Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 11:24 AM EDT

PDB ID	:	2OAX
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 (i) 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 (i)) were used in the production of this report:

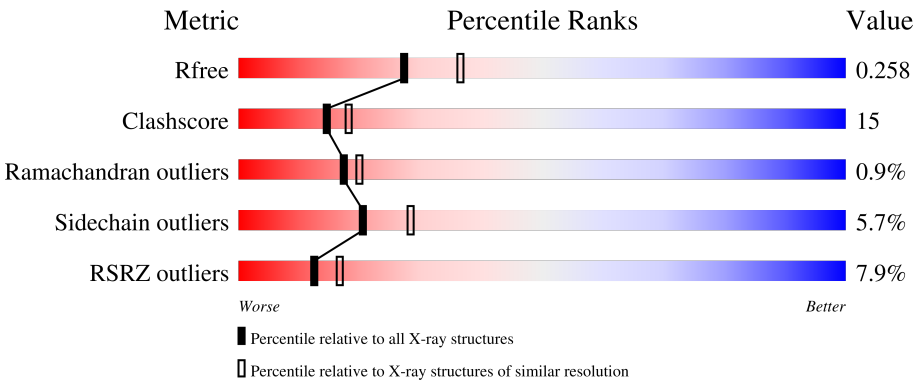
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.29 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	8%, 62%, 27%, •, 9%
1	B	256	4%, 62%, 26%, •, 9%
1	C	256	3%, 68%, 22%, •, 9%
1	D	256	7%, 64%, 26%, •, 9%
1	E	256	14%, 53%, 36%, •, 9%

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Mol	Chain	Length	Quality of chain
1	F	256	7% 66% 25% 7%

2 Entry composition (i)

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

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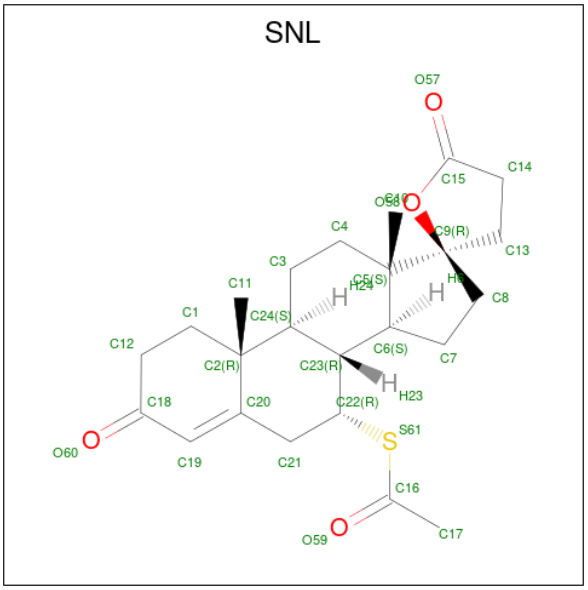
Chain	Residue	Modelled	Actual	Comment	Reference
E	730	SER	-	expression tag	UNP P08235
E	810	LEU	SER	engineered mutation	UNP P08235
E	910	ALA	CYS	engineered mutation	UNP P08235
F	729	GLY	-	expression tag	UNP P08235
F	730	SER	-	expression tag	UNP P08235
F	810	LEU	SER	engineered mutation	UNP P08235
F	910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

- Molecule 2 is SPIRONOLACTONE (three-letter code: SNL) (formula: $C_{24}H_{32}O_4S$).



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

- Molecule 3 is water.

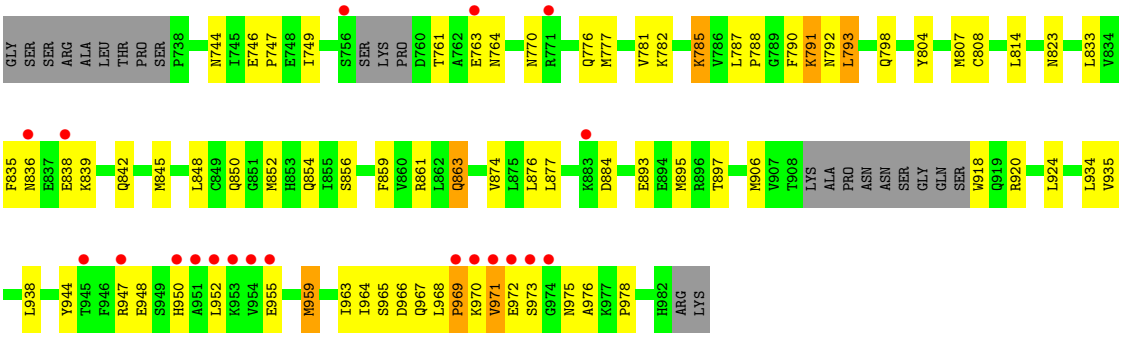
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	54	54	54	0	0
			Total	O		
3	B	53	53	53	0	0
			Total	O		
3	C	72	72	72	0	0
			Total	O		
3	D	66	66	66	0	0
			Total	O		
3	E	34	34	34	0	0
			Total	O		
3	F	60	60	60	0	0

3 Residue-property plots (i)

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

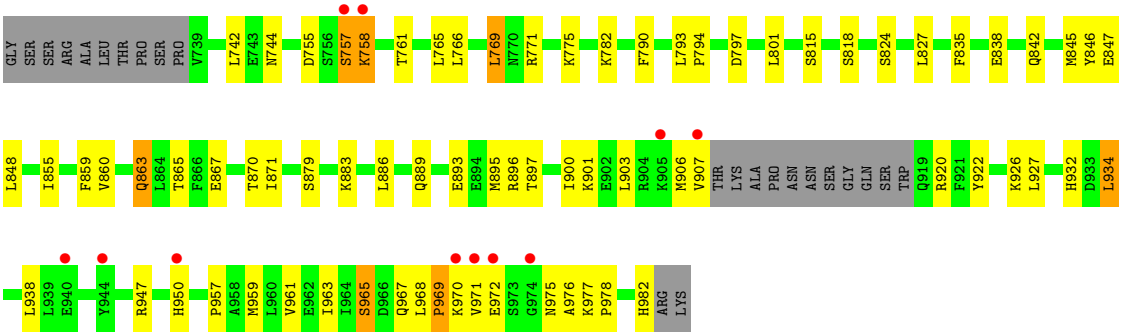
- Molecule 1: Mineralocorticoid receptor

Chain A:



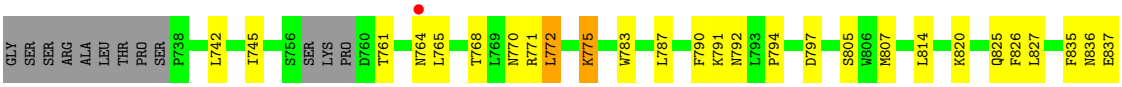
- Molecule 1: Mineralocorticoid receptor

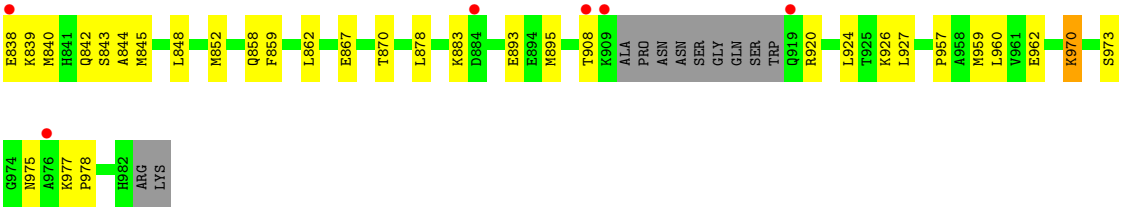
Chain B:



- Molecule 1: Mineralocorticoid receptor

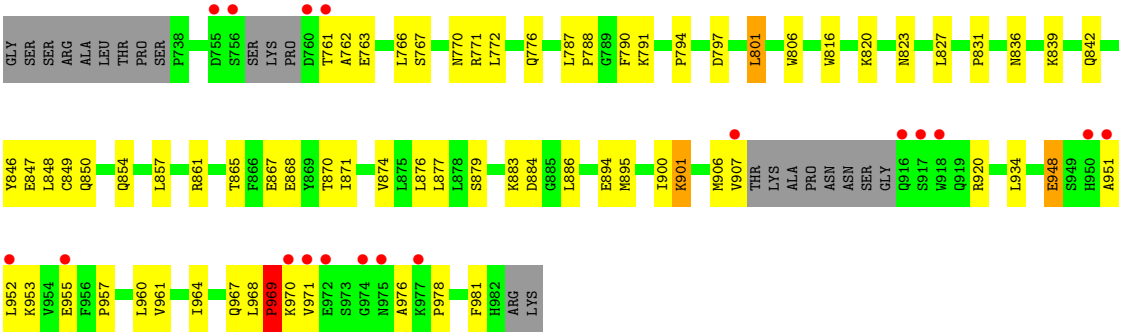
Chain C:





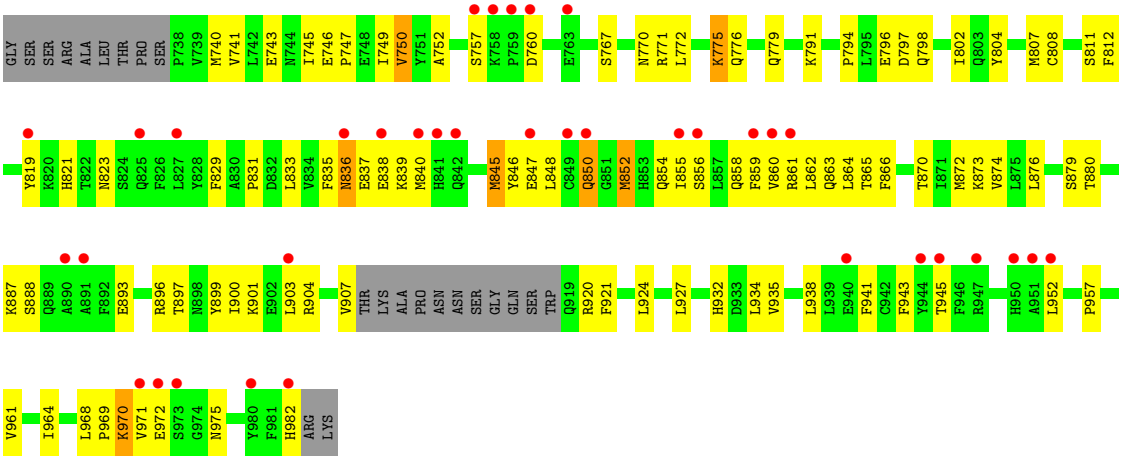
- Molecule 1: Mineralocorticoid receptor

Chain D:



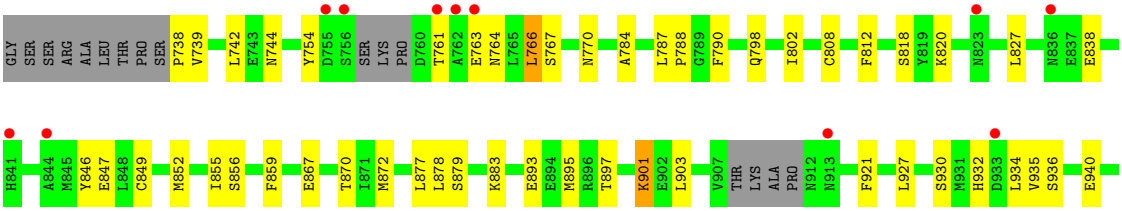
- Molecule 1: Mineralocorticoid receptor

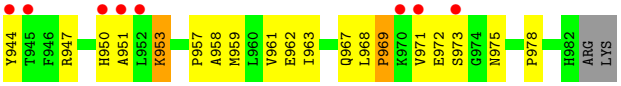
Chain E:



- Molecule 1: Mineralocorticoid receptor

Chain F:




Y944
T945
F946
R947
H950
A951
L952
K953
P957
A958
M959
L960
V961
E962
I963
Q967
L968
P969
K970
V971
E972
S973
G974
N975
P978
H982
ARG
LYS

4 Data and refinement statistics (i)

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) 91.3 (14.92-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.263 0.234 , 0.258	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 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/1948	0.55	0/2636
1	B	0.39	0/1960	0.56	0/2647
1	C	0.42	0/1956	0.59	0/2641
1	D	0.40	0/1963	0.60	0/2651
1	E	0.40	0/1956	0.58	0/2643
1	F	0.36	0/1984	0.54	0/2680
All	All	0.39	0/11767	0.57	0/15898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1903	0	1887	62	0
1	B	1916	0	1929	64	0
1	C	1913	0	1920	38	0
1	D	1919	0	1921	56	0
1	E	1912	0	1919	75	0
1	F	1940	0	1932	56	0
2	A	29	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	32	1	0
2	C	29	0	32	6	0
2	D	29	0	32	4	0
2	E	29	0	32	6	0
2	F	29	0	32	10	0
3	A	54	0	0	2	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
All	All	12016	0	11700	359	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 15.

All (359) 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:CE	1:A:934:LEU:HD23	1.58	1.31
1:A:852:MET:HE1	1:A:934:LEU:CD2	1.65	1.25
1:A:852:MET:HE1	1:A:934:LEU:HD23	1.11	1.09
1:F:761:THR:H	1:F:764:ASN:ND2	1.49	1.09
1:A:852:MET:CE	1:A:934:LEU:CD2	2.22	1.08
1:F:761:THR:N	1:F:764:ASN:HD22	1.54	1.05
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:878:LEU:HD11	1:F:895:MET:HE2	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:A:852:MET:HE2	1:A:934:LEU:CD2	2.09	0.81
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:E:807:MET:HE1	2:E:5001:SNL:H23	1.64	0.78
1:A:965:SER:O	1:A:969:PRO:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:878:LEU:HD11	1:F:895:MET:CE	2.13	0.78
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:A:808:CYS:HB3	1:A:876:LEU:HD22	1.70	0.74
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
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: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:A:852:MET:HE2	1:A:934:LEU:HD21	1.72	0.70
1:B:927:LEU:HD23	1:B:927:LEU:O	1.91	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:E:837:GLU:HG2	1:E:840:MET:HE1	1.76	0.67
1:A:863:GLN:NE2	1:A:863:GLN:HA	2.08	0.67
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:E:752:ALA:HB2	1:E:772:LEU:HD13	1.81	0.62
1:B:797:ASP:OD1	1:B:886:LEU:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:793:LEU:HD11	1:B:895:MET:HE2	1.83	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:A:852:MET:CE	1:A:934:LEU:HD21	2.23	0.60
1:E:876:LEU:HA	1:E:879:SER:OG	2.02	0.60
1:E:852:MET:HE1	1:E:934:LEU:HD23	1.83	0.59
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: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: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: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:B:838:GLU:O	1:B:842:GLN:HG3	2.05	0.57
1:B:927:LEU:HD23	1:B:927:LEU:C	2.24	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:A:852:MET:HE1	1:A:934:LEU:HD22	1.77	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
1:E:845:MET:HG2	1:E:848:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:GLU:CD	1:A:747:PRO:HD2	2.25	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: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:F:878:LEU:CD1	1:F:895:MET:HE2	2.33	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
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:B:790:PHE:HD1	1:B:895:MET:HE1	1.73	0.53
1:B:897:THR:O	1:B:901:LYS:HG3	2.09	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:B:969:PRO:C	1:B:971:VAL:H	2.12	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
1:A:967:GLN:HG3	3:A:7267:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:LEU:HB3	1:B:870:THR:OG1	2.10	0.51
1:E:852:MET:HE3	1:E:855:ILE:HG13	1.93	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: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:D:790:PHE:HB2	1:D:895:MET:HE1	1.92	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: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: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
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:A:807:MET:HE1	2:A:1001:SNL:H111	1.94	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:D:790:PHE:HA	1:D:895:MET:HE2	1.95	0.49
1:A:790:PHE:HD1	1:A:895:MET:HE1	1.77	0.48
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
1:F:846:TYR:O	1:F:847:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:838:GLU:H	1:F:838:GLU:CD	2.16	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:E:794:PRO:HG3	1:E:888:SER:OG	2.13	0.48
1:C:883:LYS:HB2	1:C:975:ASN:CG	2.33	0.48
1:D:968:LEU:HB3	1:D:969:PRO:HD3	1.94	0.48
1:A:845:MET:HE3	2:A:1001:SNL:H171	1.95	0.48
1:B:976:ALA:O	1:B:978:PRO:HD3	2.14	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:F:738:PRO:O	1:F:742:LEU:HG	2.15	0.47
1:A:793:LEU:HD11	1:A:895:MET:HE2	1.96	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:C:790:PHE:HA	1:C:895:MET:HE2	1.97	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: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:B:855:ILE:HD11	1:B:934:LEU:HD21	1.97	0.46
1:C:977:LYS:N	1:C:978:PRO:HD3	2.31	0.46
1:B:793:LEU:HD11	1:B:895:MET:CE	2.44	0.46
1:F:812:PHE:HZ	1:F:872:MET:CE	2.29	0.46
1:A:971:VAL:HG13	1:A:975:ASN:HB2	1.98	0.46
1:E:750:VAL:HG21	1:E:776:GLN:HG2	1.97	0.46
1:F:812:PHE:HZ	1:F:872:MET:HE1	1.81	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:790:PHE:C	1:A:792:ASN:H	2.19	0.45
1:D:901:LYS:HE3	1:D:901:LYS:HA	1.98	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:B:766:LEU:HD22	2:B:2001:SNL:H142	1.99	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:B:782:LYS:HB3	1:B:782:LYS:HZ2	1.82	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
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:F:878:LEU:HD11	1:F:895:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:797:ASP:CG	1:D:886:LEU:HB3	2.39	0.43
1:D:968:LEU:N	1:D:969:PRO:HD2	2.33	0.43
1:A:964:ILE:C	1:A:966:ASP:H	2.21	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:C:878:LEU:HD11	1:C:895:MET:HE3	2.01	0.43
1:A:746:GLU:CG	1:A:747:PRO:HD2	2.48	0.43
1:E:746:GLU:OE1	1:E:747:PRO:HD2	2.19	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:D:967:GLN:C	1:D:971:VAL:HG23	2.40	0.42
1:E:836:ASN:C	1:E:838:GLU:N	2.73	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: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:F:878:LEU:HD21	1:F:895:MET:HE2	2.00	0.42
1:C:745:ILE:HD11	1:C:787:LEU:HD23	2.02	0.42
1:E:807:MET:CE	2:E:5001:SNL:H23	2.43	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: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
1:D:968:LEU:CB	1:D:969:PRO:HD3	2.48	0.42
1:E:872:MET:HE2	1:E:927:LEU:HD22	2.01	0.42
1:F:827:LEU:HD11	1:F:849:CYS:O	2.19	0.42
1:C:807:MET:HE1	2:C:3001:SNL:H101	2.02	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:F:927:LEU:O	1:F:927:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:790:PHE:HA	1:D:895:MET:CE	2.50	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:769:LEU:CD2	1:B:845:MET:HE1	2.51	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: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: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: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:D:790:PHE:CB	1:D:895:MET:HE1	2.51	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
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:818:SER:OG	1:B:827:LEU:HA	2.21	0.40
1:D:790:PHE:HE1	1:D:801:LEU:HD23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:948:GLU:C	1:A:950:HIS:N	2.75	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: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

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	227/256 (89%)	214 (94%)	9 (4%)	4 (2%)	8 7
1	B	229/256 (90%)	217 (95%)	10 (4%)	2 (1%)	17 20
1	C	227/256 (89%)	217 (96%)	9 (4%)	1 (0%)	34 42
1	D	228/256 (89%)	214 (94%)	13 (6%)	1 (0%)	34 42
1	E	230/256 (90%)	211 (92%)	18 (8%)	1 (0%)	34 42
1	F	232/256 (91%)	210 (90%)	19 (8%)	3 (1%)	12 12
All	All	1373/1536 (89%)	1283 (93%)	78 (6%)	12 (1%)	17 20

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	969	PRO
1	C	908	THR
1	F	969	PRO

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Mol	Chain	Res	Type
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 (i)

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%)	201 (96%)	9 (4%)	29	40
1	B	215/234 (92%)	202 (94%)	13 (6%)	19	26
1	C	214/234 (92%)	202 (94%)	12 (6%)	21	29
1	D	214/234 (92%)	202 (94%)	12 (6%)	21	29
1	E	214/234 (92%)	197 (92%)	17 (8%)	12	15
1	F	216/234 (92%)	206 (95%)	10 (5%)	27	38
All	All	1283/1404 (91%)	1210 (94%)	73 (6%)	20	28

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	ASN
1	A	785	LYS
1	A	793	LEU
1	A	861	ARG
1	A	863	GLN
1	A	884	ASP
1	A	906	MET
1	A	955	GLU
1	A	959	MET

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Mol	Chain	Res	Type
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	801	LEU
1	B	863	GLN
1	B	879	SER
1	B	934	LEU
1	B	947	ARG
1	B	950	HIS
1	B	965	SER
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	926	LYS
1	C	959	MET
1	C	962	GLU
1	C	970	LYS
1	C	973	SER
1	D	771	ARG
1	D	801	LEU
1	D	823	ASN
1	D	842	GLN
1	D	848	LEU
1	D	894	GLU
1	D	901	LYS
1	D	906	MET
1	D	934	LEU
1	D	948	GLU
1	D	969	PRO
1	D	970	LYS
1	E	740	MET
1	E	750	VAL
1	E	757	SER
1	E	760	ASP
1	E	775	LYS

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Mol	Chain	Res	Type
1	E	791	LYS
1	E	835	PHE
1	E	836	ASN
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	893	GLU
1	E	975	ASN
1	F	744	ASN
1	F	766	LEU
1	F	767	SER
1	F	852	MET
1	F	879	SER
1	F	893	GLU
1	F	901	LYS
1	F	936	SER
1	F	947	ARG
1	F	953	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	798	GLN
1	A	803	GLN
1	A	841	HIS
1	A	854	GLN
1	A	950	HIS
1	B	764	ASN
1	B	803	GLN
1	B	950	HIS
1	B	967	GLN
1	C	803	GLN
1	C	825	GLN
1	C	842	GLN
1	C	850	GLN
1	C	853	HIS
1	C	854	GLN
1	C	889	GLN

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Mol	Chain	Res	Type
1	D	803	GLN
1	D	825	GLN
1	D	842	GLN
1	D	850	GLN
1	D	854	GLN
1	D	975	ASN
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	923	GLN
1	F	744	ASN
1	F	764	ASN
1	F	803	GLN
1	F	842	GLN
1	F	850	GLN
1	F	854	GLN
1	F	863	GLN
1	F	923	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	E	5001	-	32,33,33	4.46	20 (62%)	48,54,54	2.38	12 (25%)
2	SNL	C	3001	-	32,33,33	5.60	25 (78%)	48,54,54	2.25	14 (29%)
2	SNL	D	4001	-	32,33,33	4.92	21 (65%)	48,54,54	2.51	16 (33%)
2	SNL	A	1001	-	32,33,33	4.08	18 (56%)	48,54,54	2.19	13 (27%)
2	SNL	B	2001	-	32,33,33	4.90	21 (65%)	48,54,54	2.72	18 (37%)
2	SNL	F	6001	-	32,33,33	5.58	21 (65%)	48,54,54	1.99	13 (27%)

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

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	SNL	C22-S61	20.41	2.08	1.83
2	F	6001	SNL	C22-S61	16.94	2.04	1.83
2	F	6001	SNL	C23-C24	10.75	1.74	1.53
2	E	5001	SNL	C22-S61	10.68	1.96	1.83
2	A	1001	SNL	C22-S61	10.28	1.95	1.83
2	D	4001	SNL	C23-C24	10.17	1.73	1.53
2	D	4001	SNL	C4-C5	10.05	1.72	1.54
2	B	2001	SNL	C23-C24	9.49	1.72	1.53
2	F	6001	SNL	C1-C2	9.22	1.71	1.54
2	C	3001	SNL	C2-C20	9.16	1.71	1.52
2	B	2001	SNL	C4-C5	9.02	1.71	1.54
2	B	2001	SNL	C22-S61	8.95	1.94	1.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SNL	C4-C5	8.94	1.70	1.54
2	B	2001	SNL	C1-C2	8.88	1.71	1.54
2	F	6001	SNL	C4-C5	8.74	1.70	1.54
2	F	6001	SNL	C12-C18	8.69	1.68	1.49
2	F	6001	SNL	C10-C5	8.53	1.71	1.54
2	C	3001	SNL	C23-C24	8.44	1.70	1.53
2	D	4001	SNL	C3-C24	8.41	1.67	1.53
2	D	4001	SNL	C22-S61	8.35	1.93	1.83
2	B	2001	SNL	C11-C2	8.31	1.68	1.54
2	E	5001	SNL	C4-C5	8.29	1.69	1.54
2	A	1001	SNL	C23-C24	8.25	1.70	1.53
2	B	2001	SNL	C2-C20	7.88	1.68	1.52
2	C	3001	SNL	C4-C5	7.83	1.68	1.54
2	D	4001	SNL	C2-C20	7.78	1.68	1.52
2	B	2001	SNL	C10-C5	7.60	1.69	1.54
2	C	3001	SNL	C1-C2	7.58	1.68	1.54
2	E	5001	SNL	C12-C18	7.51	1.66	1.49
2	A	1001	SNL	C1-C2	7.34	1.68	1.54
2	E	5001	SNL	C1-C2	7.33	1.68	1.54
2	F	6001	SNL	C2-C20	7.21	1.67	1.52
2	E	5001	SNL	C23-C24	7.14	1.67	1.53
2	F	6001	SNL	C19-C20	7.07	1.44	1.34
2	D	4001	SNL	C9-C5	6.78	1.68	1.54
2	D	4001	SNL	C12-C18	6.69	1.64	1.49
2	B	2001	SNL	C13-C9	6.62	1.66	1.53
2	D	4001	SNL	C1-C2	6.57	1.66	1.54
2	C	3001	SNL	C3-C24	6.48	1.64	1.53
2	C	3001	SNL	C19-C20	6.32	1.43	1.34
2	B	2001	SNL	O58-C15	6.29	1.46	1.35
2	E	5001	SNL	C10-C5	6.20	1.66	1.54
2	E	5001	SNL	C19-C20	6.17	1.43	1.34
2	B	2001	SNL	C21-C22	-5.98	1.45	1.53
2	E	5001	SNL	O58-C9	5.85	1.55	1.47
2	B	2001	SNL	O58-C9	-5.80	1.38	1.47
2	D	4001	SNL	C21-C20	5.58	1.63	1.51
2	C	3001	SNL	C13-C9	5.45	1.64	1.53
2	D	4001	SNL	C19-C20	5.28	1.42	1.34
2	E	5001	SNL	C21-C20	5.18	1.62	1.51
2	D	4001	SNL	C21-C22	-5.15	1.46	1.53
2	B	2001	SNL	C21-C20	5.10	1.62	1.51
2	D	4001	SNL	C5-C6	4.94	1.63	1.54
2	F	6001	SNL	C13-C9	4.92	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5001	SNL	C11-C2	4.92	1.63	1.54
2	A	1001	SNL	C12-C18	4.90	1.60	1.49
2	A	1001	SNL	C5-C6	4.90	1.63	1.54
2	D	4001	SNL	C7-C6	4.69	1.64	1.54
2	A	1001	SNL	C2-C20	4.66	1.62	1.52
2	A	1001	SNL	C10-C5	4.66	1.63	1.54
2	E	5001	SNL	C2-C20	4.64	1.62	1.52
2	F	6001	SNL	C5-C6	4.58	1.63	1.54
2	F	6001	SNL	O58-C9	4.57	1.53	1.47
2	A	1001	SNL	C21-C20	4.57	1.61	1.51
2	A	1001	SNL	C3-C24	4.50	1.61	1.53
2	C	3001	SNL	C10-C5	4.49	1.63	1.54
2	F	6001	SNL	C4-C3	-4.45	1.43	1.53
2	D	4001	SNL	C1-C12	4.11	1.61	1.53
2	C	3001	SNL	C16-S61	4.00	1.84	1.77
2	A	1001	SNL	C16-S61	3.99	1.84	1.77
2	D	4001	SNL	C16-S61	3.99	1.84	1.77
2	F	6001	SNL	C16-S61	3.97	1.84	1.77
2	C	3001	SNL	C21-C20	3.93	1.60	1.51
2	D	4001	SNL	C19-C18	3.88	1.54	1.45
2	C	3001	SNL	C13-C14	3.85	1.62	1.52
2	E	5001	SNL	C5-C6	3.83	1.61	1.54
2	C	3001	SNL	C12-C18	3.78	1.58	1.49
2	E	5001	SNL	C9-C5	3.72	1.62	1.54
2	A	1001	SNL	C19-C20	3.69	1.39	1.34
2	E	5001	SNL	C23-C6	3.67	1.61	1.53
2	D	4001	SNL	O58-C9	-3.66	1.41	1.47
2	C	3001	SNL	O58-C9	-3.61	1.42	1.47
2	A	1001	SNL	C11-C2	3.61	1.60	1.54
2	C	3001	SNL	O58-C15	3.60	1.41	1.35
2	F	6001	SNL	C19-C18	3.60	1.53	1.45
2	C	3001	SNL	C5-C6	3.56	1.61	1.54
2	C	3001	SNL	C8-C9	3.53	1.60	1.53
2	E	5001	SNL	C3-C24	3.38	1.59	1.53
2	A	1001	SNL	O58-C15	3.35	1.41	1.35
2	B	2001	SNL	C8-C7	-3.34	1.43	1.54
2	E	5001	SNL	C13-C9	3.33	1.60	1.53
2	D	4001	SNL	C4-C3	-3.21	1.46	1.53
2	C	3001	SNL	C1-C12	3.15	1.59	1.53
2	F	6001	SNL	C8-C9	3.10	1.59	1.53
2	E	5001	SNL	C13-C14	3.08	1.60	1.52
2	C	3001	SNL	C14-C15	3.05	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3001	SNL	C23-C6	3.03	1.59	1.53
2	F	6001	SNL	C9-C5	3.01	1.60	1.54
2	F	6001	SNL	C7-C6	3.00	1.60	1.54
2	F	6001	SNL	C13-C14	3.00	1.60	1.52
2	C	3001	SNL	C21-C22	-2.89	1.49	1.53
2	E	5001	SNL	C14-C15	2.86	1.55	1.50
2	C	3001	SNL	C2-C24	2.83	1.60	1.56
2	B	2001	SNL	C3-C24	2.74	1.58	1.53
2	F	6001	SNL	C3-C24	2.73	1.58	1.53
2	A	1001	SNL	C21-C22	2.69	1.56	1.53
2	F	6001	SNL	C2-C24	2.67	1.60	1.56
2	B	2001	SNL	C19-C18	2.63	1.51	1.45
2	E	5001	SNL	O58-C15	-2.62	1.31	1.35
2	D	4001	SNL	C11-C2	2.55	1.59	1.54
2	B	2001	SNL	C5-C6	2.51	1.59	1.54
2	A	1001	SNL	C2-C24	2.51	1.60	1.56
2	B	2001	SNL	C1-C12	2.49	1.58	1.53
2	B	2001	SNL	C9-C5	2.46	1.59	1.54
2	C	3001	SNL	C11-C2	2.45	1.58	1.54
2	A	1001	SNL	C13-C9	2.45	1.58	1.53
2	C	3001	SNL	C19-C18	2.33	1.50	1.45
2	A	1001	SNL	C1-C12	2.33	1.58	1.53
2	C	3001	SNL	C4-C3	-2.32	1.48	1.53
2	E	5001	SNL	O60-C18	2.30	1.26	1.23
2	B	2001	SNL	C14-C15	2.21	1.54	1.50
2	F	6001	SNL	O57-C15	-2.15	1.16	1.22
2	B	2001	SNL	C12-C18	2.07	1.54	1.49
2	D	4001	SNL	C8-C9	2.05	1.57	1.53
2	D	4001	SNL	O60-C18	2.03	1.26	1.23
2	B	2001	SNL	C19-C20	2.03	1.37	1.34

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5001	SNL	C17-C16-S61	10.24	125.44	113.01
2	B	2001	SNL	C17-C16-S61	10.10	125.28	113.01
2	C	3001	SNL	C17-C16-S61	7.31	121.89	113.01
2	F	6001	SNL	C17-C16-S61	7.30	121.87	113.01
2	D	4001	SNL	C17-C16-S61	7.29	121.86	113.01
2	A	1001	SNL	C17-C16-S61	7.26	121.82	113.01
2	E	5001	SNL	O59-C16-S61	-6.76	117.93	123.01
2	B	2001	SNL	O59-C16-S61	-6.37	118.22	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4001	SNL	O58-C9-C8	-6.15	101.65	109.14
2	D	4001	SNL	O58-C9-C5	5.73	116.92	110.95
2	B	2001	SNL	O58-C15-O57	5.46	125.67	120.80
2	C	3001	SNL	O58-C15-O57	4.94	125.21	120.80
2	E	5001	SNL	O58-C15-O57	4.93	125.20	120.80
2	D	4001	SNL	C9-C5-C6	-4.83	95.02	99.94
2	B	2001	SNL	C7-C6-C23	4.61	124.78	118.33
2	A	1001	SNL	O58-C15-O57	4.43	124.75	120.80
2	C	3001	SNL	C7-C6-C23	4.24	124.26	118.33
2	B	2001	SNL	C7-C8-C9	4.12	112.23	105.57
2	B	2001	SNL	C7-C6-C5	4.09	109.21	103.73
2	C	3001	SNL	C10-C5-C9	4.04	114.01	108.66
2	C	3001	SNL	C12-C18-C19	4.00	122.91	116.74
2	D	4001	SNL	C7-C6-C5	4.00	109.10	103.73
2	D	4001	SNL	C8-C9-C5	3.99	107.31	103.67
2	C	3001	SNL	C7-C6-C5	3.98	109.07	103.73
2	C	3001	SNL	O59-C16-S61	-3.94	120.05	123.01
2	F	6001	SNL	O59-C16-S61	-3.92	120.06	123.01
2	D	4001	SNL	O59-C16-S61	-3.92	120.06	123.01
2	A	1001	SNL	O59-C16-S61	-3.92	120.07	123.01
2	B	2001	SNL	C11-C2-C20	-3.86	102.10	108.34
2	A	1001	SNL	C7-C6-C23	3.78	123.62	118.33
2	C	3001	SNL	C4-C5-C9	-3.78	114.30	117.76
2	D	4001	SNL	O58-C15-O57	3.75	124.15	120.80
2	B	2001	SNL	C8-C9-C5	3.61	106.96	103.67
2	A	1001	SNL	C12-C18-C19	3.60	122.28	116.74
2	A	1001	SNL	C8-C9-C5	3.52	106.88	103.67
2	F	6001	SNL	O58-C15-O57	3.47	123.90	120.80
2	B	2001	SNL	C9-C5-C6	-3.47	96.41	99.94
2	D	4001	SNL	C7-C8-C9	3.46	111.16	105.57
2	A	1001	SNL	C11-C2-C20	-3.30	103.00	108.34
2	D	4001	SNL	C7-C6-C23	3.29	122.93	118.33
2	B	2001	SNL	C12-C18-C19	3.29	121.81	116.74
2	A	1001	SNL	C7-C8-C9	3.29	110.89	105.57
2	C	3001	SNL	C1-C2-C24	3.22	113.22	108.73
2	E	5001	SNL	C11-C2-C20	-3.16	103.22	108.34
2	B	2001	SNL	C10-C5-C9	3.12	112.80	108.66
2	E	5001	SNL	C7-C8-C9	2.99	110.41	105.57
2	E	5001	SNL	C12-C18-C19	2.99	121.35	116.74
2	B	2001	SNL	C1-C2-C24	2.96	112.86	108.73
2	D	4001	SNL	C12-C18-C19	2.91	121.22	116.74
2	F	6001	SNL	C7-C8-C9	2.90	110.26	105.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	SNL	C9-C5-C6	-2.88	97.00	99.94
2	F	6001	SNL	C4-C5-C9	-2.76	115.23	117.76
2	F	6001	SNL	C9-C5-C6	-2.76	97.13	99.94
2	D	4001	SNL	C11-C2-C20	-2.62	104.10	108.34
2	A	1001	SNL	C1-C2-C24	2.60	112.35	108.73
2	F	6001	SNL	C7-C6-C5	2.57	107.17	103.73
2	F	6001	SNL	C12-C18-C19	2.57	120.69	116.74
2	A	1001	SNL	C10-C5-C9	2.56	112.05	108.66
2	C	3001	SNL	O60-C18-C12	-2.56	116.28	121.57
2	E	5001	SNL	C4-C5-C6	-2.53	104.72	108.47
2	F	6001	SNL	C10-C5-C9	2.53	112.01	108.66
2	C	3001	SNL	C8-C9-C5	2.51	105.96	103.67
2	B	2001	SNL	C13-C9-C5	2.51	120.77	116.19
2	F	6001	SNL	C7-C6-C23	2.51	121.83	118.33
2	D	4001	SNL	C10-C5-C9	2.48	111.94	108.66
2	C	3001	SNL	C9-C5-C6	-2.46	97.43	99.94
2	A	1001	SNL	O58-C9-C8	-2.43	106.19	109.14
2	F	6001	SNL	O58-C15-C14	2.38	112.58	110.19
2	C	3001	SNL	C11-C2-C20	-2.37	104.51	108.34
2	E	5001	SNL	O58-C9-C5	2.35	113.39	110.95
2	B	2001	SNL	C4-C5-C9	-2.25	115.70	117.76
2	B	2001	SNL	C5-C6-C23	2.24	115.48	113.43
2	E	5001	SNL	C10-C5-C9	2.23	111.61	108.66
2	B	2001	SNL	C10-C5-C4	2.23	112.89	109.73
2	D	4001	SNL	C4-C5-C6	-2.21	105.21	108.47
2	A	1001	SNL	O58-C9-C5	2.19	113.23	110.95
2	C	3001	SNL	C13-C9-C8	-2.17	106.96	113.80
2	F	6001	SNL	C10-C5-C4	2.16	112.79	109.73
2	B	2001	SNL	C4-C5-C6	-2.15	105.29	108.47
2	E	5001	SNL	O58-C9-C8	-2.14	106.54	109.14
2	F	6001	SNL	C5-C6-C23	-2.11	111.50	113.43
2	B	2001	SNL	C21-C20-C2	2.11	119.22	116.42
2	E	5001	SNL	C7-C6-C23	2.08	121.24	118.33
2	D	4001	SNL	C21-C20-C2	2.08	119.18	116.42
2	E	5001	SNL	C1-C2-C24	2.02	111.55	108.73
2	D	4001	SNL	C21-C20-C19	-2.01	117.81	121.17

There are no chirality outliers.

There are no torsion outliers.

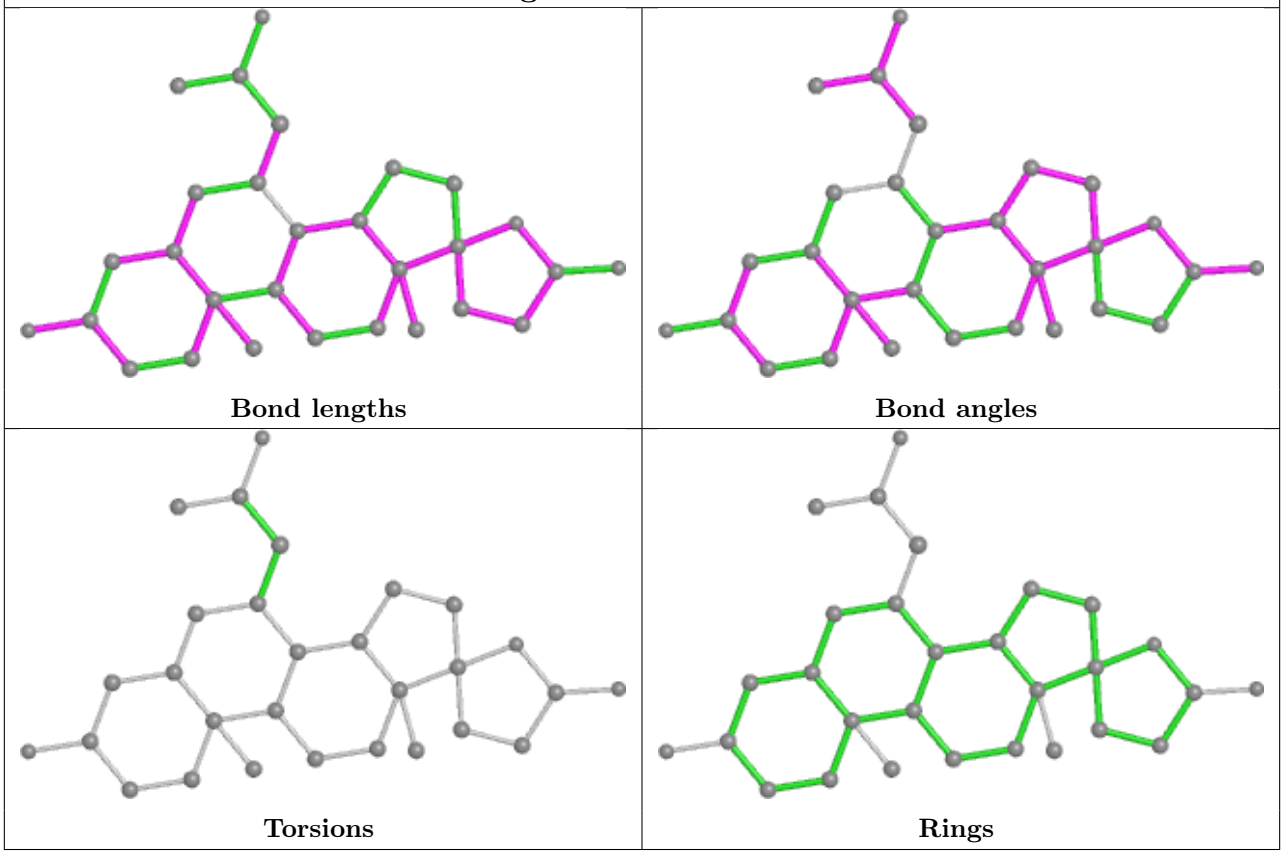
There are no ring outliers.

6 monomers are involved in 30 short contacts:

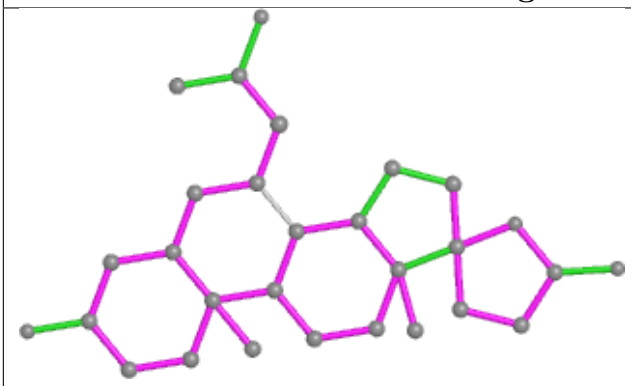
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	5001	SNL	6	0
2	C	3001	SNL	6	0
2	D	4001	SNL	4	0
2	A	1001	SNL	3	0
2	B	2001	SNL	1	0
2	F	6001	SNL	10	0

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 then 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.

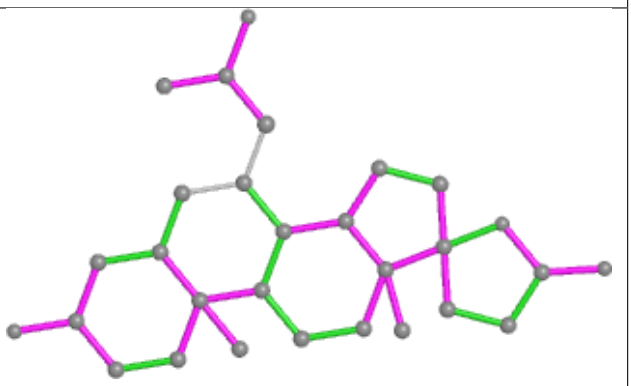
Ligand SNL E 5001



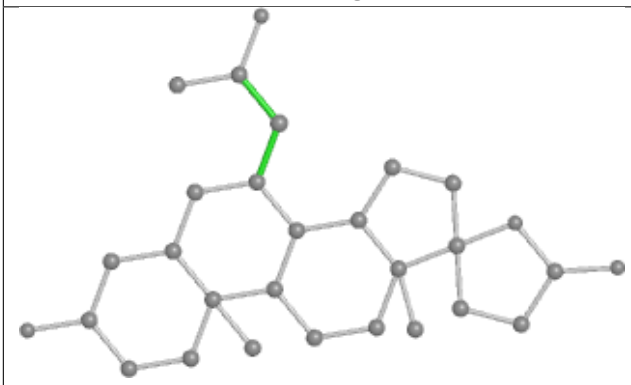
Ligand SNL C 3001



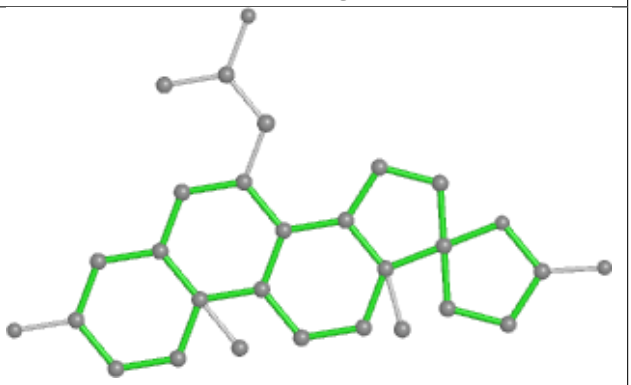
Bond lengths



Bond angles

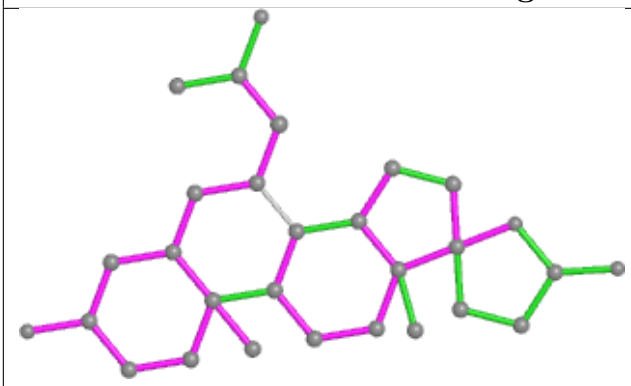


Torsions

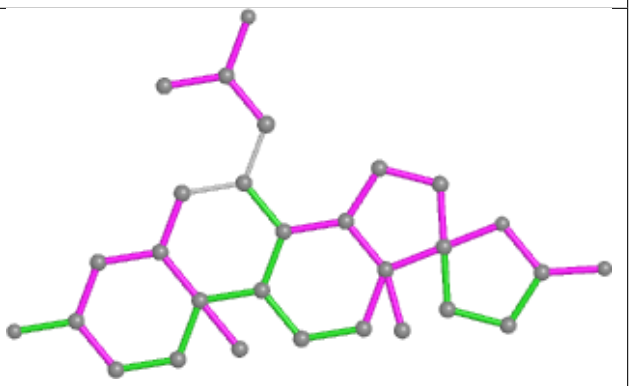


Rings

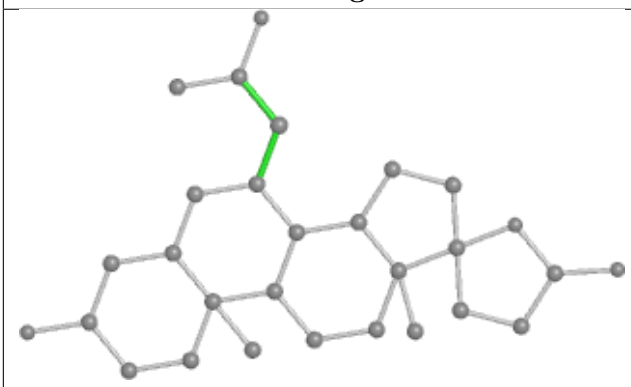
Ligand SNL D 4001



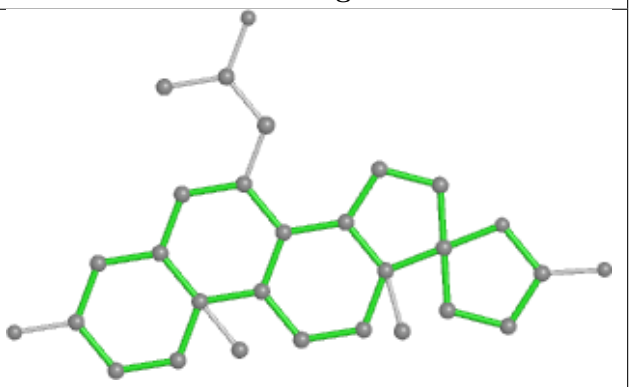
Bond lengths



Bond angles

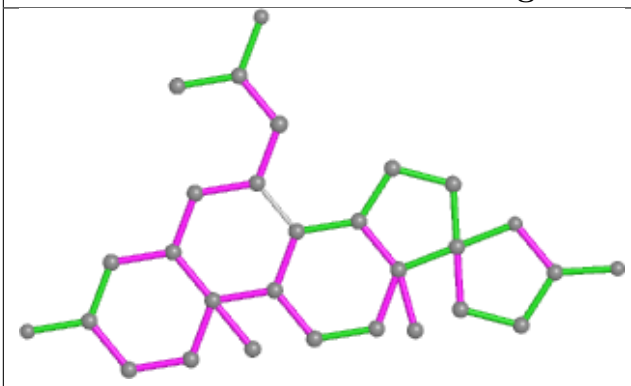


Torsions

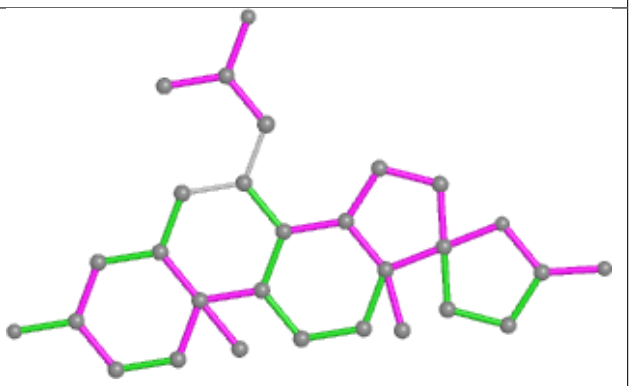


Rings

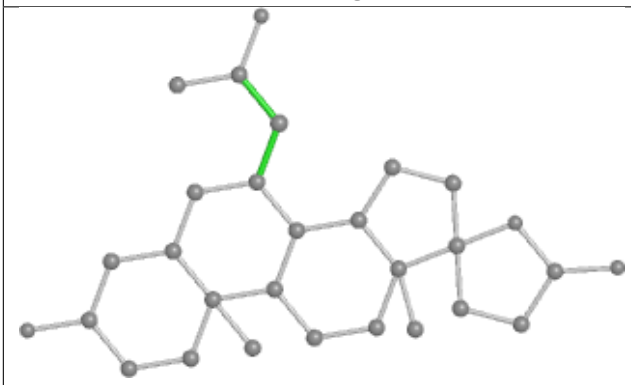
Ligand SNL A 1001



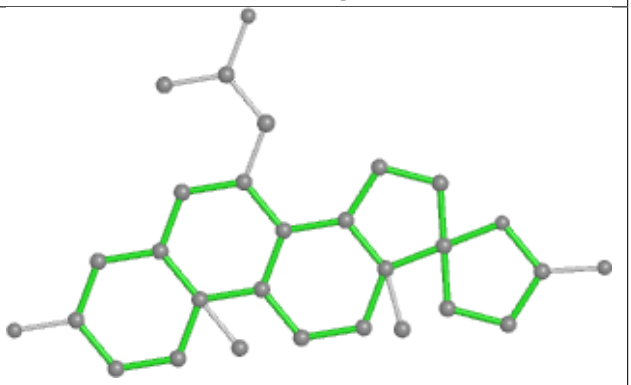
Bond lengths



Bond angles

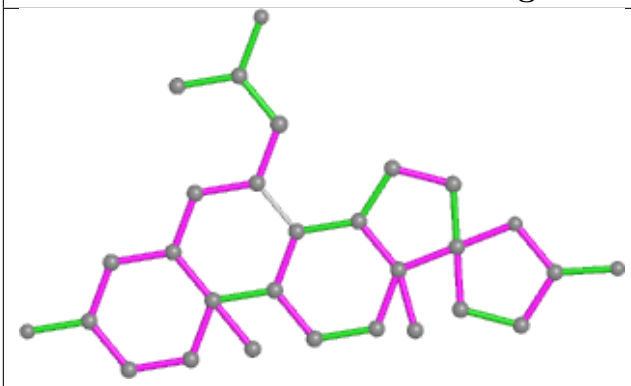


Torsions

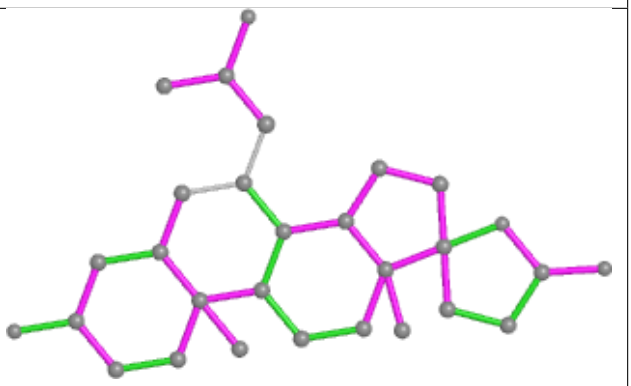


Rings

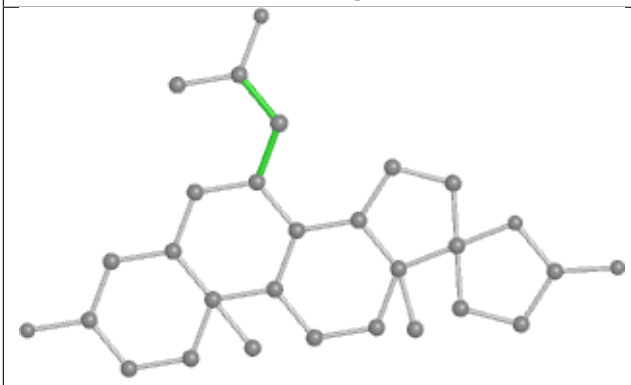
Ligand SNL B 2001



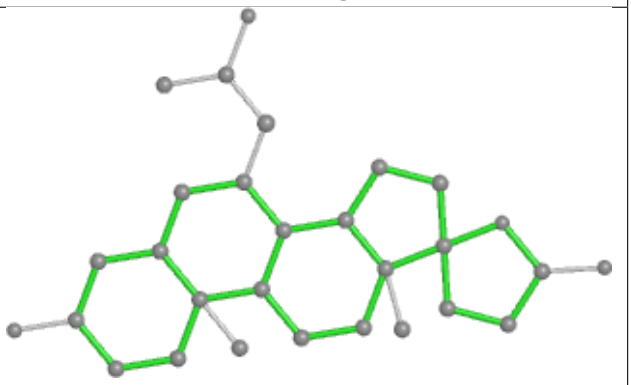
Bond lengths



Bond angles

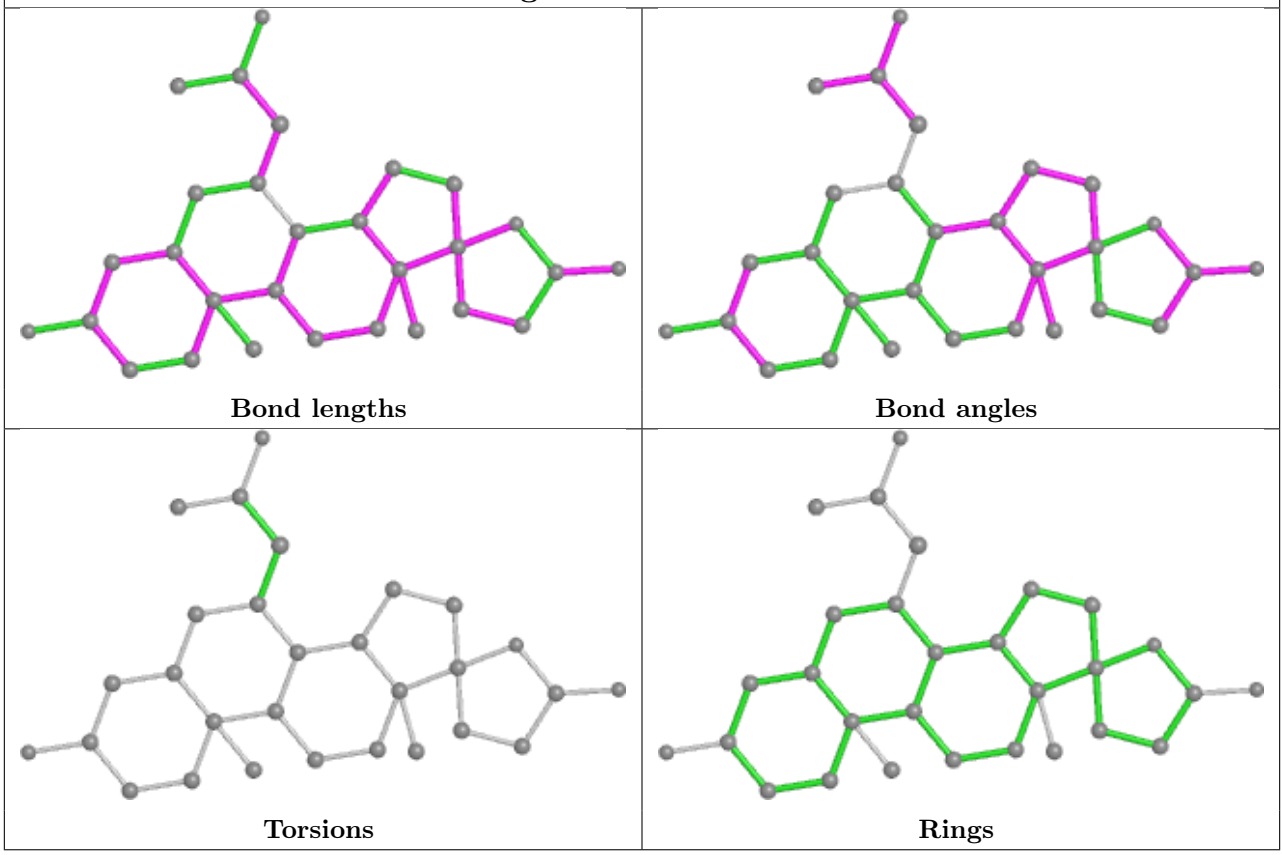


Torsions



Rings

Ligand SNL F 6001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.39	20 (8%)	10	14	23, 41, 69, 82	0
1	B	233/256 (91%)	0.28	11 (4%)	31	38	24, 40, 58, 71	0
1	C	233/256 (91%)	0.16	7 (3%)	50	57	20, 37, 60, 71	0
1	D	234/256 (91%)	0.33	18 (7%)	13	17	20, 39, 71, 86	0
1	E	234/256 (91%)	0.82	36 (15%)	2	3	22, 57, 78, 82	0
1	F	238/256 (92%)	0.46	19 (7%)	12	16	23, 43, 75, 79	0
All	All	1405/1536 (91%)	0.41	111 (7%)	12	17	20, 41, 73, 86	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	951	ALA	7.5
1	D	951	ALA	6.4
1	E	951	ALA	6.3
1	B	970	LYS	6.3
1	E	760	ASP	6.2
1	F	952	LEU	5.7
1	C	909	LYS	5.6
1	A	950	HIS	5.3
1	F	970	LYS	5.0
1	A	951	ALA	4.7
1	D	974	GLY	4.7
1	D	971	VAL	4.7
1	E	757	SER	4.7
1	E	950	HIS	4.6
1	D	950	HIS	4.4
1	F	973	SER	4.3
1	D	972	GLU	4.3
1	B	757	SER	3.9
1	F	950	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	758	LYS	3.8
1	E	841	HIS	3.7
1	E	819	TYR	3.6
1	F	836	ASN	3.6
1	D	952	LEU	3.4
1	D	761	THR	3.3
1	F	763	GLU	3.3
1	A	838	GLU	3.3
1	E	856	SER	3.2
1	F	755	ASP	3.2
1	A	971	VAL	3.2
1	E	849	CYS	3.2
1	E	972	GLU	3.2
1	F	762	ALA	3.2
1	F	841	HIS	3.1
1	D	760	ASP	3.1
1	E	842	GLN	3.1
1	E	847	GLU	3.0
1	B	907	VAL	3.0
1	F	944	TYR	3.0
1	D	755	ASP	3.0
1	E	827	LEU	3.0
1	A	973	SER	3.0
1	B	950	HIS	3.0
1	A	953	LYS	3.0
1	F	971	VAL	2.9
1	A	970	LYS	2.9
1	E	947	ARG	2.8
1	A	974	GLY	2.8
1	D	917	SER	2.8
1	E	891	ALA	2.7
1	D	756	SER	2.7
1	E	952	LEU	2.7
1	D	916	GLN	2.7
1	A	883	LYS	2.7
1	F	756	SER	2.7
1	F	844	ALA	2.7
1	A	756	SER	2.6
1	A	969	PRO	2.6
1	E	855	ILE	2.6
1	A	954	VAL	2.6
1	D	975	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	836	ASN	2.6
1	C	884	ASP	2.6
1	E	825	GLN	2.6
1	E	840	MET	2.6
1	E	890	ALA	2.6
1	E	763	GLU	2.5
1	C	976	ALA	2.5
1	B	758	LYS	2.5
1	E	850	GLN	2.5
1	A	836	ASN	2.5
1	B	972	GLU	2.5
1	F	933	ASP	2.5
1	A	771	ARG	2.4
1	F	761	THR	2.4
1	A	972	GLU	2.4
1	B	974	GLY	2.4
1	C	764	ASN	2.4
1	F	823	ASN	2.3
1	B	944	TYR	2.3
1	E	759	PRO	2.3
1	E	945	THR	2.3
1	E	980	TYR	2.3
1	E	971	VAL	2.3
1	C	838	GLU	2.3
1	A	952	LEU	2.2
1	D	970	LYS	2.2
1	F	913	ASN	2.2
1	D	955	GLU	2.2
1	E	944	TYR	2.2
1	A	945	THR	2.2
1	D	918	TRP	2.2
1	A	947	ARG	2.2
1	A	763	GLU	2.1
1	E	940	GLU	2.1
1	B	940	GLU	2.1
1	C	919	GLN	2.1
1	C	908	THR	2.1
1	E	838	GLU	2.1
1	E	859	PHE	2.1
1	E	973	SER	2.1
1	B	905	LYS	2.1
1	D	977	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	971	VAL	2.1
1	D	907	VAL	2.0
1	E	860	VAL	2.0
1	E	982	HIS	2.0
1	E	903	LEU	2.0
1	F	945	THR	2.0
1	A	955	GLU	2.0
1	E	861	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

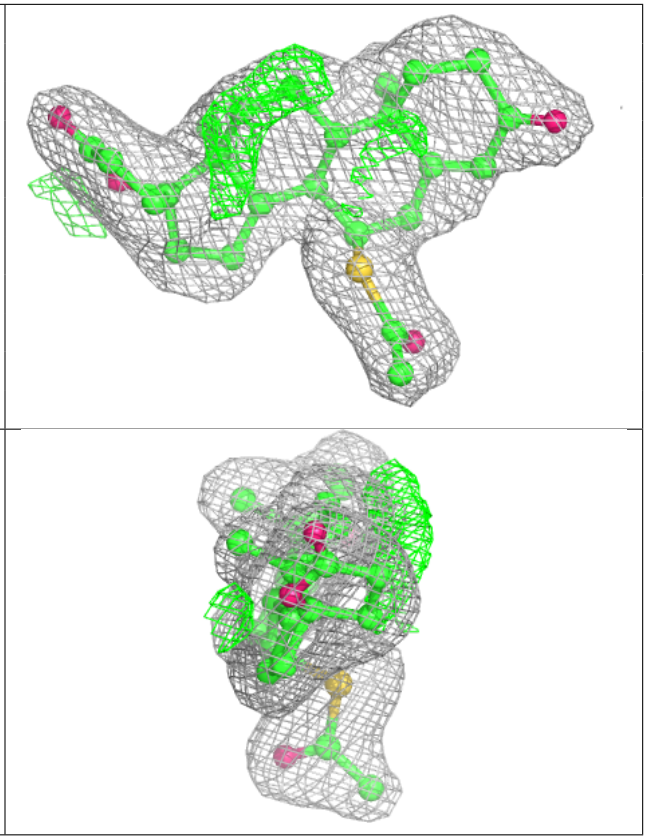
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

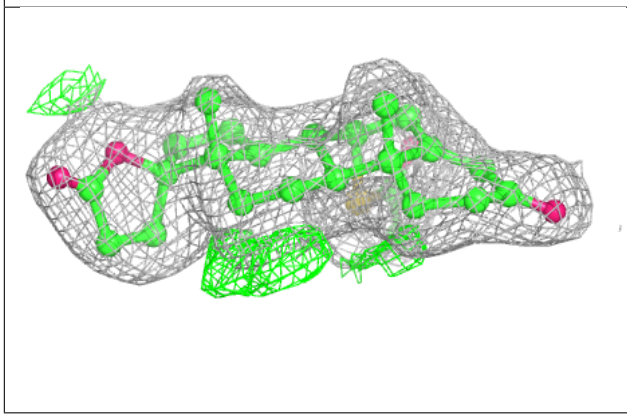
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SNL	D	4001	29/29	0.92	0.15	22,27,29,30	0
2	SNL	E	5001	29/29	0.92	0.16	42,43,45,47	0
2	SNL	F	6001	29/29	0.93	0.13	29,34,38,40	0
2	SNL	B	2001	29/29	0.95	0.13	19,21,23,24	0
2	SNL	A	1001	29/29	0.95	0.14	25,29,31,32	0
2	SNL	C	3001	29/29	0.96	0.11	18,23,25,30	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:

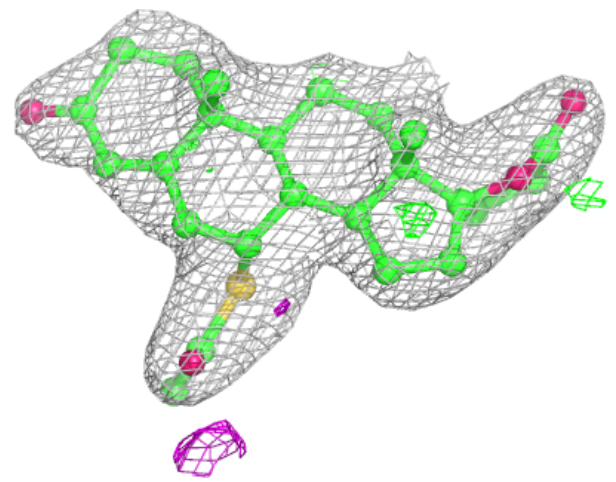
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

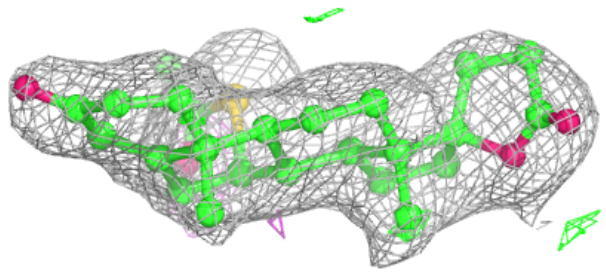


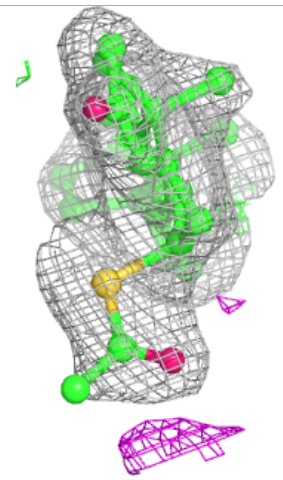


Electron density around SNL E 5001:

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

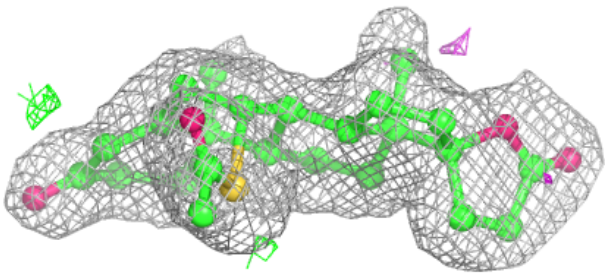


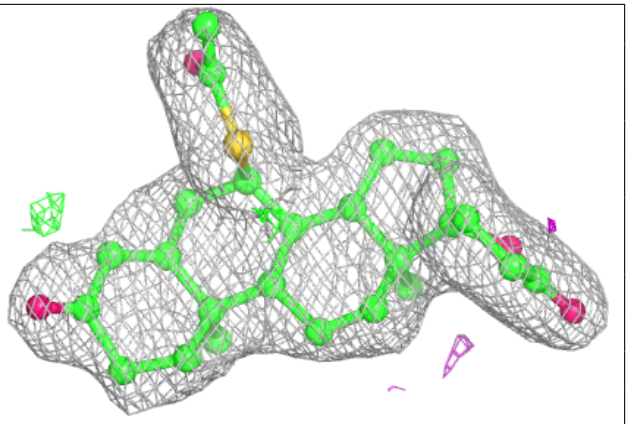


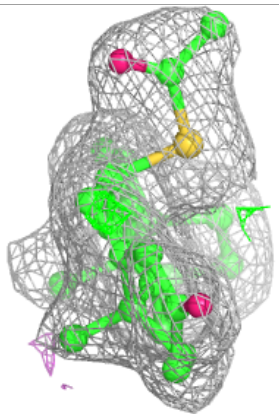


Electron density around SNL F 6001:

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

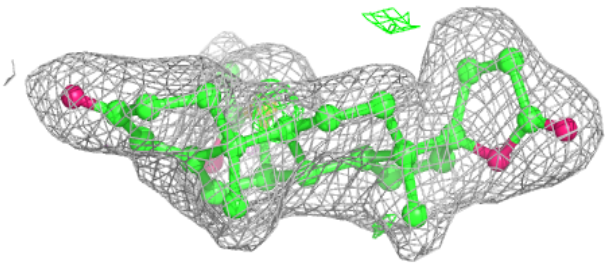


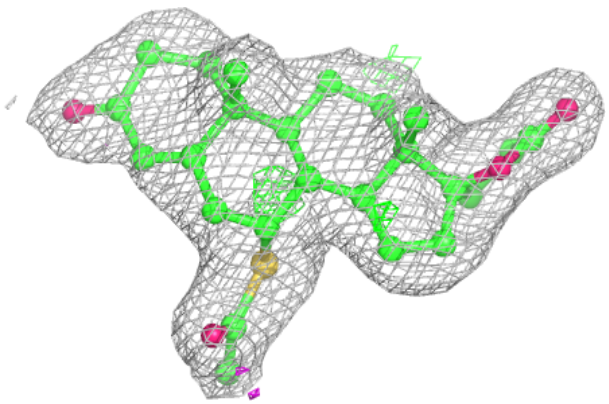


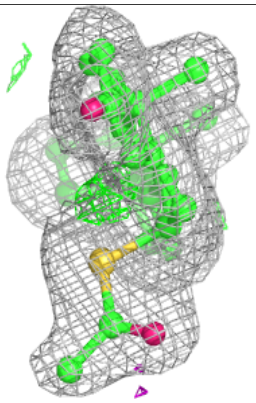


Electron density around SNL B 2001:

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

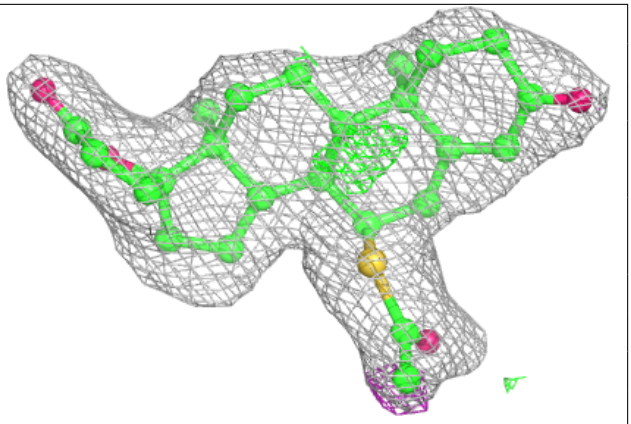


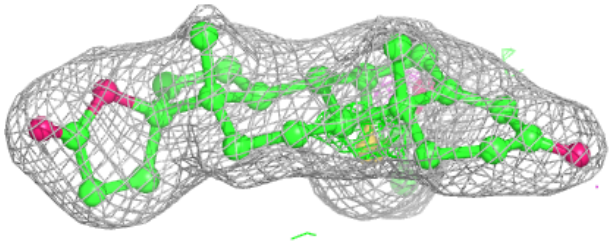


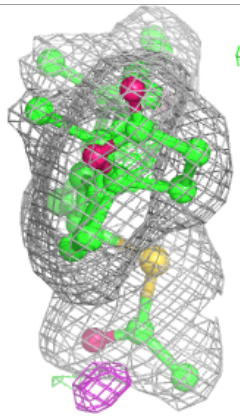


Electron density around SNL A 1001:

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

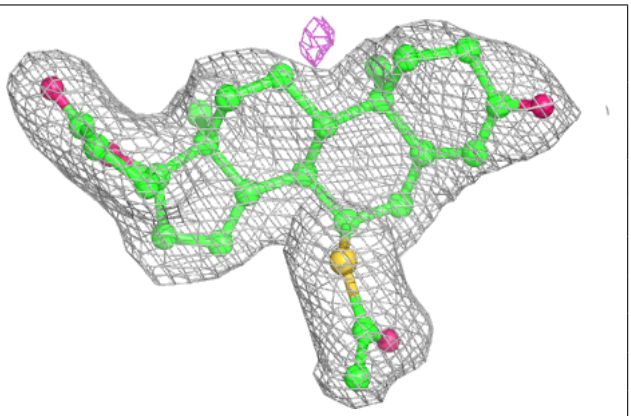


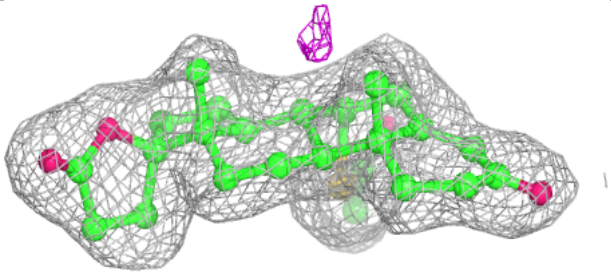


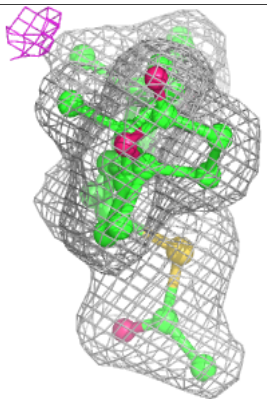


Electron density around SNL C 3001:

$2mF_o$-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.