67	116.28	121.59
2	A	1001	SNL	O58-C9-C5	2.67	113.23	110.83
2	F	6001	SNL	C22-C21-C20	2.65	114.37	112.62
2	F	6001	SNL	O58-C15-C14	2.64	112.58	110.17
2	E	5001	SNL	C4-C5-C6	-2.64	104.72	108.43
2	F	6001	SNL	C12-C18-C19	2.61	120.69	116.73
2	E	5001	SNL	O58-C9-C8	-2.57	106.54	109.42
2	E	5001	SNL	C6-C23-C22	2.56	114.56	112.94
2	F	6001	SNL	C9-C5-C6	-2.55	97.13	99.78
2	C	3001	SNL	C11-C2-C20	-2.54	104.51	108.38
2	F	6001	SNL	C7-C6-C23	2.54	121.83	118.36
2	D	4001	SNL	C22-C21-C20	2.51	114.28	112.62
2	C	3001	SNL	C13-C9-C8	-2.50	106.96	113.44
2	B	2001	SNL	C4-C5-C9	-2.50	115.70	117.86
2	E	5001	SNL	C10-C5-C9	2.46	111.61	108.69
2	C	3001	SNL	C24-C23-C22	-2.42	109.46	111.27
2	C	3001	SNL	C22-S61-C16	2.37	103.47	100.68
2	A	1001	SNL	C14-C13-C9	2.34	106.61	103.81
2	B	2001	SNL	C10-C5-C4	2.34	112.89	109.69
2	D	4001	SNL	C4-C5-C6	-2.29	105.21	108.43
2	F	6001	SNL	C10-C5-C4	2.27	112.79	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3001	SNL	C9-C5-C6	-2.26	97.43	99.78
2	E	5001	SNL	C21-C22-S61	-2.25	108.56	110.43
2	B	2001	SNL	C4-C5-C6	-2.24	105.29	108.43
2	C	3001	SNL	C6-C23-C22	2.24	114.36	112.94
2	B	2001	SNL	C5-C6-C23	2.21	115.48	113.41
2	F	6001	SNL	C21-C22-S61	-2.19	108.61	110.43
2	B	2001	SNL	C21-C20-C2	2.18	119.22	116.42
2	F	6001	SNL	O58-C9-C8	-2.18	106.97	109.42
2	D	4001	SNL	C21-C20-C2	2.15	119.18	116.42
2	B	2001	SNL	C13-C9-C8	-2.14	107.90	113.44
2	E	5001	SNL	C1-C2-C24	2.12	111.55	108.74
2	E	5001	SNL	C7-C6-C23	2.10	121.24	118.36
2	B	2001	SNL	C22-C21-C20	2.08	114.00	112.62
2	F	6001	SNL	C8-C9-C5	2.07	105.33	103.67
2	A	1001	SNL	C4-C5-C6	-2.06	105.54	108.43
2	F	6001	SNL	C4-C5-C6	-2.04	105.56	108.43
2	F	6001	SNL	C5-C6-C23	-2.04	111.50	113.41
2	D	4001	SNL	C6-C23-C22	2.03	114.23	112.94
2	D	4001	SNL	C21-C20-C19	-2.03	117.81	120.91

There are no chirality outliers.

There are no torsion outliers.

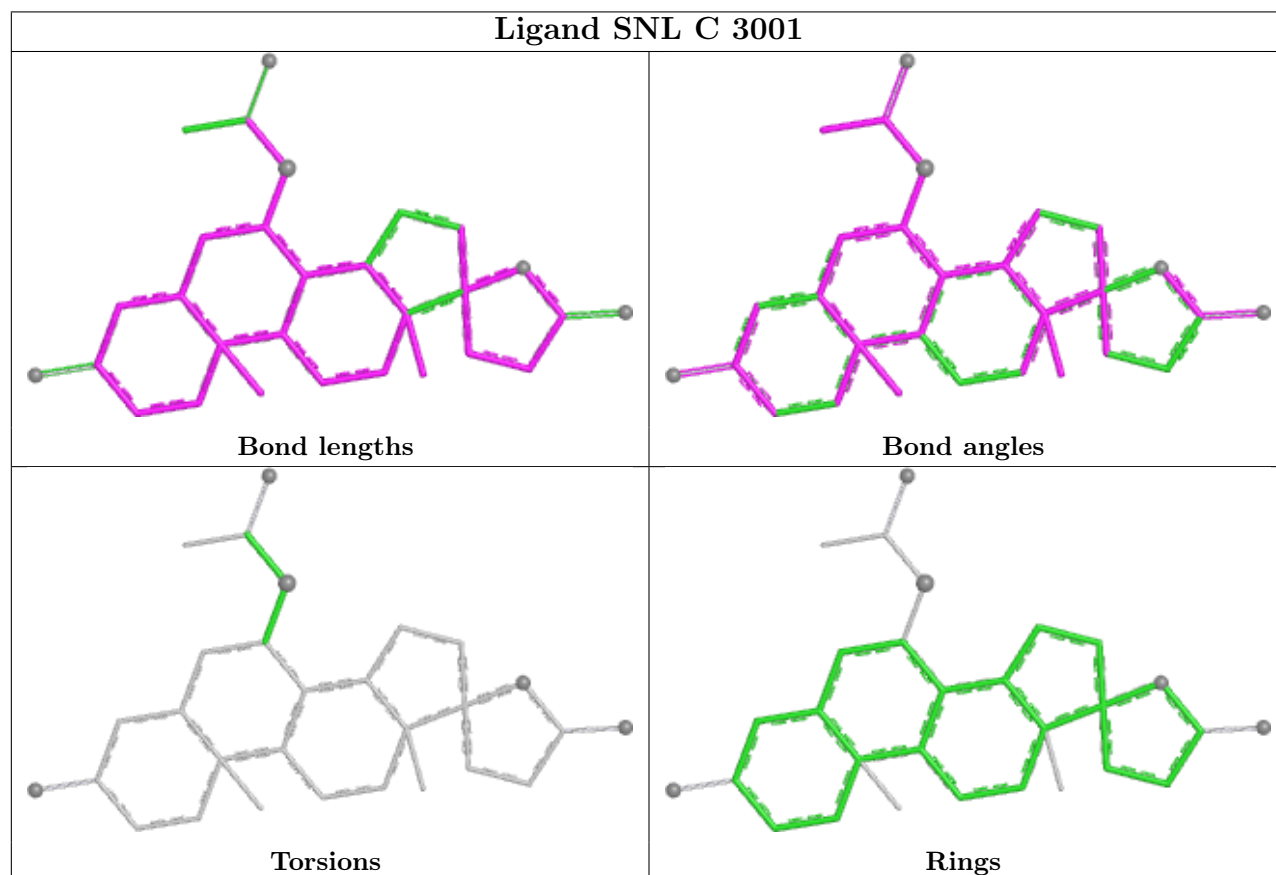
There are no ring outliers.

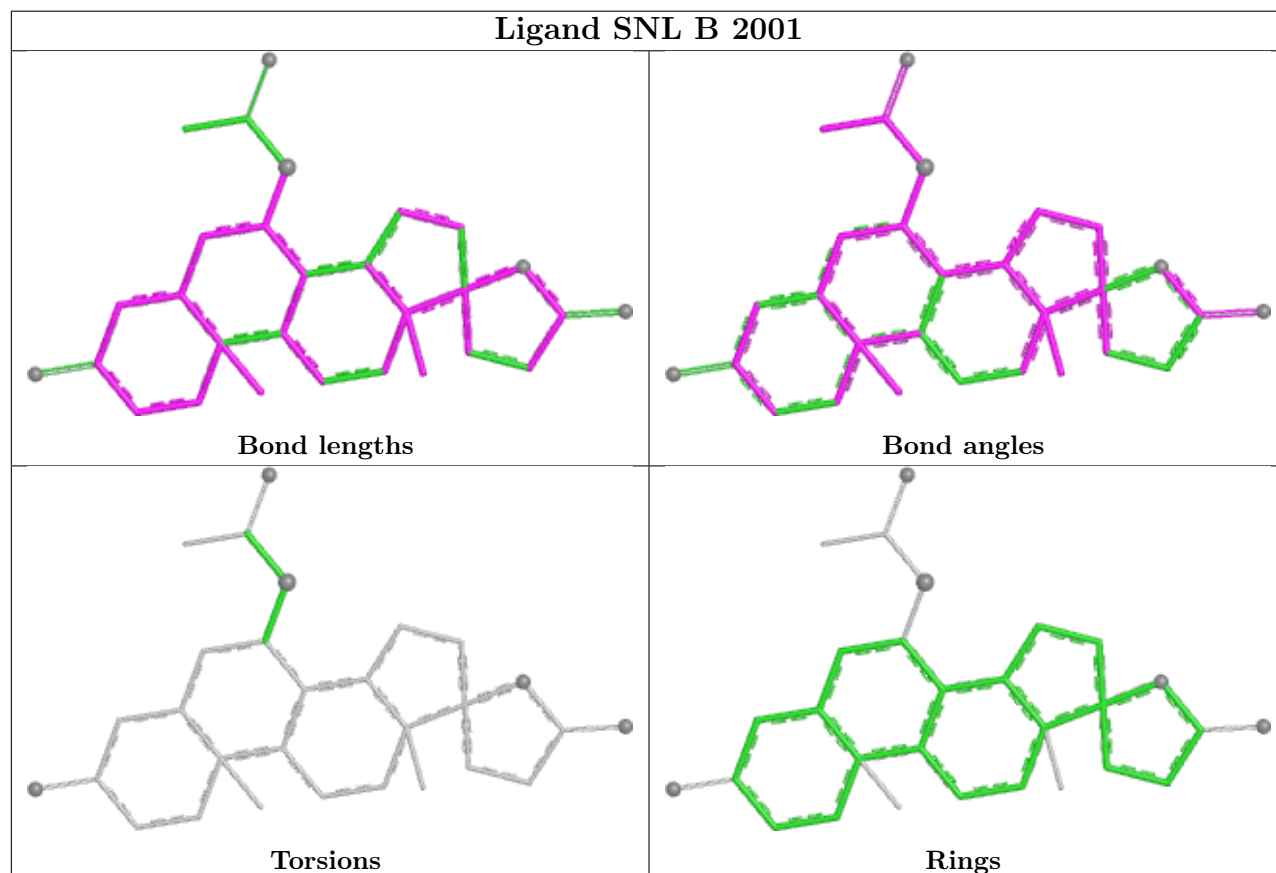
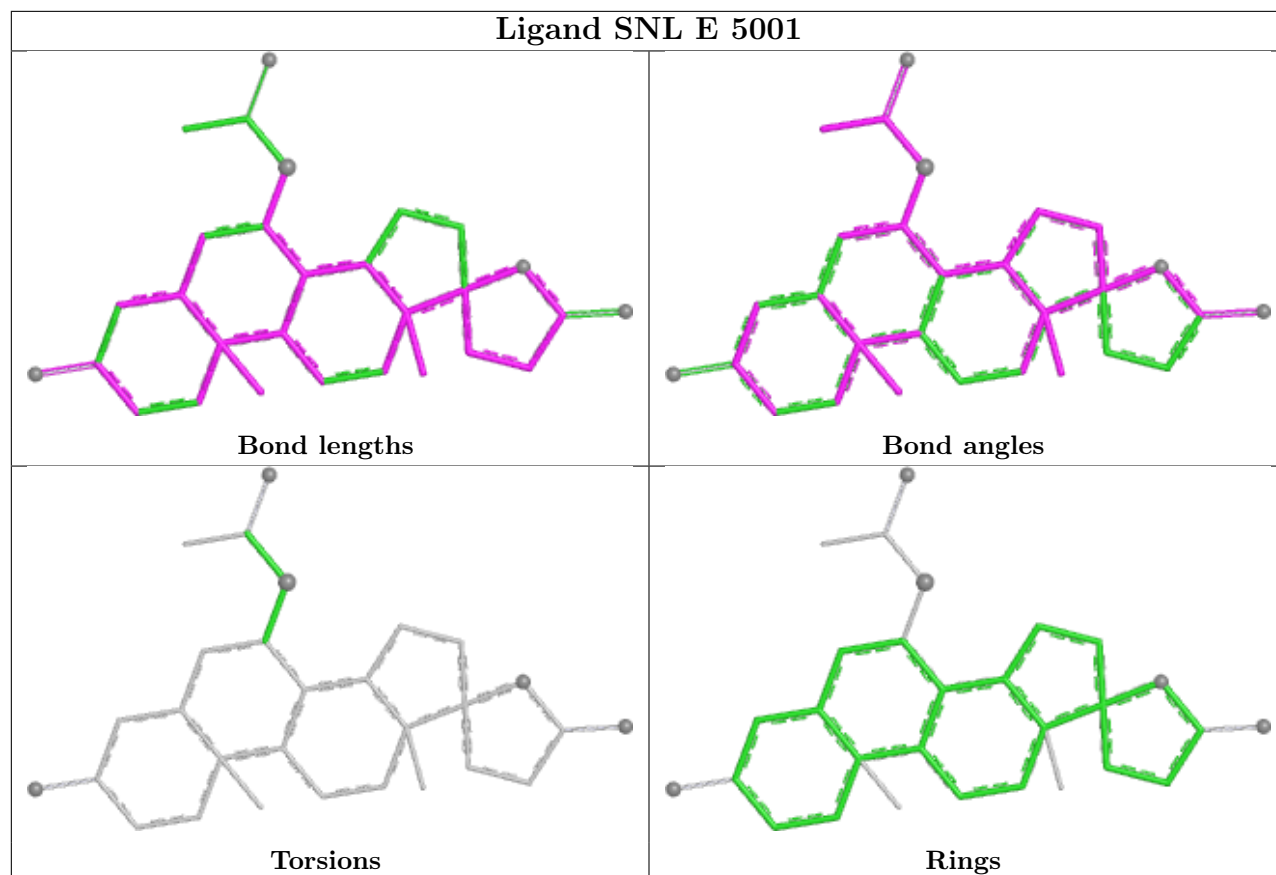
6 monomers are involved in 33 short contacts:

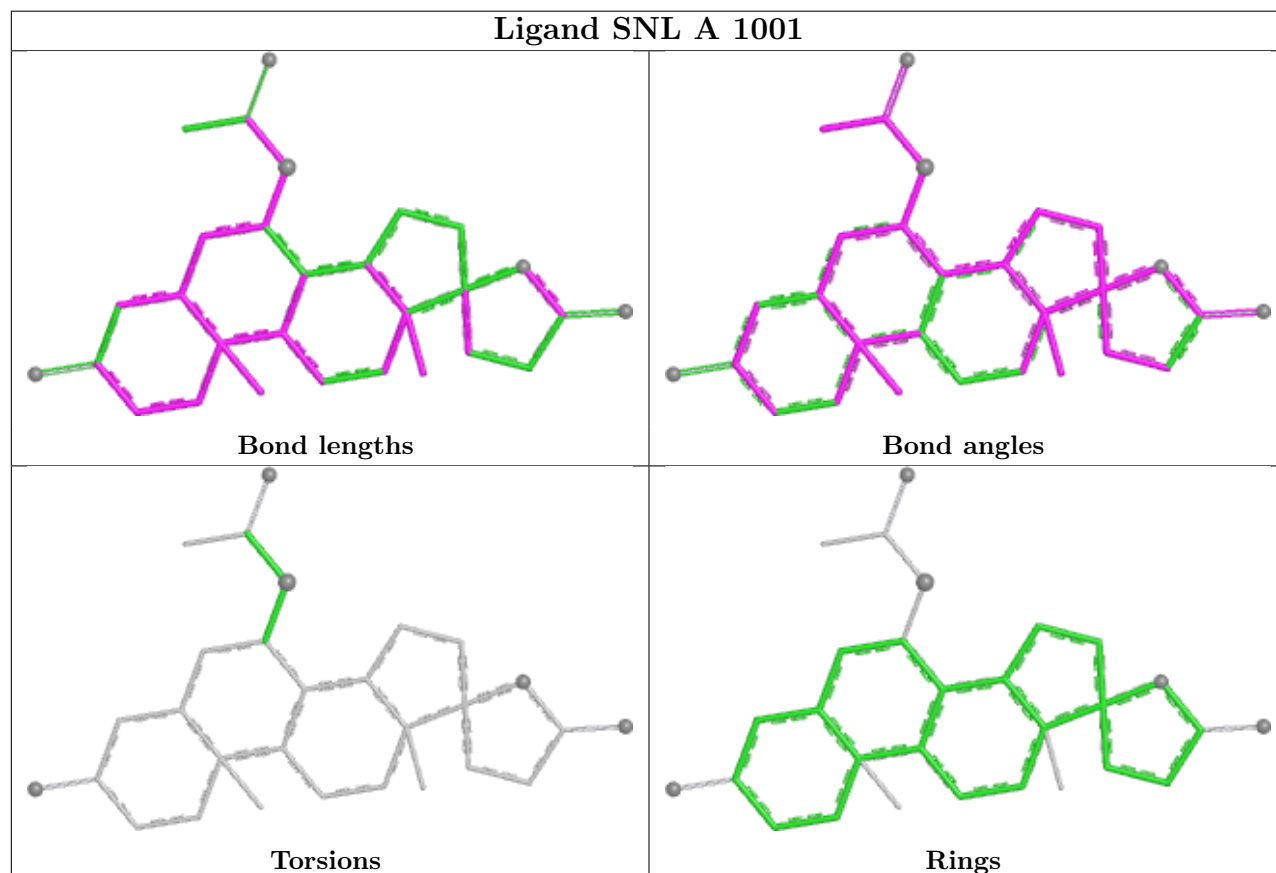
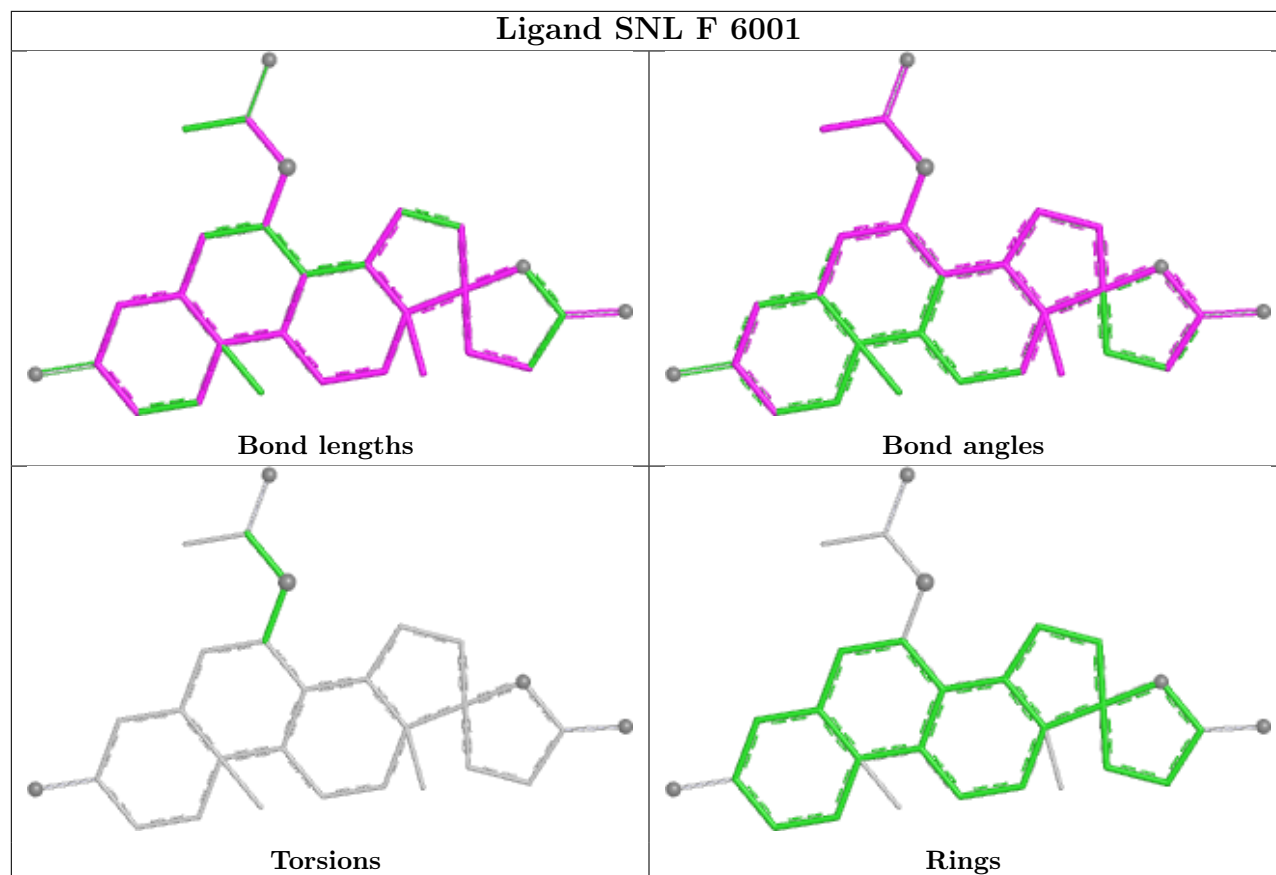
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3001	SNL	6	0
2	E	5001	SNL	5	0
2	B	2001	SNL	2	0
2	F	6001	SNL	11	0
2	A	1001	SNL	4	0
2	D	4001	SNL	5	0

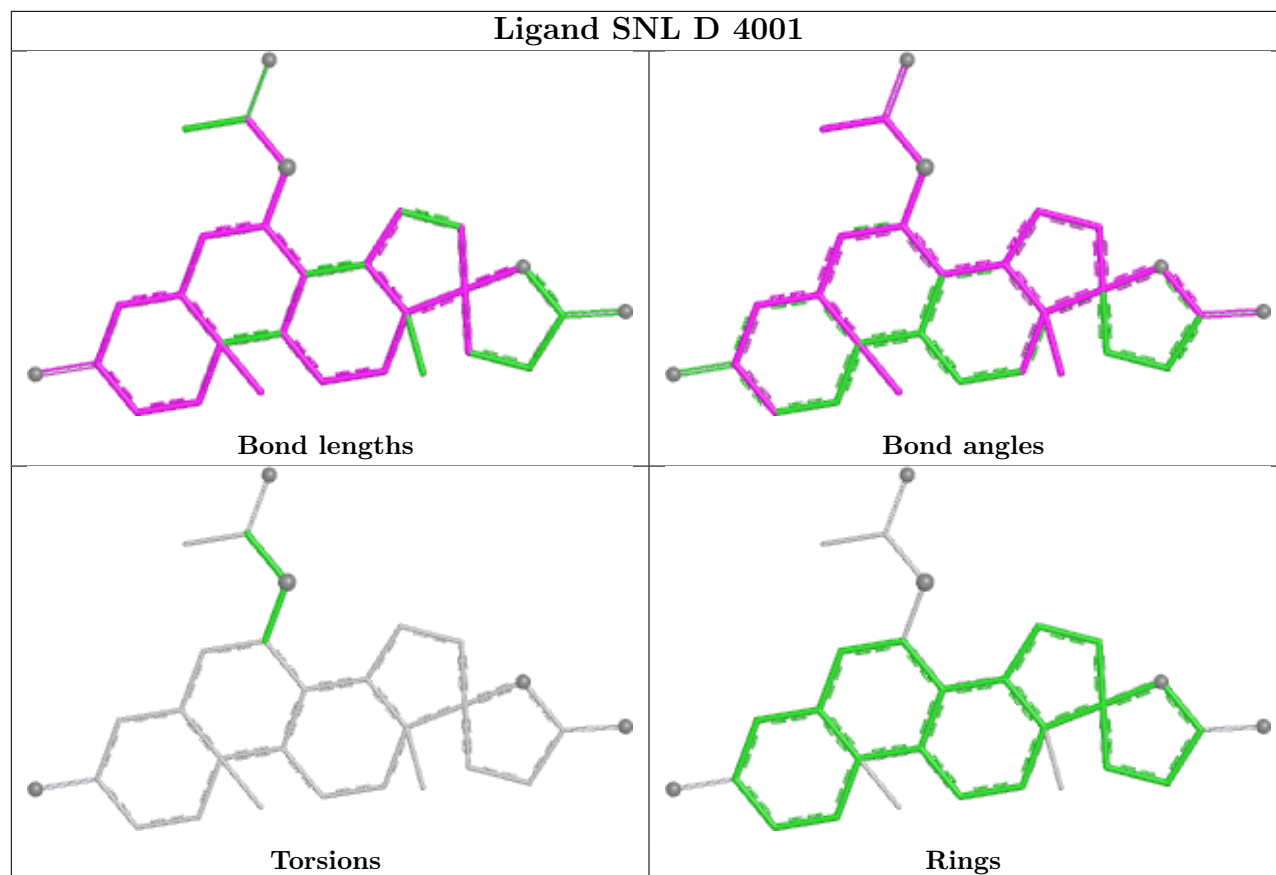
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	233/256 (91%)	0.30	6 (2%) 57 59	23, 41, 69, 82	0
1	B	233/256 (91%)	0.22	2 (0%) 81 82	24, 40, 58, 71	0
1	C	233/256 (91%)	0.13	3 (1%) 75 76	20, 37, 60, 71	0
1	D	234/256 (91%)	0.23	7 (2%) 52 54	20, 39, 71, 86	0
1	E	234/256 (91%)	0.72	18 (7%) 19 21	22, 57, 78, 82	0
1	F	238/256 (92%)	0.36	8 (3%) 48 50	23, 43, 75, 79	0
All	All	1405/1536 (91%)	0.33	44 (3%) 51 53	20, 41, 73, 86	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	971	VAL	4.2
1	F	971	VAL	4.2
1	D	971	VAL	4.1
1	E	971	VAL	3.8
1	E	760	ASP	3.3
1	E	951	ALA	3.2
1	D	951	ALA	3.1
1	C	976	ALA	3.1
1	E	758	LYS	3.0
1	B	971	VAL	3.0
1	F	952	LEU	3.0
1	A	951	ALA	2.9
1	D	974	GLY	2.9
1	F	951	ALA	2.8
1	F	765	LEU	2.8
1	E	952	LEU	2.6
1	A	952	LEU	2.6
1	C	884	ASP	2.6
1	D	907	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	952	LEU	2.5
1	A	972	GLU	2.5
1	E	944	TYR	2.5
1	F	846	TYR	2.5
1	E	849	CYS	2.4
1	D	950	HIS	2.4
1	E	894	GLU	2.4
1	E	819	TYR	2.4
1	E	860	VAL	2.4
1	D	976	ALA	2.3
1	E	848	LEU	2.3
1	F	970	LYS	2.2
1	B	970	LYS	2.2
1	F	973	SER	2.2
1	E	932	HIS	2.2
1	E	903	LEU	2.2
1	A	969	PRO	2.1
1	F	761	THR	2.1
1	A	968	LEU	2.1
1	E	950	HIS	2.1
1	E	907	VAL	2.1
1	E	818	SER	2.0
1	C	885	GLY	2.0
1	E	919	GLN	2.0
1	E	759	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

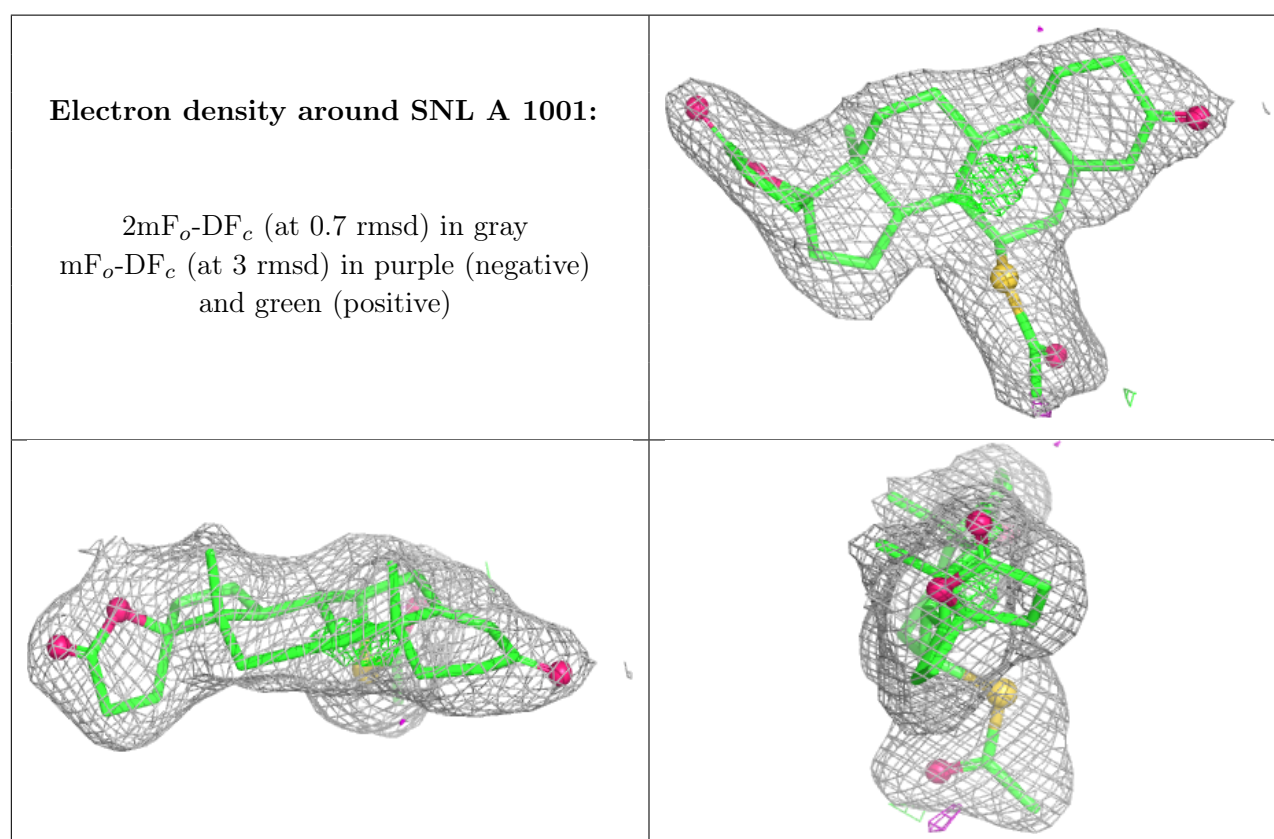
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

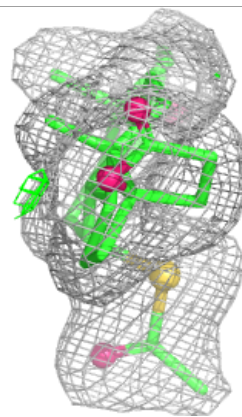
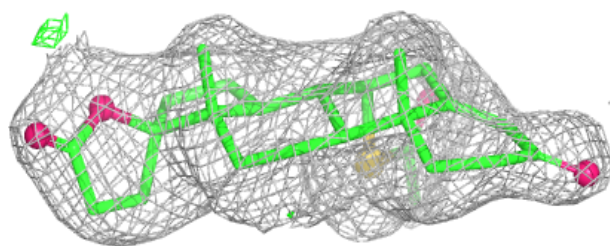
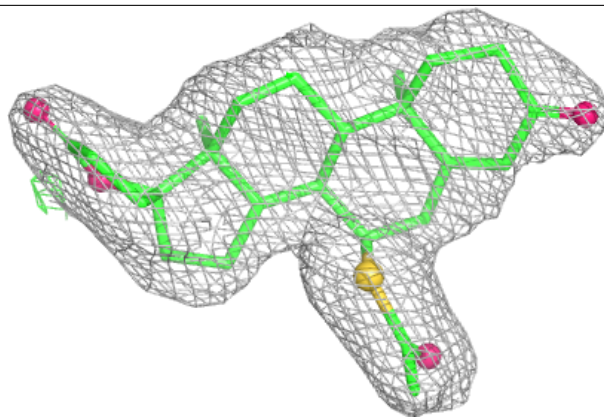
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SNL	A	1001	29/29	0.93	0.09	25,29,31,32	0
2	SNL	D	4001	29/29	0.93	0.08	22,27,29,30	0
2	SNL	E	5001	29/29	0.93	0.10	42,43,45,47	0
2	SNL	F	6001	29/29	0.93	0.09	29,34,38,40	0
2	SNL	C	3001	29/29	0.95	0.07	18,23,25,30	0
2	SNL	B	2001	29/29	0.95	0.07	19,21,23,24	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.



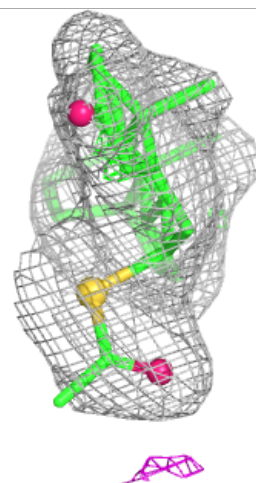
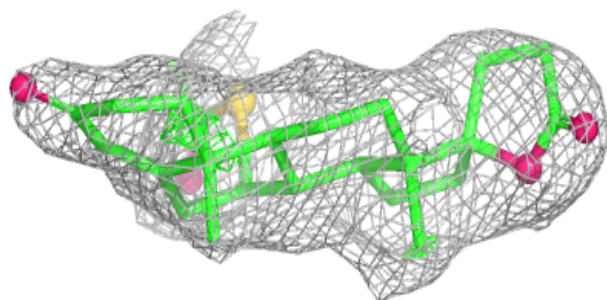
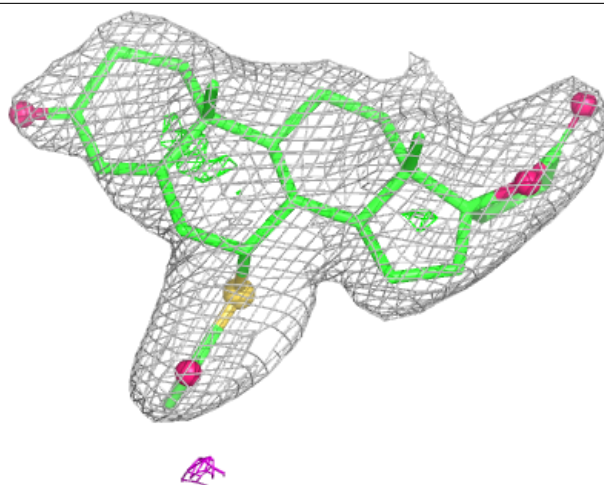
Electron density around SNL D 4001:

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



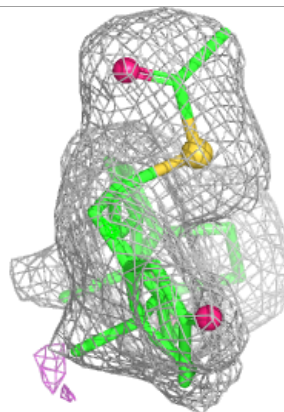
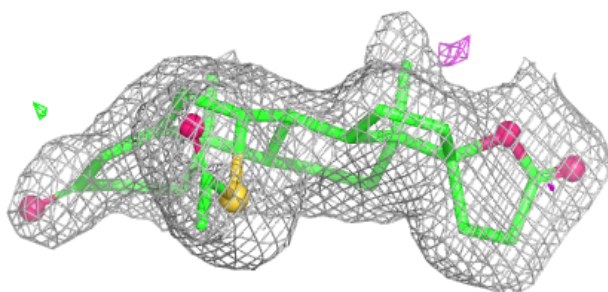
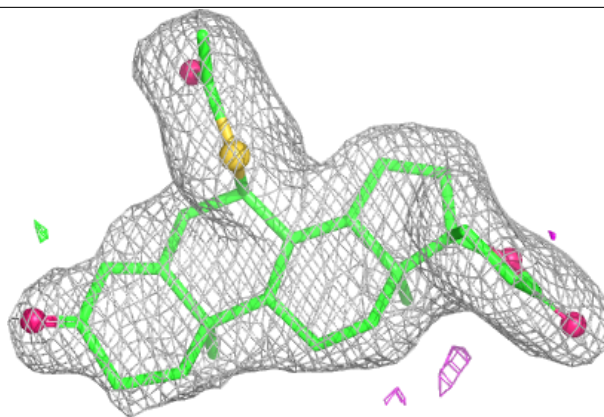
Electron density around SNL E 5001:

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

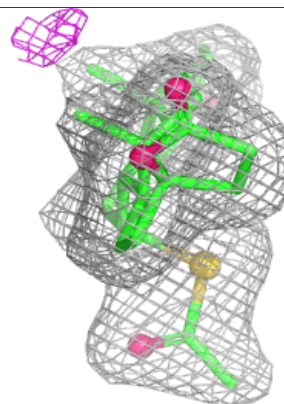
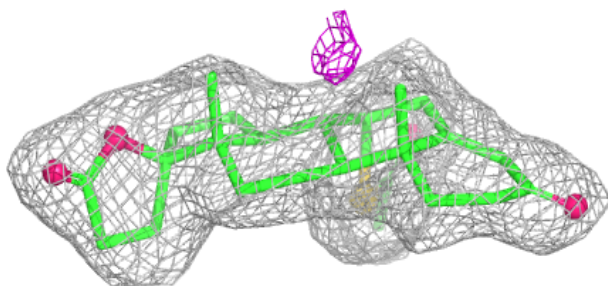
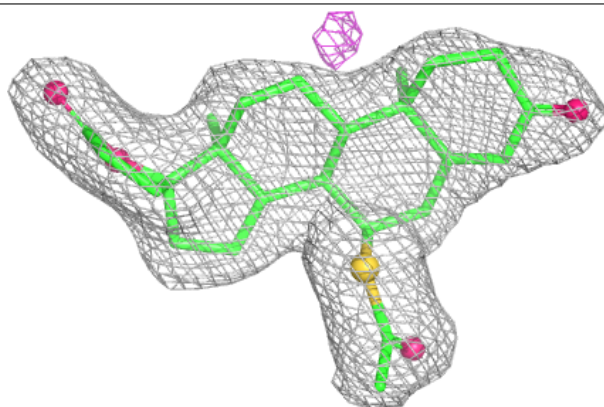


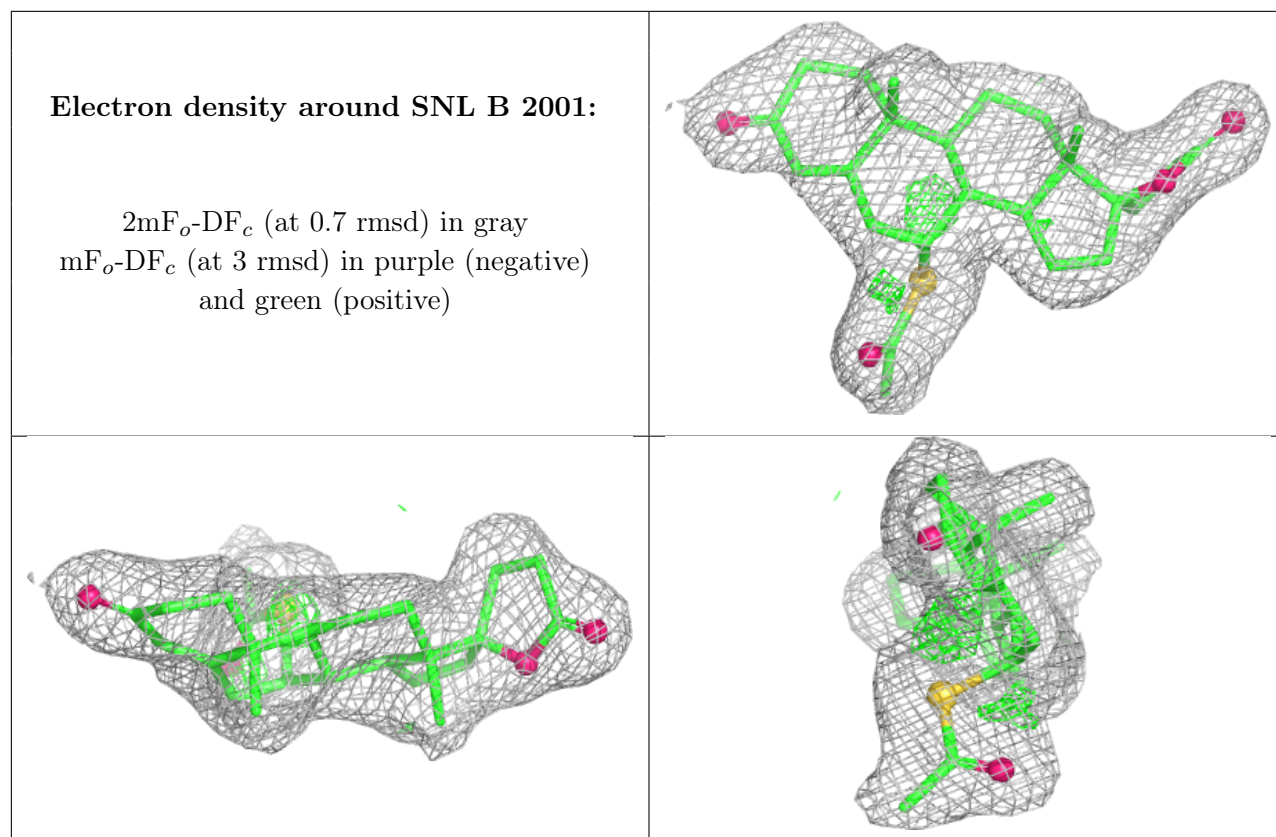
Electron density around SNL F 6001:

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

**Electron density around SNL C 3001:**

$2mF_o-DF_c$ (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.