



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:28 am BST

PDB ID : 3BJW
Title : Crystal Structure of ecarpholin S complexed with suramin
Authors : Zhou, X.; Sivaraman, J.
Deposited on : 2007-12-04
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

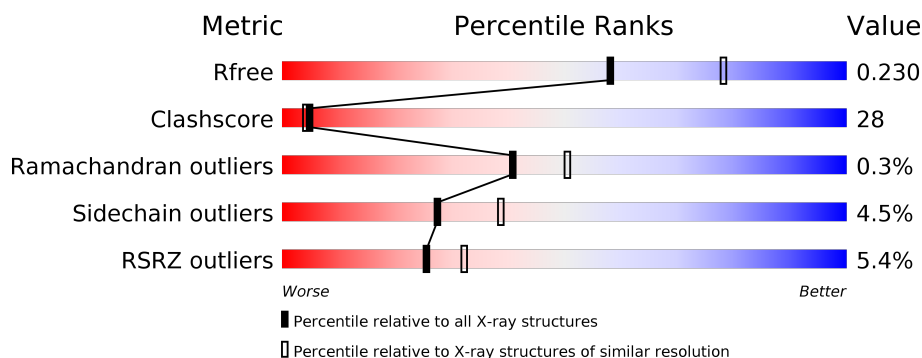
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	122	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>29%</div> <div>•</div> </div> </div>
1	B	122	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>•</div> </div> </div>
1	C	122	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>43%</div> <div>•</div> </div> </div>
1	D	122	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>37%</div> <div>6%</div> </div> </div>
1	E	122	<div> <div>20%</div> <div> <div></div> <div>59%</div> <div>38%</div> <div>•</div> </div> </div>
1	F	122	<div> <div>7%</div> <div> <div></div> <div>60%</div> <div>38%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	122	<div><div></div><div>2%</div><div>47%</div><div>48%</div><div></div><div></div></div>
1	H	122	<div><div></div><div>5%</div><div>58%</div><div>37%</div><div>5%</div><div></div></div>

2 Entry composition

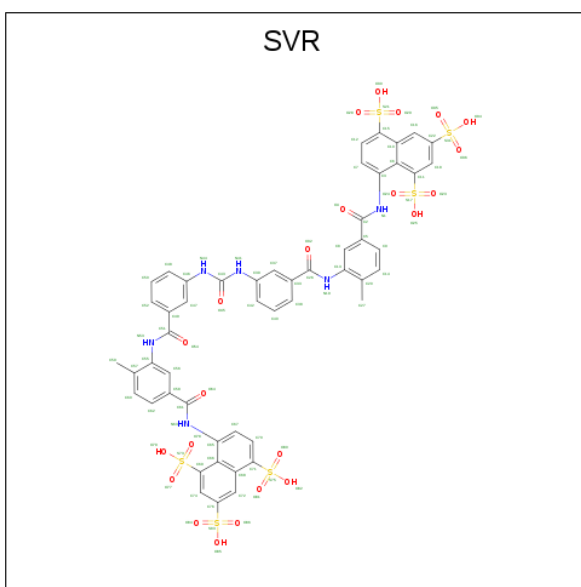
There are 3 unique types of molecules in this entry. The entry contains 9074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			
1	B	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			
1	C	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			
1	D	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			
1	E	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			
1	F	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			
1	G	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			
1	H	122	Total	C	N	O	S	0	0	0
			959	596	163	185	15			

- Molecule 2 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: C₅₁H₄₀N₆O₂₃S₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	B	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	B	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	C	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	C	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	E	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	E	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	F	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	F	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	G	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	H	1	Total	C	N	O	S	0	0
			86	51	6	23	6		
2	H	1	Total	C	N	O	S	0	0
			86	51	6	23	6		

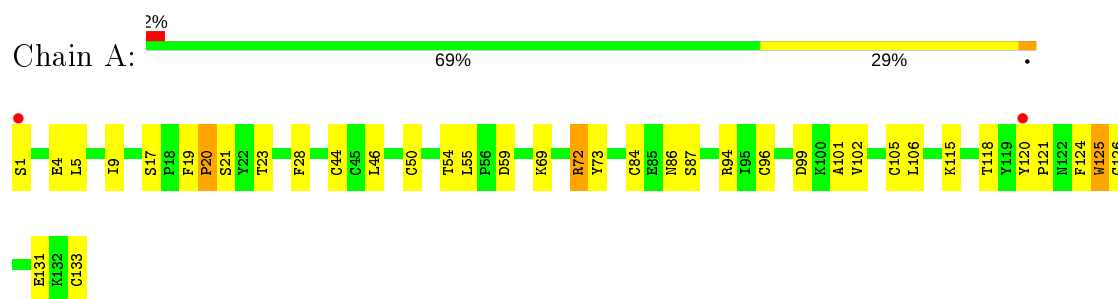
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total 54	O 54	0	0
3	B	59	Total 59	O 59	0	0
3	C	56	Total 56	O 56	0	0
3	D	39	Total 39	O 39	0	0
3	E	33	Total 33	O 33	0	0
3	F	51	Total 51	O 51	0	0
3	G	39	Total 39	O 39	0	0
3	H	39	Total 39	O 39	0	0

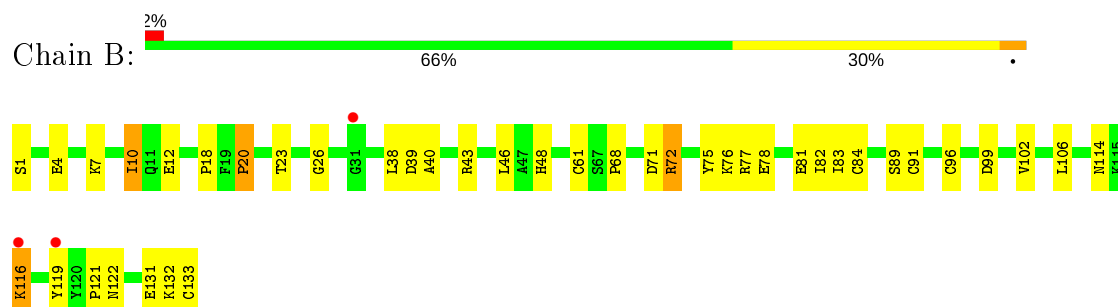
3 Residue-property plots [i](#)

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

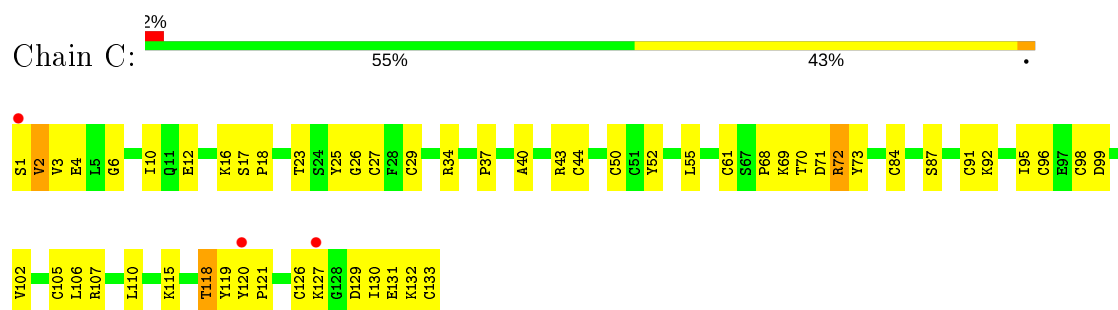
• Molecule 1: Phospholipase A2



• Molecule 1: Phospholipase A2

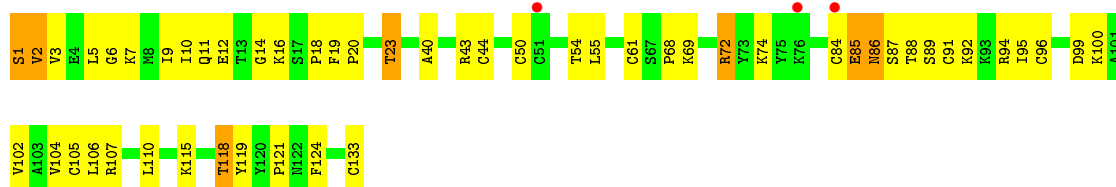


• Molecule 1: Phospholipase A2

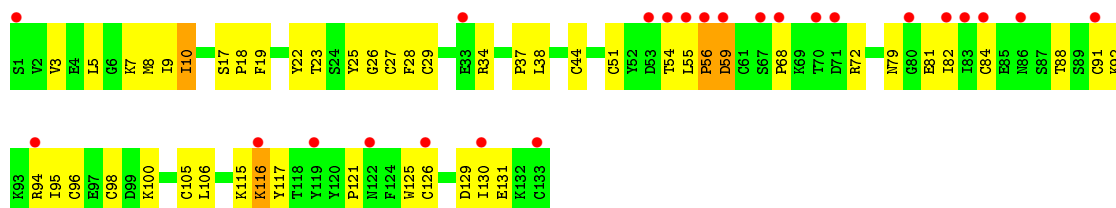


• Molecule 1: Phospholipase A2

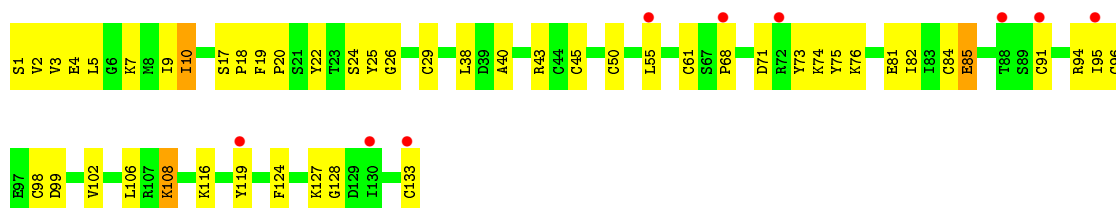




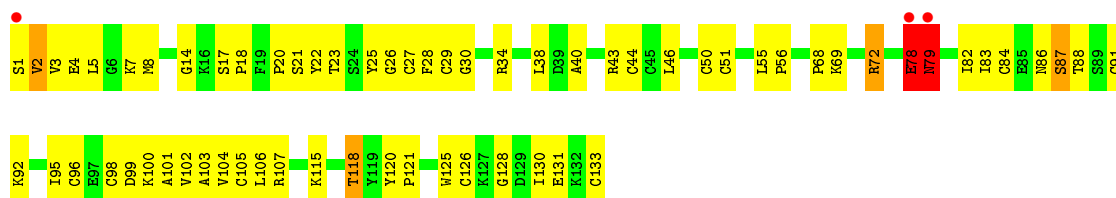
• Molecule 1: Phospholipase A2



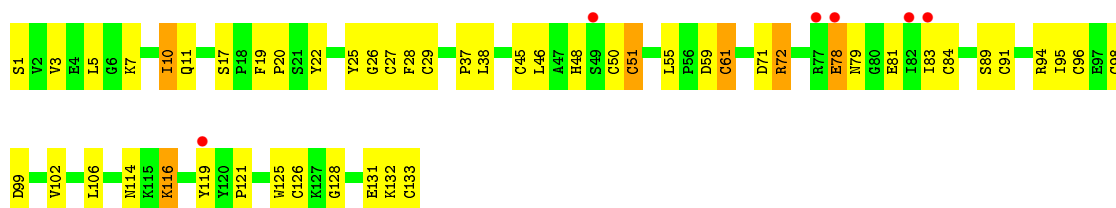
• Molecule 1: Phospholipase A2



• Molecule 1: Phospholipase A2



• Molecule 1: Phospholipase A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.45Å 132.25Å 86.10Å 90.00° 99.33° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 47.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.6 (20.00-2.30) 98.6 (47.40-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.275 0.228 , 0.230	Depositor DCC
R_{free} test set	2514 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9074	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/980	0.66	1/1318 (0.1%)
1	B	0.40	0/980	0.63	0/1318
1	C	0.41	0/980	0.65	0/1318
1	D	0.37	0/980	0.59	0/1318
1	E	0.41	0/980	0.71	2/1318 (0.2%)
1	F	0.37	0/980	0.60	0/1318
1	G	0.35	0/980	0.73	2/1318 (0.2%)
1	H	0.37	0/980	0.82	2/1318 (0.2%)
All	All	0.39	0/7840	0.68	7/10544 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	78	GLU	CB-CA-C	13.74	137.87	110.40
1	H	79	ASN	N-CA-CB	-11.42	90.04	110.60
1	G	79	ASN	N-CA-CB	-10.61	91.50	110.60
1	G	78	GLU	CB-CA-C	9.91	130.22	110.40
1	E	59	ASP	O-C-N	7.38	134.51	122.70
1	E	56	PRO	C-N-CA	6.58	138.16	121.70
1	A	125	TRP	N-CA-C	5.08	124.72	111.00

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	959	0	933	33	0
1	B	959	0	933	45	0
1	C	959	0	933	53	0
1	D	959	0	933	57	0
1	E	959	0	931	62	0
1	F	959	0	933	40	0
1	G	959	0	933	64	0
1	H	959	0	933	50	0
2	A	86	0	40	7	0
2	B	172	0	80	4	0
2	C	172	0	80	23	0
2	E	172	0	80	7	0
2	F	172	0	80	13	0
2	G	86	0	40	3	0
2	H	172	0	80	13	0
3	A	54	0	0	0	0
3	B	59	0	0	3	0
3	C	56	0	0	4	0
3	D	39	0	0	1	0
3	E	33	0	0	2	0
3	F	51	0	0	2	0
3	G	39	0	0	1	0
3	H	39	0	0	3	0
All	All	9074	0	7942	404	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 28.

All (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:GLU:O	3:H:549:HOH:O	1.65	1.13
1:H:116:LYS:HB2	1:H:116:LYS:NZ	1.64	1.06
1:H:116:LYS:HB2	1:H:116:LYS:HZ2	1.19	1.04
1:D:10:ILE:HG23	1:E:116:LYS:HE2	1.37	1.03
1:G:55:LEU:HD13	1:G:95:ILE:HD13	1.41	1.01
1:B:116:LYS:HE2	1:C:10:ILE:HG23	1.44	0.96
1:F:84:CYS:HG	1:F:96:CYS:HG	1.01	0.92
1:D:68:PRO:HA	1:D:95:ILE:HD12	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:CYS:HG	1:G:133:CYS:HG	0.98	0.90
1:F:10:ILE:HD11	2:F:502:SVR:H44	1.36	0.89
1:H:61:CYS:HG	1:H:91:CYS:HG	1.07	0.87
1:F:26:GLY:HA2	1:F:38:LEU:HD12	1.57	0.86
1:C:130:ILE:HD12	1:C:130:ILE:H	1.41	0.85
1:B:116:LYS:NZ	1:B:116:LYS:HB2	1.92	0.84
1:C:50:CYS:HG	1:C:133:CYS:HG	0.90	0.83
1:D:61:CYS:HG	1:D:91:CYS:HG	0.85	0.83
1:B:72:ARG:HH11	1:B:72:ARG:HB3	1.43	0.82
1:F:61:CYS:HG	1:F:91:CYS:HG	0.97	0.82
1:G:68:PRO:HB3	1:G:95:ILE:HD12	1.62	0.81
2:A:508:SVR:O45	1:G:2:VAL:HG13	1.80	0.81
1:G:84:CYS:HG	1:G:96:CYS:HG	0.98	0.81
1:B:1:SER:HB3	1:B:68:PRO:O	1.81	0.81
1:C:84:CYS:HG	1:C:96:CYS:HG	0.88	0.80
1:A:50:CYS:HG	1:A:133:CYS:HG	1.01	0.80
1:H:50:CYS:HG	1:H:133:CYS:HG	1.18	0.80
1:H:84:CYS:HG	1:H:96:CYS:HG	0.87	0.80
1:G:79:ASN:N	1:G:79:ASN:OD1	2.16	0.79
1:D:1:SER:HB3	1:D:68:PRO:O	1.83	0.79
1:G:44:CYS:HG	1:G:105:CYS:HG	0.88	0.79
1:D:10:ILE:HG23	1:E:116:LYS:CE	2.13	0.78
1:D:40:ALA:HA	1:D:43:ARG:NH1	1.99	0.78
1:D:74:LYS:O	1:D:85:GLU:HG2	1.84	0.77
1:B:116:LYS:CE	1:C:10:ILE:HG23	2.15	0.77
1:E:130:ILE:H	1:E:130:ILE:HD12	1.50	0.76
1:D:115:LYS:O	1:D:118:THR:HB	1.86	0.76
1:G:46:LEU:HD21	1:G:131:GLU:HG2	1.66	0.76
1:H:1:SER:HB2	1:H:71:ASP:O	1.86	0.75
1:F:18:PRO:HG2	2:F:502:SVR:H47	1.68	0.75
1:G:3:VAL:HB	1:G:72:ARG:HH12	1.51	0.75
1:A:1:SER:HB2	1:A:73:TYR:CE2	2.21	0.75
1:G:1:SER:HB3	1:G:68:PRO:O	1.86	0.75
1:C:1:SER:HA	1:C:4:GLU:OE1	1.87	0.74
1:G:14:GLY:O	1:H:116:LYS:HE2	1.87	0.74
1:H:78:GLU:HB3	1:H:83:ILE:HD12	1.70	0.74
1:E:34:ARG:HH12	1:E:129:ASP:HA	1.52	0.74
1:H:26:GLY:HA2	1:H:38:LEU:HD12	1.69	0.73
1:B:7:LYS:HA	1:B:10:ILE:HD11	1.69	0.73
1:E:18:PRO:HG2	2:E:503:SVR:H47	1.70	0.73
1:B:72:ARG:HH11	1:B:72:ARG:CB	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:CYS:CB	1:E:98:CYS:HG	2.03	0.72
1:G:78:GLU:C	1:G:79:ASN:OD1	2.29	0.71
1:A:72:ARG:HG3	1:A:72:ARG:HH11	1.55	0.71
1:C:2:VAL:HG13	2:C:507:SVR:O45	1.89	0.71
1:F:1:SER:HA	1:F:4:GLU:OE1	1.90	0.71
1:A:1:SER:HB2	1:A:73:TYR:HE2	1.55	0.71
1:A:9:ILE:HD12	1:A:106:LEU:HD12	1.72	0.71
1:G:3:VAL:HG21	1:G:72:ARG:HH22	1.56	0.70
1:D:118:THR:HG22	1:D:119:TYR:HD2	1.54	0.70
1:E:34:ARG:NH1	1:E:129:ASP:HA	2.07	0.70
1:E:3:VAL:HG12	1:E:7:LYS:NZ	2.07	0.69
1:A:115:LYS:O	1:A:118:THR:HB	1.93	0.69
1:D:10:ILE:CG2	1:E:116:LYS:HE2	2.19	0.68
1:C:40:ALA:HA	1:C:43:ARG:NH1	2.09	0.67
1:C:72:ARG:HG3	1:C:72:ARG:HH11	1.59	0.67
1:F:124:PHE:O	1:F:127:LYS:HE3	1.95	0.67
1:E:54:THR:O	1:E:55:LEU:HD23	1.95	0.67
1:H:99:ASP:O	1:H:102:VAL:HG12	1.95	0.67
1:H:3:VAL:CG1	1:H:7:LYS:HE3	2.25	0.66
1:G:87:SER:OG	1:G:92:LYS:HD2	1.96	0.66
1:A:28:PHE:CE2	1:A:46:LEU:HD13	2.30	0.66
1:E:10:ILE:H	1:E:10:ILE:HD13	1.61	0.66
1:F:29:CYS:HG	1:F:45:CYS:HG	1.04	0.66
1:F:74:LYS:O	1:F:85:GLU:HG2	1.95	0.66
1:D:14:GLY:C	1:E:116:LYS:HZ2	2.00	0.65
1:C:130:ILE:CD1	1:C:130:ILE:H	2.10	0.64
1:F:10:ILE:HD13	2:F:502:SVR:H41	1.62	0.64
1:H:27:CYS:CB	1:H:126:CYS:HG	2.11	0.64
1:F:10:ILE:HD11	2:F:502:SVR:N44	2.12	0.63
1:D:14:GLY:HA2	1:E:116:LYS:NZ	2.13	0.63
1:D:72:ARG:NH2	2:H:511:SVR:O86	2.31	0.63
1:H:10:ILE:HD12	1:H:11:GLN:H	1.61	0.63
1:B:132:LYS:O	1:B:133:CYS:HB2	1.98	0.62
1:F:5:LEU:O	1:F:9:ILE:HG12	1.98	0.62
1:C:130:ILE:N	1:C:130:ILE:HD12	2.13	0.62
1:D:12:GLU:OE1	1:D:107:ARG:NH1	2.33	0.62
1:A:46:LEU:HD21	1:A:131:GLU:HG2	1.80	0.62
1:E:116:LYS:HZ3	1:E:117:TYR:HE1	1.44	0.62
1:A:69:LYS:HB3	2:G:506:SVR:H272	1.80	0.62
1:D:7:LYS:O	1:D:11:GLN:HG3	2.00	0.61
1:F:25:TYR:HB3	1:F:29:CYS:SG	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:LYS:O	1:H:10:ILE:HD12	2.00	0.61
1:B:116:LYS:HZ3	1:B:116:LYS:HB2	1.65	0.61
1:E:3:VAL:HB	1:E:72:ARG:NH1	2.14	0.61
1:A:1:SER:HA	1:A:4:GLU:OE1	2.01	0.61
1:A:72:ARG:CG	1:A:72:ARG:HH11	2.14	0.61
1:D:9:ILE:HD12	1:D:106:LEU:HD12	1.83	0.60
1:E:84:CYS:CB	1:E:96:CYS:HG	2.13	0.60
1:G:86:ASN:O	1:G:88:THR:N	2.34	0.60
1:B:7:LYS:O	1:B:10:ILE:HD12	2.01	0.60
1:F:108:LYS:HA	1:F:108:LYS:HE2	1.83	0.60
1:G:5:LEU:HD13	1:G:99:ASP:HB3	1.83	0.60
1:H:116:LYS:NZ	1:H:116:LYS:CB	2.53	0.60
1:F:22:TYR:O	1:F:29:CYS:HB3	2.01	0.60
1:C:72:ARG:CG	1:C:72:ARG:HH11	2.15	0.60
1:D:91:CYS:O	1:D:95:ILE:HG12	2.01	0.60
1:C:69:LYS:HB3	2:C:507:SVR:H272	1.85	0.59
1:D:7:LYS:HD3	1:E:125:TRP:CE2	2.38	0.59
1:G:34:ARG:HG2	1:G:128:GLY:O	2.02	0.59
2:A:508:SVR:O54	1:G:3:VAL:HG22	2.02	0.58
1:B:72:ARG:HH11	1:B:72:ARG:CG	2.15	0.58
1:B:83:ILE:N	1:B:83:ILE:HD12	2.19	0.58
1:C:25:TYR:O	1:C:29:CYS:HB2	2.03	0.58
1:G:84:CYS:CB	1:G:96:CYS:HG	2.16	0.58
1:C:127:LYS:HD2	3:C:520:HOH:O	2.03	0.58
1:D:55:LEU:CD1	1:D:95:ILE:HD13	2.34	0.58
1:F:99:ASP:O	1:F:102:VAL:HG12	2.04	0.58
1:H:102:VAL:O	1:H:106:LEU:HG	2.04	0.58
1:C:70:THR:O	1:C:72:ARG:HD2	2.04	0.57
1:C:23:THR:HG21	2:F:509:SVR:H591	1.87	0.57
1:C:40:ALA:HA	1:C:43:ARG:HH11	1.69	0.57
1:C:118:THR:HG22	1:C:119:TYR:CD2	2.39	0.57
1:D:55:LEU:HD13	1:D:95:ILE:HD13	1.86	0.57
1:E:3:VAL:HB	1:E:72:ARG:HH12	1.70	0.57
1:E:3:VAL:HG12	1:E:7:LYS:HZ3	1.68	0.56
1:C:102:VAL:O	1:C:106:LEU:HG	2.06	0.56
2:C:505:SVR:H44	2:H:504:SVR:C40	2.17	0.56
1:G:115:LYS:O	1:G:118:THR:HB	2.04	0.56
1:B:26:GLY:HA2	1:B:38:LEU:HD12	1.87	0.56
1:C:132:LYS:HA	3:C:539:HOH:O	2.05	0.56
2:C:505:SVR:O54	1:D:3:VAL:HG22	2.06	0.56
1:C:99:ASP:O	1:C:102:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:O	1:E:9:ILE:HG12	2.05	0.56
1:H:7:LYS:HA	1:H:10:ILE:HD11	1.87	0.56
1:F:91:CYS:O	1:F:95:ILE:HD13	2.06	0.56
1:C:118:THR:HG22	1:C:119:TYR:HD2	1.71	0.55
1:E:28:PHE:CE1	1:E:37:PRO:HG3	2.41	0.55
1:D:3:VAL:CG2	1:D:72:ARG:HH22	2.19	0.55
1:G:7:LYS:NZ	1:H:125:TRP:NE1	2.53	0.55
1:D:14:GLY:O	1:E:116:LYS:HG2	2.07	0.55
1:D:84:CYS:HG	1:D:96:CYS:HG	0.56	0.55
1:E:22:TYR:O	1:E:29:CYS:HB3	2.07	0.55
1:E:26:GLY:HA2	1:E:38:LEU:HD12	1.89	0.55
1:B:7:LYS:HA	1:B:10:ILE:CD1	2.35	0.55
1:B:116:LYS:HE2	1:C:10:ILE:CG2	2.28	0.55
1:B:75:TYR:O	1:B:76:LYS:HD3	2.06	0.55
1:G:51:CYS:CB	1:G:98:CYS:HG	2.20	0.54
1:C:34:ARG:NH1	1:C:129:ASP:HA	2.21	0.54
1:D:14:GLY:HA2	1:E:116:LYS:HZ2	1.72	0.54
1:H:91:CYS:O	1:H:95:ILE:HG13	2.06	0.54
1:B:116:LYS:HZ2	1:B:116:LYS:HB2	1.71	0.54
1:A:23:THR:HG21	2:B:512:SVR:H591	1.90	0.54
2:C:507:SVR:O4	1:D:124:PHE:CD2	2.61	0.54
1:G:34:ARG:HH11	1:G:34:ARG:HG2	1.72	0.54
2:C:507:SVR:O4	1:D:124:PHE:CE2	2.61	0.54
1:B:48:HIS:HE1	1:B:99:ASP:OD1	1.91	0.54
2:C:505:SVR:O45	1:D:2:VAL:HG13	2.07	0.54
1:G:121:PRO:HD2	1:G:125:TRP:CE3	2.43	0.54
1:G:46:LEU:CD2	1:G:131:GLU:HG2	2.37	0.53
1:G:72:ARG:HG3	1:G:72:ARG:HH11	1.72	0.53
1:D:14:GLY:CA	1:E:116:LYS:HZ2	2.20	0.53
1:C:44:CYS:HG	1:C:105:CYS:HG	0.54	0.53
1:E:27:CYS:CB	1:E:126:CYS:HG	2.20	0.53
1:G:82:ILE:O	1:G:83:ILE:HD13	2.09	0.53
1:A:124:PHE:CD2	2:A:508:SVR:O4	2.62	0.53
1:A:50:CYS:CB	1:A:133:CYS:HG	2.21	0.53
1:E:121:PRO:HD3	1:H:19:PHE:CE2	2.44	0.53
1:C:26:GLY:O	1:C:120:TYR:CE1	2.62	0.52
1:D:5:LEU:O	1:D:9:ILE:HG12	2.10	0.52
1:B:46:LEU:HD11	1:B:131:GLU:HG2	1.91	0.52
1:C:1:SER:HB2	1:C:71:ASP:O	2.10	0.52
1:B:84:CYS:CB	1:B:96:CYS:HG	2.19	0.52
1:F:75:TYR:C	1:F:76:LYS:HD3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:LYS:HE2	2:H:511:SVR:C72	2.39	0.52
1:H:81:GLU:O	1:H:83:ILE:HG13	2.09	0.52
1:G:27:CYS:HG	1:G:126:CYS:HG	0.55	0.52
1:H:3:VAL:HG13	1:H:7:LYS:HE3	1.91	0.52
1:D:10:ILE:O	1:E:116:LYS:NZ	2.38	0.52
1:E:130:ILE:N	1:E:130:ILE:HD12	2.24	0.52
1:B:119:TYR:CZ	1:F:119:TYR:CE1	2.98	0.52
1:C:115:LYS:O	1:C:118:THR:HB	2.10	0.51
1:G:22:TYR:CE2	1:G:106:LEU:HD22	2.44	0.51
1:H:114:ASN:OD1	1:H:116:LYS:HE3	2.10	0.51
1:B:82:ILE:N	1:B:82:ILE:HD12	2.25	0.51
1:D:87:SER:OG	1:D:92:LYS:HD2	2.10	0.51
1:C:52:TYR:CE2	1:C:68:PRO:HB2	2.45	0.51
1:E:130:ILE:H	1:E:130:ILE:CD1	2.21	0.51
1:E:91:CYS:O	1:E:95:ILE:HG13	2.10	0.51
1:D:121:PRO:HG3	2:F:509:SVR:H593	1.92	0.51
1:D:72:ARG:NH2	3:D:134:HOH:O	2.43	0.51
1:H:94:ARG:HG3	1:H:94:ARG:HH11	1.76	0.51
1:A:99:ASP:O	1:A:102:VAL:HG12	2.11	0.51
1:E:68:PRO:HA	1:E:95:ILE:HD13	1.92	0.51
2:C:505:SVR:H62	2:H:504:SVR:O78	2.10	0.51
1:E:55:LEU:N	1:E:56:PRO:CD	2.74	0.51
1:B:122:ASN:HB3	2:F:502:SVR:O81	2.11	0.51
1:G:120:TYR:HB2	1:G:125:TRP:CE3	2.46	0.51
1:D:14:GLY:CA	1:E:116:LYS:NZ	2.74	0.50
1:G:91:CYS:O	1:G:95:ILE:HG12	2.11	0.50
1:D:23:THR:HG21	2:H:511:SVR:H591	1.92	0.50
1:H:89:SER:OG	1:H:94:ARG:NH1	2.42	0.50
1:B:12:GLU:OE2	1:B:82:ILE:HD11	2.11	0.50
1:F:1:SER:HB2	1:F:71:ASP:O	2.11	0.50
1:G:8:MET:HG2	1:G:82:ILE:HD13	1.92	0.50
1:C:52:TYR:CZ	1:C:68:PRO:HB2	2.46	0.50
1:D:102:VAL:O	1:D:106:LEU:HG	2.11	0.50
1:A:44:CYS:CB	1:A:105:CYS:HG	2.24	0.50
1:A:54:THR:O	1:A:55:LEU:HD23	2.11	0.50
2:C:505:SVR:C48	1:D:6:GLY:HA3	2.42	0.50
1:E:22:TYR:CE2	1:E:106:LEU:HD22	2.47	0.50
1:E:88:THR:OG1	1:E:92:LYS:HG3	2.11	0.49
1:G:1:SER:HA	1:G:4:GLU:OE1	2.12	0.49
1:B:72:ARG:NH1	1:B:72:ARG:HB3	2.21	0.49
1:D:14:GLY:C	1:E:116:LYS:NZ	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:PHE:CE1	1:H:37:PRO:HG3	2.47	0.49
1:A:1:SER:O	1:A:4:GLU:N	2.46	0.49
1:C:27:CYS:CB	1:C:126:CYS:HG	2.20	0.49
1:H:10:ILE:HD12	1:H:11:GLN:N	2.27	0.49
1:H:3:VAL:HG12	1:H:7:LYS:HE3	1.95	0.49
1:B:78:GLU:HB3	1:B:83:ILE:HD11	1.95	0.49
1:E:81:GLU:HG2	1:E:82:ILE:H	1.76	0.49
1:B:102:VAL:O	1:B:106:LEU:HG	2.13	0.49
2:E:510:SVR:S17	2:E:510:SVR:N1	2.86	0.49
1:A:120:TYR:CE2	1:A:126:CYS:SG	3.06	0.49
1:H:1:SER:HB3	3:H:533:HOH:O	2.13	0.49
2:H:504:SVR:S73	2:H:504:SVR:N63	2.86	0.49
1:E:18:PRO:HG2	3:E:513:HOH:O	2.13	0.49
1:B:40:ALA:HA	1:B:43:ARG:HH11	1.78	0.48
2:C:505:SVR:S73	2:C:505:SVR:N63	2.86	0.48
1:D:44:CYS:HG	1:D:105:CYS:CB	2.23	0.48
1:G:100:LYS:O	1:G:104:VAL:HG23	2.12	0.48
1:B:77:ARG:HG3	2:G:506:SVR:O34	2.14	0.48
1:F:94:ARG:HG3	1:F:94:ARG:HH11	1.77	0.48
1:E:8:MET:HG2	1:E:82:ILE:HD13	1.95	0.48
1:G:26:GLY:HA2	1:G:38:LEU:HD12	1.95	0.48
1:G:86:ASN:O	1:G:87:SER:C	2.51	0.48
1:B:89:SER:HB3	3:B:557:HOH:O	2.12	0.48
1:C:10:ILE:HA	1:C:16:LYS:O	2.14	0.48
1:E:44:CYS:HG	1:E:105:CYS:HG	0.56	0.48
1:C:6:GLY:HA3	2:C:507:SVR:C48	2.43	0.48
1:B:20:PRO:HB2	1:B:119:TYR:HE2	1.78	0.48
2:C:505:SVR:H41	2:H:504:SVR:C40	2.26	0.48
1:C:1:SER:HB3	1:C:68:PRO:O	2.13	0.48
2:C:507:SVR:H37	2:F:509:SVR:O77	2.13	0.48
1:F:9:ILE:HD12	1:F:106:LEU:HD12	1.96	0.48
1:B:46:LEU:CD1	1:B:131:GLU:HG2	2.44	0.48
1:D:99:ASP:O	1:D:102:VAL:HG12	2.14	0.47
1:F:24:SER:HB3	3:F:514:HOH:O	2.14	0.47
1:G:40:ALA:HA	1:G:43:ARG:NH1	2.28	0.47
1:A:59:ASP:CG	1:A:94:ARG:HH22	2.17	0.47
2:B:501:SVR:N63	2:B:501:SVR:S73	2.87	0.47
1:E:81:GLU:HG2	1:E:82:ILE:N	2.29	0.47
1:E:3:VAL:HG12	1:E:7:LYS:HZ2	1.77	0.47
1:C:12:GLU:OE1	1:C:107:ARG:NH1	2.47	0.47
1:H:10:ILE:HG23	1:H:17:SER:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:VAL:HG13	1:G:103:ALA:N	2.30	0.47
1:B:132:LYS:O	1:B:133:CYS:CB	2.62	0.47
1:E:28:PHE:CZ	1:E:131:GLU:HG3	2.50	0.47
1:D:50:CYS:CB	1:D:133:CYS:HG	2.26	0.47
1:B:18:PRO:HD2	3:B:522:HOH:O	2.15	0.47
1:E:55:LEU:HD13	1:E:95:ILE:HG12	1.97	0.46
1:F:50:CYS:CB	1:F:133:CYS:HG	2.28	0.46
1:G:92:LYS:O	1:G:96:CYS:HB2	2.15	0.46
2:A:508:SVR:H48	1:G:18:PRO:HG2	1.97	0.46
2:C:507:SVR:N63	2:C:507:SVR:S73	2.89	0.46
1:G:68:PRO:CB	1:G:95:ILE:HD12	2.41	0.46
1:E:28:PHE:CE2	1:E:131:GLU:HG3	2.50	0.46
1:E:18:PRO:O	1:E:23:THR:HG23	2.16	0.46
1:C:3:VAL:HG22	2:C:507:SVR:O54	2.16	0.46
1:F:3:VAL:O	1:F:7:LYS:HG3	2.15	0.46
1:H:22:TYR:O	1:H:29:CYS:HB3	2.16	0.46
1:A:121:PRO:O	1:A:125:TRP:HB2	2.15	0.46
1:E:25:TYR:HB3	1:E:29:CYS:SG	2.55	0.46
1:D:89:SER:O	1:D:94:ARG:HG3	2.16	0.46
1:F:55:LEU:HD13	1:F:95:ILE:HD12	1.98	0.46
1:D:40:ALA:HA	1:D:43:ARG:HH12	1.76	0.45
1:H:61:CYS:HB3	1:H:91:CYS:SG	2.56	0.45
1:H:25:TYR:O	1:H:29:CYS:HB2	2.16	0.45
1:A:9:ILE:CD1	1:A:106:LEU:HD12	2.44	0.45
2:E:503:SVR:S73	2:E:503:SVR:N63	2.90	0.45
1:A:124:PHE:HD1	1:G:30:GLY:O	1.99	0.45
1:G:14:GLY:O	1:H:116:LYS:CE	2.61	0.45
1:A:19:PHE:HA	1:A:20:PRO:HA	1.75	0.45
1:E:19:PHE:CZ	1:H:121:PRO:HG3	2.52	0.45
1:C:37:PRO:HG2	3:C:537:HOH:O	2.16	0.45
1:H:46:LEU:HD11	1:H:131:GLU:HG2	1.98	0.45
1:H:61:CYS:CB	1:H:91:CYS:HG	2.27	0.45
1:E:34:ARG:O	1:E:126:CYS:HB3	2.17	0.45
2:C:505:SVR:H44	2:H:504:SVR:C42	2.30	0.45
1:B:114:ASN:OD1	1:B:116:LYS:HG2	2.17	0.45
1:G:3:VAL:HB	1:G:72:ARG:NH1	2.28	0.45
1:C:72:ARG:CG	1:C:72:ARG:NH1	2.78	0.44
1:E:121:PRO:HG2	1:E:125:TRP:CD2	2.52	0.44
1:A:72:ARG:CZ	1:A:72:ARG:HB3	2.47	0.44
1:B:61:CYS:HG	1:B:91:CYS:CB	2.25	0.44
1:C:55:LEU:HD11	1:C:98:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:ARG:HB3	1:H:72:ARG:HH11	1.82	0.44
1:G:17:SER:O	1:G:18:PRO:C	2.55	0.44
2:C:505:SVR:O45	1:D:2:VAL:O	2.35	0.44
1:E:10:ILE:HG23	1:E:17:SER:HA	1.99	0.44
2:B:512:SVR:N1	2:B:512:SVR:S17	2.91	0.44
1:G:102:VAL:CG1	1:G:103:ALA:N	2.80	0.44
1:G:115:LYS:O	1:G:115:LYS:HG3	2.18	0.44
1:C:121:PRO:HG3	2:H:511:SVR:H593	2.00	0.44
1:B:72:ARG:NH1	1:B:72:ARG:CG	2.80	0.44
1:D:84:CYS:CB	1:D:96:CYS:SG	3.05	0.44
2:F:509:SVR:H48	2:F:509:SVR:O45	2.17	0.44
1:G:72:ARG:HG3	1:G:72:ARG:NH1	2.33	0.44
1:A:72:ARG:CG	1:A:72:ARG:NH1	2.76	0.44
1:B:40:ALA:HA	1:B:43:ARG:NH1	2.33	0.44
1:G:34:ARG:HG3	1:G:130:ILE:HD13	1.99	0.44
1:G:28:PHE:CE2	1:G:46:LEU:HD13	2.52	0.44
2:A:508:SVR:H272	1:G:69:LYS:HB3	1.98	0.44
1:H:29:CYS:CB	1:H:45:CYS:HG	2.28	0.44
1:D:88:THR:OG1	1:D:92:LYS:HG3	2.18	0.44
2:G:506:SVR:N63	2:G:506:SVR:S73	2.91	0.44
1:A:17:SER:O	1:A:21:SER:HB2	2.18	0.44
1:D:94:ARG:HG3	1:D:94:ARG:HH11	1.82	0.44
1:G:55:LEU:N	1:G:56:PRO:CD	2.81	0.44
1:A:5:LEU:O	1:A:9:ILE:HG12	2.18	0.43
1:B:99:ASP:O	1:B:102:VAL:HG12	2.17	0.43
1:C:17:SER:O	1:C:18:PRO:C	2.57	0.43
2:F:502:SVR:S73	2:F:502:SVR:N63	2.90	0.43
1:H:51:CYS:CB	1:H:98:CYS:HG	2.24	0.43
1:E:17:SER:HA	1:E:18:PRO:HD2	1.87	0.43
1:E:18:PRO:CG	2:E:503:SVR:H47	2.45	0.43
1:F:102:VAL:O	1:F:106:LEU:HG	2.18	0.43
1:G:107:ARG:NE	3:G:516:HOH:O	2.47	0.43
1:H:50:CYS:CB	1:H:133:CYS:HG	2.31	0.43
1:B:121:PRO:HG3	1:F:19:PHE:CZ	2.53	0.43
1:D:9:ILE:HD12	1:D:106:LEU:CD1	2.47	0.43
1:H:102:VAL:HA	3:H:544:HOH:O	2.17	0.43
2:C:505:SVR:H41	2:H:504:SVR:H40	1.83	0.43
2:A:508:SVR:N63	2:A:508:SVR:S73	2.92	0.43
1:A:1:SER:CB	1:A:73:TYR:HE2	2.28	0.43
1:C:72:ARG:HB3	1:C:72:ARG:NH1	2.34	0.43
1:E:3:VAL:CG1	1:E:7:LYS:NZ	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:LEU:HD13	1:G:95:ILE:CD1	2.30	0.43
1:A:101:ALA:O	1:A:105:CYS:HB2	2.18	0.43
1:C:16:LYS:HE2	1:C:110:LEU:CD2	2.49	0.43
1:D:19:PHE:HA	1:D:20:PRO:HA	1.85	0.43
1:G:26:GLY:HA2	1:G:38:LEU:CD1	2.49	0.43
1:G:3:VAL:CB	1:G:72:ARG:HH12	2.28	0.43
2:C:505:SVR:H272	1:D:69:LYS:HB3	2.00	0.42
2:E:503:SVR:S17	2:E:503:SVR:N1	2.93	0.42
2:C:507:SVR:H44	2:F:502:SVR:C40	2.32	0.42
1:H:55:LEU:C	1:H:59:ASP:N	2.71	0.42
1:C:18:PRO:CG	2:C:507:SVR:H48	2.49	0.42
1:G:17:SER:O	1:G:21:SER:HB2	2.19	0.42
1:H:48:HIS:HE1	1:H:99:ASP:OD1	2.02	0.42
1:G:3:VAL:HG12	1:G:7:LYS:HE2	2.01	0.42
2:B:501:SVR:S17	2:B:501:SVR:N1	2.93	0.42
1:B:81:GLU:O	1:B:83:ILE:HD12	2.20	0.42
1:F:40:ALA:HA	1:F:43:ARG:NH1	2.35	0.42
1:F:18:PRO:CG	2:F:502:SVR:H47	2.45	0.42
1:A:120:TYR:HB2	1:A:125:TRP:CE3	2.55	0.42
2:F:509:SVR:N1	2:F:509:SVR:S17	2.93	0.42
1:G:95:ILE:O	1:G:98:CYS:HB2	2.20	0.42
1:H:61:CYS:CB	1:H:91:CYS:SG	3.08	0.42
1:H:94:ARG:NH1	1:H:94:ARG:HG3	2.35	0.42
1:E:82:ILE:HB	1:E:100:LYS:HG3	2.01	0.41
1:A:84:CYS:CB	1:A:96:CYS:SG	3.08	0.41
1:C:133:CYS:N	3:C:539:HOH:O	2.48	0.41
1:D:86:ASN:ND2	1:D:86:ASN:O	2.52	0.41
1:B:18:PRO:O	1:B:23:THR:HG23	2.20	0.41
1:C:91:CYS:O	1:C:95:ILE:HD13	2.19	0.41
1:B:39:ASP:HB2	3:B:558:HOH:O	2.19	0.41
1:G:25:TYR:O	1:G:29:CYS:HB2	2.20	0.41
1:H:5:LEU:HD23	2:H:504:SVR:H591	2.02	0.41
1:B:1:SER:HA	1:B:4:GLU:OE1	2.21	0.41
1:C:40:ALA:CA	1:C:43:ARG:NH1	2.82	0.41
1:F:81:GLU:HG2	1:F:82:ILE:N	2.36	0.41
1:G:87:SER:HG	1:G:92:LYS:HD2	1.82	0.41
1:E:115:LYS:HB2	3:E:516:HOH:O	2.20	0.41
2:E:510:SVR:H591	1:G:23:THR:HG21	2.02	0.41
1:E:59:ASP:CG	1:E:94:ARG:HH22	2.23	0.41
1:G:34:ARG:HH11	1:G:34:ARG:CG	2.33	0.41
1:C:61:CYS:HB3	1:C:95:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:TYR:CE1	1:C:96:CYS:SG	3.13	0.41
1:E:3:VAL:CB	1:E:72:ARG:HH12	2.34	0.41
2:H:504:SVR:S17	2:H:504:SVR:N1	2.93	0.41
1:H:51:CYS:CB	1:H:98:CYS:SG	3.09	0.41
1:A:86:ASN:O	1:A:87:SER:C	2.57	0.41
1:F:10:ILE:HG12	1:F:18:PRO:HD2	2.02	0.41
1:F:17:SER:HA	1:F:18:PRO:HD2	1.88	0.41
1:C:16:LYS:HE2	1:C:110:LEU:HD22	2.03	0.41
1:D:54:THR:O	1:D:55:LEU:HD23	2.20	0.41
1:F:10:ILE:HG13	1:F:10:ILE:H	1.43	0.41
2:A:508:SVR:H37	2:E:510:SVR:O77	2.21	0.41
1:C:4:GLU:HG2	1:C:73:TYR:O	2.20	0.40
2:C:505:SVR:H48	1:D:18:PRO:HG2	2.03	0.40
2:C:505:SVR:H37	2:H:511:SVR:O77	2.20	0.40
1:D:100:LYS:O	1:D:104:VAL:HG23	2.21	0.40
1:E:55:LEU:C	1:E:59:ASP:H	2.21	0.40
1:F:116:LYS:HD3	1:F:116:LYS:HA	1.97	0.40
1:F:68:PRO:HB3	1:F:95:ILE:HG13	2.03	0.40
1:F:73:TYR:CE1	1:F:96:CYS:SG	3.14	0.40
1:F:95:ILE:O	1:F:98:CYS:HB2	2.20	0.40
1:G:98:CYS:O	1:G:101:ALA:HB3	2.21	0.40
1:B:121:PRO:HG3	1:F:19:PHE:CE2	2.56	0.40
1:C:87:SER:OG	1:C:92:LYS:HD2	2.22	0.40
1:D:16:LYS:HE2	1:D:110:LEU:CD2	2.52	0.40
1:F:128:GLY:HA3	3:F:539:HOH:O	2.22	0.40
1:D:9:ILE:CD1	1:D:106:LEU:HD12	2.51	0.40
1:E:116:LYS:O	1:E:116:LYS:HD2	2.22	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	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	B	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	C	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	D	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	E	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
1	F	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	G	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	9	8
1	H	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	23
All	All	960/976 (98%)	901 (94%)	56 (6%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	87	SER
1	G	78	GLU
1	H	128	GLY

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	109/109 (100%)	107 (98%)	2 (2%)	59	75
1	B	109/109 (100%)	104 (95%)	5 (5%)	27	38
1	C	109/109 (100%)	105 (96%)	4 (4%)	34	48
1	D	109/109 (100%)	102 (94%)	7 (6%)	17	23
1	E	109/109 (100%)	106 (97%)	3 (3%)	43	60
1	F	109/109 (100%)	104 (95%)	5 (5%)	27	38
1	G	109/109 (100%)	104 (95%)	5 (5%)	27	38
1	H	109/109 (100%)	101 (93%)	8 (7%)	14	18
All	All	872/872 (100%)	833 (96%)	39 (4%)	27	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	72	ARG
1	B	10	ILE
1	B	20	PRO
1	B	71	ASP
1	B	72	ARG
1	B	116	LYS
1	C	2	VAL
1	C	72	ARG
1	C	118	THR
1	C	131	GLU
1	D	1	SER
1	D	2	VAL
1	D	23	THR
1	D	72	ARG
1	D	85	GLU
1	D	86	ASN
1	D	118	THR
1	E	10	ILE
1	E	79	ASN
1	E	116	LYS
1	F	2	VAL
1	F	10	ILE
1	F	20	PRO
1	F	85	GLU
1	F	108	LYS
1	G	2	VAL
1	G	20	PRO
1	G	72	ARG
1	G	79	ASN
1	G	118	THR
1	H	10	ILE
1	H	20	PRO
1	H	51	CYS
1	H	61	CYS
1	H	72	ARG
1	H	116	LYS
1	H	119	TYR
1	H	132	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	B	48	HIS
1	C	48	HIS
1	D	48	HIS
1	D	79	ASN
1	D	86	ASN
1	E	79	ASN
1	F	79	ASN
1	F	122	ASN
1	G	48	HIS
1	G	86	ASN
1	H	48	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	SVR	G	506	-	89,93,93	1.94	23 (25%)	129,145,145	1.13	10 (7%)
2	SVR	C	507	-	89,93,93	2.05	28 (31%)	129,145,145	1.27	10 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SVR	E	510	-	89,93,93	1.91	24 (26%)	129,145,145	1.07	8 (6%)
2	SVR	H	504	-	89,93,93	1.92	25 (28%)	129,145,145	1.06	8 (6%)
2	SVR	E	503	-	89,93,93	1.97	28 (31%)	129,145,145	1.02	6 (4%)
2	SVR	F	509	-	89,93,93	1.92	24 (26%)	129,145,145	1.18	7 (5%)
2	SVR	H	511	-	89,93,93	1.92	22 (24%)	129,145,145	1.13	7 (5%)
2	SVR	B	501	-	89,93,93	1.95	25 (28%)	129,145,145	0.99	7 (5%)
2	SVR	F	502	-	89,93,93	1.95	25 (28%)	129,145,145	1.06	8 (6%)
2	SVR	B	512	-	89,93,93	1.96	26 (29%)	129,145,145	1.12	7 (5%)
2	SVR	A	508	-	89,93,93	2.04	27 (30%)	129,145,145	1.32	12 (9%)
2	SVR	C	505	-	89,93,93	2.09	29 (32%)	129,145,145	1.19	9 (6%)

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	SVR	G	506	-	-	4/76/76/76	0/8/8/8
2	SVR	C	507	-	-	11/76/76/76	0/8/8/8
2	SVR	E	510	-	-	7/76/76/76	0/8/8/8
2	SVR	H	504	-	-	3/76/76/76	0/8/8/8
2	SVR	E	503	-	-	3/76/76/76	0/8/8/8
2	SVR	F	509	-	-	1/76/76/76	0/8/8/8
2	SVR	H	511	-	-	7/76/76/76	0/8/8/8
2	SVR	B	501	-	-	3/76/76/76	0/8/8/8
2	SVR	F	502	-	-	3/76/76/76	0/8/8/8
2	SVR	B	512	-	-	8/76/76/76	0/8/8/8
2	SVR	A	508	-	-	7/76/76/76	0/8/8/8
2	SVR	C	505	-	-	8/76/76/76	0/8/8/8

All (306) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	502	SVR	O32-C26	7.04	1.37	1.23
2	H	504	SVR	O32-C26	7.00	1.37	1.23
2	B	512	SVR	O32-C26	6.95	1.37	1.23
2	F	509	SVR	O32-C26	6.94	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	511	SVR	O32-C26	6.81	1.37	1.23
2	G	506	SVR	O45-C43	6.67	1.37	1.23
2	E	510	SVR	O32-C26	6.66	1.36	1.23
2	A	508	SVR	O32-C26	6.64	1.36	1.23
2	E	503	SVR	O32-C26	6.63	1.36	1.23
2	B	501	SVR	O32-C26	6.48	1.36	1.23
2	C	507	SVR	O32-C26	6.46	1.36	1.23
2	B	501	SVR	O45-C43	6.36	1.36	1.23
2	G	506	SVR	O32-C26	6.35	1.36	1.23
2	E	503	SVR	O45-C43	6.31	1.36	1.23
2	C	505	SVR	O32-C26	6.11	1.35	1.23
2	F	502	SVR	O45-C43	6.09	1.36	1.23
2	E	510	SVR	O45-C43	6.07	1.36	1.23
2	H	511	SVR	O45-C43	6.07	1.36	1.23
2	F	509	SVR	O45-C43	6.01	1.36	1.23
2	A	508	SVR	O45-C43	6.00	1.36	1.23
2	C	505	SVR	O45-C43	5.97	1.35	1.23
2	C	507	SVR	O45-C43	5.85	1.35	1.23
2	B	512	SVR	O45-C43	5.84	1.35	1.23
2	H	504	SVR	O45-C43	5.73	1.35	1.23
2	C	507	SVR	C3-C6	4.94	1.49	1.42
2	C	505	SVR	C56-C55	4.44	1.46	1.39
2	A	508	SVR	C3-C6	4.20	1.48	1.42
2	A	508	SVR	C11-C6	4.14	1.49	1.43
2	C	507	SVR	C11-C6	4.08	1.49	1.43
2	C	505	SVR	C8-C5	3.90	1.45	1.39
2	C	507	SVR	C37-C33	3.77	1.45	1.39
2	H	504	SVR	C13-N19	-3.71	1.34	1.41
2	A	508	SVR	C37-C33	3.68	1.44	1.39
2	C	505	SVR	C8-C13	3.66	1.45	1.39
2	C	507	SVR	C46-N44	-3.62	1.34	1.41
2	E	510	SVR	C39-N41	-3.56	1.34	1.41
2	F	509	SVR	C37-C39	3.52	1.45	1.39
2	B	512	SVR	C37-C39	3.50	1.45	1.39
2	G	506	SVR	C8-C13	3.49	1.45	1.39
2	B	512	SVR	C56-C55	3.48	1.44	1.39
2	G	506	SVR	C55-N53	-3.47	1.35	1.41
2	H	511	SVR	C56-C55	3.46	1.44	1.39
2	A	508	SVR	C37-C39	3.46	1.45	1.39
2	C	505	SVR	C46-N44	-3.46	1.34	1.41
2	F	502	SVR	C55-N53	-3.46	1.35	1.41
2	E	510	SVR	C37-C39	3.41	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	508	SVR	C55-N53	-3.39	1.35	1.41
2	E	510	SVR	C56-C55	3.39	1.44	1.39
2	B	501	SVR	C55-N53	-3.39	1.35	1.41
2	B	501	SVR	C13-N19	-3.38	1.35	1.41
2	C	507	SVR	C39-N41	-3.38	1.34	1.41
2	C	505	SVR	C70-C71	3.37	1.41	1.37
2	E	503	SVR	C70-C71	3.35	1.41	1.37
2	H	504	SVR	C37-C33	3.33	1.44	1.39
2	C	505	SVR	C5-C2	3.31	1.57	1.50
2	B	512	SVR	C65-C66	3.30	1.47	1.42
2	E	503	SVR	C37-C39	3.29	1.44	1.39
2	C	505	SVR	C39-N41	-3.29	1.35	1.41
2	E	503	SVR	C13-N19	-3.28	1.35	1.41
2	A	508	SVR	C46-N44	-3.23	1.35	1.41
2	C	505	SVR	C58-C61	3.23	1.57	1.50
2	C	505	SVR	C55-N53	-3.23	1.35	1.41
2	H	511	SVR	C37-C39	3.23	1.44	1.39
2	F	509	SVR	C56-C55	3.22	1.44	1.39
2	H	511	SVR	C39-N41	-3.21	1.35	1.41
2	H	504	SVR	C55-N53	-3.21	1.35	1.41
2	E	503	SVR	C55-N53	-3.21	1.35	1.41
2	B	501	SVR	C46-N44	-3.16	1.35	1.41
2	B	512	SVR	C37-C33	3.16	1.44	1.39
2	C	507	SVR	C55-N53	-3.15	1.35	1.41
2	C	507	SVR	C13-N19	-3.14	1.35	1.41
2	F	509	SVR	C13-C20	3.12	1.46	1.40
2	F	502	SVR	C5-C2	3.10	1.56	1.50
2	F	509	SVR	C48-C46	3.09	1.44	1.39
2	E	503	SVR	C37-C33	3.09	1.44	1.39
2	B	501	SVR	C12-C15	3.06	1.41	1.37
2	B	512	SVR	C12-C15	3.05	1.41	1.37
2	F	502	SVR	C12-C15	3.02	1.41	1.37
2	B	512	SVR	C39-N41	-3.02	1.35	1.41
2	F	509	SVR	C37-C33	3.02	1.43	1.39
2	B	501	SVR	C37-C33	3.02	1.43	1.39
2	A	508	SVR	C39-N41	-3.02	1.35	1.41
2	E	503	SVR	C46-N44	-3.00	1.35	1.41
2	B	501	SVR	C70-C71	3.00	1.41	1.37
2	H	504	SVR	C12-C15	2.99	1.41	1.37
2	F	502	SVR	C70-C71	2.98	1.41	1.37
2	F	502	SVR	C37-C39	2.98	1.44	1.39
2	E	503	SVR	C3-C6	2.98	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	505	SVR	C56-C58	2.96	1.43	1.39
2	F	502	SVR	C37-C33	2.95	1.43	1.39
2	H	504	SVR	C3-C6	2.95	1.47	1.42
2	H	504	SVR	C5-C2	2.92	1.56	1.50
2	H	511	SVR	C37-C33	2.91	1.43	1.39
2	G	506	SVR	C8-C5	2.91	1.43	1.39
2	G	506	SVR	C13-N19	-2.90	1.36	1.41
2	C	507	SVR	C37-C39	2.90	1.44	1.39
2	B	512	SVR	C48-C46	2.87	1.44	1.39
2	G	506	SVR	C46-N44	-2.87	1.35	1.41
2	F	502	SVR	C46-N44	-2.85	1.35	1.41
2	C	507	SVR	C56-C55	2.85	1.44	1.39
2	C	505	SVR	C3-C6	2.84	1.46	1.42
2	C	507	SVR	C70-C71	2.83	1.40	1.37
2	H	511	SVR	C48-C46	2.83	1.44	1.39
2	E	503	SVR	C12-C15	2.82	1.40	1.37
2	H	504	SVR	C70-C71	2.81	1.40	1.37
2	C	505	SVR	C72-C76	2.81	1.41	1.36
2	E	510	SVR	C65-C66	2.80	1.46	1.42
2	A	508	SVR	C47-C49	2.80	1.43	1.39
2	A	508	SVR	C13-N19	-2.79	1.36	1.41
2	A	508	SVR	C10-C6	2.79	1.48	1.42
2	G	506	SVR	C74-C69	2.79	1.43	1.38
2	F	509	SVR	C7-C3	2.78	1.44	1.38
2	G	506	SVR	C18-C11	2.77	1.43	1.38
2	F	502	SVR	C13-N19	-2.77	1.36	1.41
2	B	501	SVR	C39-N41	-2.77	1.36	1.41
2	H	511	SVR	C65-C66	2.76	1.46	1.42
2	E	510	SVR	C48-C46	2.75	1.43	1.39
2	E	503	SVR	C56-C55	2.74	1.43	1.39
2	B	512	SVR	C13-C20	2.73	1.46	1.40
2	E	510	SVR	C12-C15	2.72	1.40	1.37
2	H	504	SVR	C37-C39	2.71	1.43	1.39
2	E	503	SVR	C65-C66	2.69	1.46	1.42
2	B	501	SVR	C37-C39	2.69	1.43	1.39
2	A	508	SVR	C5-C2	2.69	1.55	1.50
2	F	509	SVR	C46-N44	-2.68	1.36	1.41
2	H	511	SVR	C13-C20	2.68	1.45	1.40
2	H	511	SVR	C12-C15	2.67	1.40	1.37
2	A	508	SVR	C72-C76	2.67	1.41	1.36
2	B	501	SVR	C72-C76	2.66	1.41	1.36
2	C	507	SVR	C14-C9	2.66	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	512	SVR	C16-C22	2.65	1.41	1.36
2	F	502	SVR	C7-C3	2.65	1.43	1.38
2	B	501	SVR	C7-C3	2.65	1.43	1.38
2	B	501	SVR	C67-C65	2.65	1.43	1.38
2	H	504	SVR	C48-C46	2.64	1.43	1.39
2	G	506	SVR	C70-C71	2.63	1.40	1.37
2	H	511	SVR	C18-C11	2.63	1.43	1.38
2	G	506	SVR	C39-N41	-2.62	1.36	1.41
2	C	507	SVR	C72-C76	2.61	1.41	1.36
2	A	508	SVR	C18-C11	2.61	1.43	1.38
2	G	506	SVR	C7-C3	2.60	1.43	1.38
2	A	508	SVR	C14-C9	2.60	1.43	1.38
2	C	505	SVR	C37-C39	2.59	1.43	1.39
2	F	502	SVR	C14-C9	2.57	1.43	1.38
2	C	505	SVR	C18-C11	2.57	1.42	1.38
2	E	510	SVR	C18-C11	2.56	1.42	1.38
2	H	511	SVR	C55-N53	-2.56	1.36	1.41
2	G	506	SVR	C5-C2	2.56	1.55	1.50
2	C	505	SVR	C37-C33	2.55	1.43	1.39
2	A	508	SVR	C65-N63	-2.55	1.34	1.41
2	C	505	SVR	C33-C26	2.54	1.55	1.50
2	E	503	SVR	C39-N41	-2.54	1.36	1.41
2	F	509	SVR	C11-C6	2.54	1.47	1.43
2	C	507	SVR	C18-C11	2.53	1.42	1.38
2	C	507	SVR	C10-C6	2.53	1.47	1.42
2	G	506	SVR	C48-C46	2.53	1.43	1.39
2	H	504	SVR	C16-C22	2.52	1.41	1.36
2	A	508	SVR	C56-C55	2.51	1.43	1.39
2	H	511	SVR	C7-C3	2.51	1.43	1.38
2	H	504	SVR	C14-C9	2.51	1.43	1.38
2	H	511	SVR	C3-C6	2.51	1.46	1.42
2	F	509	SVR	C39-N41	-2.50	1.36	1.41
2	H	504	SVR	C7-C3	2.50	1.43	1.38
2	E	510	SVR	C7-C3	2.50	1.43	1.38
2	F	502	SVR	C18-C11	2.49	1.42	1.38
2	G	506	SVR	C42-C39	2.49	1.43	1.39
2	B	501	SVR	C14-C9	2.49	1.43	1.38
2	C	505	SVR	C7-C3	2.48	1.43	1.38
2	F	509	SVR	C16-C22	2.48	1.41	1.36
2	E	503	SVR	C72-C76	2.48	1.41	1.36
2	C	505	SVR	C49-C51	2.47	1.55	1.50
2	H	511	SVR	C46-N44	-2.47	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	511	SVR	C13-N19	-2.47	1.37	1.41
2	B	512	SVR	C47-C46	2.47	1.43	1.39
2	C	507	SVR	C58-C61	2.46	1.55	1.50
2	H	504	SVR	C67-C65	2.46	1.43	1.38
2	C	505	SVR	C10-C6	2.46	1.47	1.42
2	E	510	SVR	C16-C22	2.46	1.41	1.36
2	F	502	SVR	C69-C66	2.46	1.47	1.43
2	G	506	SVR	C3-C6	2.46	1.46	1.42
2	E	503	SVR	C7-C3	2.46	1.43	1.38
2	A	508	SVR	C16-C22	2.46	1.41	1.36
2	H	504	SVR	C46-N44	-2.45	1.36	1.41
2	B	512	SVR	C72-C76	2.44	1.41	1.36
2	B	501	SVR	C3-C6	2.44	1.46	1.42
2	C	507	SVR	C65-C66	2.43	1.46	1.42
2	C	505	SVR	C67-C65	2.42	1.43	1.38
2	C	507	SVR	C5-C2	2.42	1.55	1.50
2	F	509	SVR	C12-C15	2.42	1.40	1.37
2	E	510	SVR	C13-C20	2.42	1.45	1.40
2	C	505	SVR	C65-C66	2.42	1.46	1.42
2	E	510	SVR	C13-N19	-2.42	1.37	1.41
2	C	507	SVR	C47-C49	2.41	1.43	1.39
2	C	505	SVR	C47-C49	2.41	1.43	1.39
2	E	503	SVR	C16-C22	2.41	1.41	1.36
2	B	512	SVR	C3-C6	2.39	1.46	1.42
2	B	501	SVR	C56-C55	2.39	1.43	1.39
2	B	501	SVR	C5-C2	2.39	1.55	1.50
2	F	502	SVR	C39-N41	-2.39	1.36	1.41
2	B	501	SVR	C69-C66	2.39	1.47	1.43
2	F	502	SVR	C67-C65	2.38	1.43	1.38
2	E	503	SVR	C67-C65	2.38	1.43	1.38
2	F	502	SVR	C8-C13	2.38	1.43	1.39
2	E	503	SVR	C14-C9	2.37	1.43	1.38
2	H	504	SVR	C69-C66	2.37	1.47	1.43
2	F	509	SVR	C74-C69	2.37	1.42	1.38
2	C	507	SVR	C16-C22	2.36	1.41	1.36
2	H	504	SVR	C8-C13	2.36	1.43	1.39
2	B	512	SVR	C33-C26	2.36	1.55	1.50
2	B	512	SVR	C74-C69	2.35	1.42	1.38
2	H	511	SVR	C11-C6	2.35	1.47	1.43
2	B	512	SVR	C5-C2	2.35	1.55	1.50
2	E	510	SVR	C67-C65	2.35	1.43	1.38
2	B	512	SVR	C7-C3	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	512	SVR	C13-N19	-2.34	1.37	1.41
2	E	510	SVR	C46-N44	-2.34	1.36	1.41
2	E	510	SVR	C58-C61	2.33	1.55	1.50
2	E	503	SVR	C18-C11	2.33	1.42	1.38
2	F	502	SVR	C56-C55	2.33	1.43	1.39
2	F	509	SVR	C13-N19	-2.33	1.37	1.41
2	B	501	SVR	C8-C13	2.32	1.43	1.39
2	E	503	SVR	C5-C2	2.32	1.55	1.50
2	A	508	SVR	C3-N1	-2.31	1.35	1.41
2	B	501	SVR	C56-C58	2.31	1.42	1.39
2	F	502	SVR	C3-C6	2.30	1.46	1.42
2	F	509	SVR	C67-C65	2.30	1.43	1.38
2	H	511	SVR	C58-C61	2.30	1.55	1.50
2	F	509	SVR	C65-C66	2.29	1.46	1.42
2	F	502	SVR	C16-C22	2.29	1.40	1.36
2	B	501	SVR	C65-N63	-2.29	1.35	1.41
2	E	510	SVR	C55-N53	-2.28	1.37	1.41
2	C	505	SVR	C48-C46	2.28	1.43	1.39
2	H	504	SVR	C10-C6	2.28	1.47	1.42
2	F	502	SVR	C62-C58	2.28	1.43	1.39
2	G	506	SVR	C10-C6	2.28	1.47	1.42
2	E	510	SVR	C11-C6	2.28	1.46	1.43
2	G	506	SVR	C65-N63	-2.27	1.35	1.41
2	C	507	SVR	C9-C5	2.26	1.43	1.39
2	C	505	SVR	C12-C15	2.26	1.40	1.37
2	H	504	SVR	C72-C76	2.25	1.40	1.36
2	E	510	SVR	C37-C33	2.24	1.42	1.39
2	B	512	SVR	C18-C11	2.24	1.42	1.38
2	E	510	SVR	C47-C46	2.23	1.43	1.39
2	C	507	SVR	C12-C15	2.23	1.40	1.37
2	F	509	SVR	C58-C61	2.22	1.54	1.50
2	C	507	SVR	C74-C69	2.22	1.42	1.38
2	C	507	SVR	C62-C58	2.22	1.43	1.39
2	C	505	SVR	C52-C49	2.21	1.43	1.39
2	E	510	SVR	C56-C58	2.21	1.42	1.39
2	G	506	SVR	C67-C65	2.20	1.42	1.38
2	H	504	SVR	C65-N63	-2.20	1.35	1.41
2	F	502	SVR	C72-C76	2.19	1.40	1.36
2	H	504	SVR	C18-C11	2.18	1.42	1.38
2	G	506	SVR	C65-C66	2.18	1.46	1.42
2	H	504	SVR	C39-N41	-2.18	1.37	1.41
2	H	511	SVR	C3-N1	-2.17	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	SVR	C10-C6	2.17	1.47	1.42
2	E	503	SVR	C48-C46	2.17	1.42	1.39
2	E	503	SVR	C74-C69	2.17	1.42	1.38
2	H	504	SVR	C56-C55	2.16	1.42	1.39
2	H	504	SVR	C9-C5	2.16	1.43	1.39
2	B	501	SVR	C58-C61	2.15	1.54	1.50
2	B	512	SVR	C46-N44	-2.14	1.37	1.41
2	B	512	SVR	C10-C6	2.14	1.47	1.42
2	F	509	SVR	C62-C58	2.14	1.43	1.39
2	F	509	SVR	C55-N53	-2.14	1.37	1.41
2	E	503	SVR	C62-C58	2.13	1.42	1.39
2	A	508	SVR	C62-C58	2.13	1.42	1.39
2	B	501	SVR	C74-C69	2.12	1.42	1.38
2	A	508	SVR	C65-C66	2.12	1.45	1.42
2	A	508	SVR	C70-C71	2.12	1.39	1.37
2	G	506	SVR	C56-C55	2.12	1.42	1.39
2	C	507	SVR	C67-C65	2.11	1.42	1.38
2	H	511	SVR	C33-C26	2.10	1.54	1.50
2	E	510	SVR	C3-C6	2.09	1.45	1.42
2	H	511	SVR	C70-C71	2.08	1.39	1.37
2	F	509	SVR	C52-C49	2.08	1.42	1.39
2	B	512	SVR	C56-C58	2.08	1.42	1.39
2	C	507	SVR	C65-N63	-2.08	1.35	1.41
2	C	505	SVR	C68-C66	2.08	1.46	1.42
2	E	503	SVR	C10-C6	2.08	1.46	1.42
2	E	503	SVR	C8-C13	2.08	1.42	1.39
2	A	508	SVR	C7-C3	2.07	1.42	1.38
2	A	508	SVR	C12-C15	2.07	1.39	1.37
2	E	503	SVR	C68-C66	2.07	1.46	1.42
2	F	509	SVR	C65-N63	-2.06	1.35	1.41
2	A	508	SVR	C48-C46	2.06	1.42	1.39
2	B	501	SVR	C16-C22	2.06	1.40	1.36
2	F	502	SVR	C65-N63	-2.05	1.36	1.41
2	B	512	SVR	C11-C6	2.05	1.46	1.43
2	E	510	SVR	C33-C26	2.04	1.54	1.50
2	E	503	SVR	C58-C61	2.04	1.54	1.50
2	C	507	SVR	C3-N1	-2.04	1.36	1.41
2	F	509	SVR	C10-C6	2.03	1.46	1.42
2	F	502	SVR	C65-C66	2.03	1.45	1.42
2	F	502	SVR	C9-C5	2.02	1.42	1.39
2	F	509	SVR	C49-C51	2.02	1.54	1.50
2	C	505	SVR	C13-N19	-2.02	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	511	SVR	C16-C22	2.02	1.40	1.36
2	B	512	SVR	C67-C65	2.02	1.42	1.38
2	B	512	SVR	C9-C5	2.01	1.42	1.39
2	A	508	SVR	C67-C65	2.01	1.42	1.38
2	E	510	SVR	C9-C5	2.01	1.42	1.39
2	G	506	SVR	C58-C61	2.01	1.54	1.50
2	E	503	SVR	C69-C66	2.01	1.46	1.43
2	G	506	SVR	C9-C5	2.00	1.42	1.39

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	507	SVR	C6-C3-N1	5.64	128.98	120.58
2	A	508	SVR	C6-C3-N1	5.42	128.65	120.58
2	A	508	SVR	C7-C3-N1	-4.14	111.85	123.29
2	C	507	SVR	C7-C3-N1	-4.12	111.91	123.29
2	G	506	SVR	C6-C3-N1	4.10	126.68	120.58
2	F	509	SVR	C20-C13-N19	4.08	125.17	118.81
2	H	511	SVR	C66-C65-N63	4.08	126.66	120.58
2	C	505	SVR	C65-N63-C61	-4.08	116.55	128.64
2	B	512	SVR	C66-C65-N63	4.04	126.60	120.58
2	F	509	SVR	C66-C65-N63	3.87	126.34	120.58
2	H	504	SVR	N44-C43-N41	3.84	119.19	112.49
2	H	511	SVR	C20-C13-N19	3.71	124.59	118.81
2	B	512	SVR	C20-C13-N19	3.65	124.49	118.81
2	C	505	SVR	C6-C3-N1	3.62	125.98	120.58
2	A	508	SVR	C39-N41-C43	3.51	133.79	126.61
2	A	508	SVR	C13-N19-C26	-3.46	117.44	126.93
2	G	506	SVR	C14-C20-C13	3.29	120.54	117.44
2	A	508	SVR	C3-N1-C2	-3.29	118.89	128.64
2	E	510	SVR	C20-C13-N19	3.23	123.84	118.81
2	C	505	SVR	C60-C57-C55	3.23	120.48	117.44
2	F	509	SVR	C60-C57-C55	3.18	120.44	117.44
2	B	512	SVR	C67-C65-N63	-3.15	114.58	123.29
2	E	510	SVR	C66-C65-N63	3.15	125.27	120.58
2	F	509	SVR	C67-C65-N63	-3.13	114.64	123.29
2	C	505	SVR	C14-C20-C13	3.13	120.39	117.44
2	C	507	SVR	C13-N19-C26	-3.11	118.39	126.93
2	F	502	SVR	C65-N63-C61	-3.11	119.42	128.64
2	E	503	SVR	N44-C43-N41	3.10	117.91	112.49
2	F	502	SVR	N44-C43-N41	3.10	117.90	112.49
2	H	511	SVR	C67-C65-N63	-3.08	114.77	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	506	SVR	C7-C3-N1	-3.02	114.94	123.29
2	E	510	SVR	C60-C57-C55	3.02	120.29	117.44
2	C	507	SVR	C20-C13-N19	3.01	123.50	118.81
2	A	508	SVR	C46-N44-C43	2.91	132.57	126.61
2	B	501	SVR	C60-C57-C55	2.91	120.18	117.44
2	H	511	SVR	C60-C57-C55	2.88	120.15	117.44
2	E	510	SVR	C14-C20-C13	2.87	120.15	117.44
2	E	503	SVR	C65-N63-C61	-2.81	120.31	128.64
2	B	501	SVR	N44-C43-N41	2.79	117.36	112.49
2	B	512	SVR	C60-C57-C55	2.75	120.04	117.44
2	H	504	SVR	C65-N63-C61	-2.74	120.52	128.64
2	C	505	SVR	C7-C3-N1	-2.73	115.74	123.29
2	F	502	SVR	C60-C57-C55	2.70	119.98	117.44
2	E	503	SVR	C60-C57-C55	2.60	119.89	117.44
2	H	504	SVR	C6-C3-N1	2.57	124.41	120.58
2	E	510	SVR	C67-C65-N63	-2.56	116.20	123.29
2	H	504	SVR	C60-C57-C55	2.56	119.85	117.44
2	A	508	SVR	C60-C57-C55	2.56	119.85	117.44
2	G	506	SVR	C57-C55-N53	2.56	122.79	118.81
2	B	501	SVR	C65-N63-C61	-2.53	121.13	128.64
2	E	510	SVR	C13-N19-C26	-2.52	120.01	126.93
2	C	507	SVR	C46-N44-C43	2.51	131.75	126.61
2	A	508	SVR	C20-C13-N19	2.50	122.71	118.81
2	F	509	SVR	C14-C20-C13	2.49	119.78	117.44
2	G	506	SVR	C67-C65-N63	-2.46	116.49	123.29
2	B	512	SVR	C14-C20-C13	2.46	119.75	117.44
2	F	502	SVR	C6-C3-N1	2.44	124.21	120.58
2	C	507	SVR	C60-C57-C55	2.44	119.73	117.44
2	C	505	SVR	C46-N44-C43	2.41	131.54	126.61
2	F	502	SVR	C7-C3-N1	-2.38	116.71	123.29
2	G	506	SVR	C55-N53-C51	-2.38	120.42	126.93
2	E	503	SVR	C14-C20-C13	2.35	119.65	117.44
2	C	507	SVR	C3-N1-C2	-2.33	121.74	128.64
2	E	510	SVR	N44-C43-N41	2.33	116.55	112.49
2	H	504	SVR	C7-C3-N1	-2.32	116.87	123.29
2	C	505	SVR	C13-N19-C26	-2.30	120.62	126.93
2	G	506	SVR	C3-N1-C2	-2.30	121.83	128.64
2	C	505	SVR	C58-C61-N63	2.28	120.95	115.92
2	A	508	SVR	C67-C65-N63	-2.26	117.05	123.29
2	B	512	SVR	N44-C43-N41	2.25	116.42	112.49
2	G	506	SVR	C66-C65-N63	2.25	123.93	120.58
2	H	511	SVR	C14-C20-C13	2.21	119.52	117.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	511	SVR	N44-C43-N41	2.20	116.33	112.49
2	A	508	SVR	C33-C26-N19	2.18	120.71	115.92
2	C	507	SVR	C14-C20-C13	2.17	119.49	117.44
2	A	508	SVR	C14-C20-C13	2.17	119.48	117.44
2	F	502	SVR	C20-C13-N19	2.16	122.18	118.81
2	H	511	SVR	C7-C3-N1	-2.16	117.32	123.29
2	B	501	SVR	C6-C3-N1	2.16	123.79	120.58
2	E	503	SVR	C6-C3-N1	2.15	123.78	120.58
2	H	504	SVR	O45-C43-N44	-2.14	120.00	123.62
2	F	502	SVR	C14-C20-C13	2.14	119.46	117.44
2	G	506	SVR	C58-C61-N63	-2.11	111.28	115.92
2	C	507	SVR	C67-C65-N63	-2.11	117.47	123.29
2	H	504	SVR	C13-N19-C26	-2.09	121.19	126.93
2	C	507	SVR	C58-C61-N63	-2.09	111.32	115.92
2	C	505	SVR	O64-C61-C58	-2.09	117.21	120.94
2	F	502	SVR	C13-N19-C26	-2.08	121.22	126.93
2	F	509	SVR	C39-N41-C43	2.07	130.85	126.61
2	B	512	SVR	C7-C3-N1	-2.06	117.59	123.29
2	F	509	SVR	C8-C13-N19	-2.05	116.48	121.90
2	E	503	SVR	C7-C3-N1	-2.05	117.62	123.29
2	H	504	SVR	C20-C13-N19	2.03	121.98	118.81
2	B	501	SVR	C69-C66-C68	2.03	118.25	116.34
2	G	506	SVR	C60-C57-C55	2.03	119.35	117.44
2	B	501	SVR	C14-C20-C13	2.02	119.34	117.44
2	B	501	SVR	C7-C3-N1	-2.02	117.72	123.29
2	E	510	SVR	C11-C6-C10	2.01	118.23	116.34
2	A	508	SVR	C58-C61-N63	-2.00	111.51	115.92

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	505	SVR	C42-C39-N41-C43
2	C	505	SVR	C37-C39-N41-C43
2	C	505	SVR	C48-C46-N44-C43
2	C	505	SVR	C47-C46-N44-C43
2	H	504	SVR	C48-C46-N44-C43
2	C	507	SVR	C42-C39-N41-C43
2	H	504	SVR	C47-C46-N44-C43
2	C	507	SVR	C37-C39-N41-C43
2	H	511	SVR	C47-C49-C51-O54
2	F	502	SVR	C48-C46-N44-C43

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Mol	Chain	Res	Type	Atoms
2	E	510	SVR	C42-C39-N41-C43
2	C	507	SVR	C47-C46-N44-C43
2	C	507	SVR	C48-C46-N44-C43
2	B	501	SVR	C48-C46-N44-C43
2	B	512	SVR	C47-C49-C51-O54
2	F	502	SVR	C47-C46-N44-C43
2	H	511	SVR	C52-C49-C51-O54
2	H	511	SVR	C47-C49-C51-N53
2	B	512	SVR	C52-C49-C51-O54
2	E	510	SVR	C37-C39-N41-C43
2	E	503	SVR	C48-C46-N44-C43
2	B	501	SVR	C47-C46-N44-C43
2	A	508	SVR	C7-C3-N1-C2
2	B	512	SVR	C47-C49-C51-N53
2	H	511	SVR	C52-C49-C51-N53
2	C	505	SVR	C20-C13-N19-C26
2	C	507	SVR	C7-C3-N1-C2
2	C	507	SVR	C8-C13-N19-C26
2	B	512	SVR	C52-C49-C51-N53
2	E	503	SVR	C47-C46-N44-C43
2	C	507	SVR	C20-C13-N19-C26
2	G	506	SVR	C56-C55-N53-C51
2	H	511	SVR	C42-C39-N41-C43
2	C	505	SVR	C8-C13-N19-C26
2	B	512	SVR	C42-C39-N41-C43
2	F	502	SVR	C67-C65-N63-C61
2	G	506	SVR	C67-C65-N63-C61
2	B	501	SVR	C67-C65-N63-C61
2	C	505	SVR	C67-C65-N63-C61
2	B	512	SVR	C37-C39-N41-C43
2	H	511	SVR	C37-C39-N41-C43
2	A	508	SVR	C56-C58-C61-O64
2	E	510	SVR	C8-C13-N19-C26
2	C	505	SVR	C7-C3-N1-C2
2	E	510	SVR	C47-C49-C51-O54
2	G	506	SVR	C57-C55-N53-C51
2	A	508	SVR	C20-C13-N19-C26
2	C	507	SVR	C56-C58-C61-O64
2	G	506	SVR	C7-C3-N1-C2
2	A	508	SVR	C8-C13-N19-C26
2	E	503	SVR	C67-C65-N63-C61
2	E	510	SVR	C20-C13-N19-C26

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Mol	Chain	Res	Type	Atoms
2	B	512	SVR	C7-C3-N1-C2
2	A	508	SVR	C62-C58-C61-O64
2	E	510	SVR	C52-C49-C51-O54
2	C	507	SVR	C67-C65-N63-C61
2	F	509	SVR	C20-C13-N19-C26
2	H	504	SVR	C67-C65-N63-C61
2	E	510	SVR	C47-C49-C51-N53
2	C	507	SVR	C62-C58-C61-O64
2	A	508	SVR	C56-C58-C61-N63
2	A	508	SVR	C67-C65-N63-C61
2	H	511	SVR	C8-C13-N19-C26
2	B	512	SVR	C20-C13-N19-C26
2	C	507	SVR	C56-C58-C61-N63

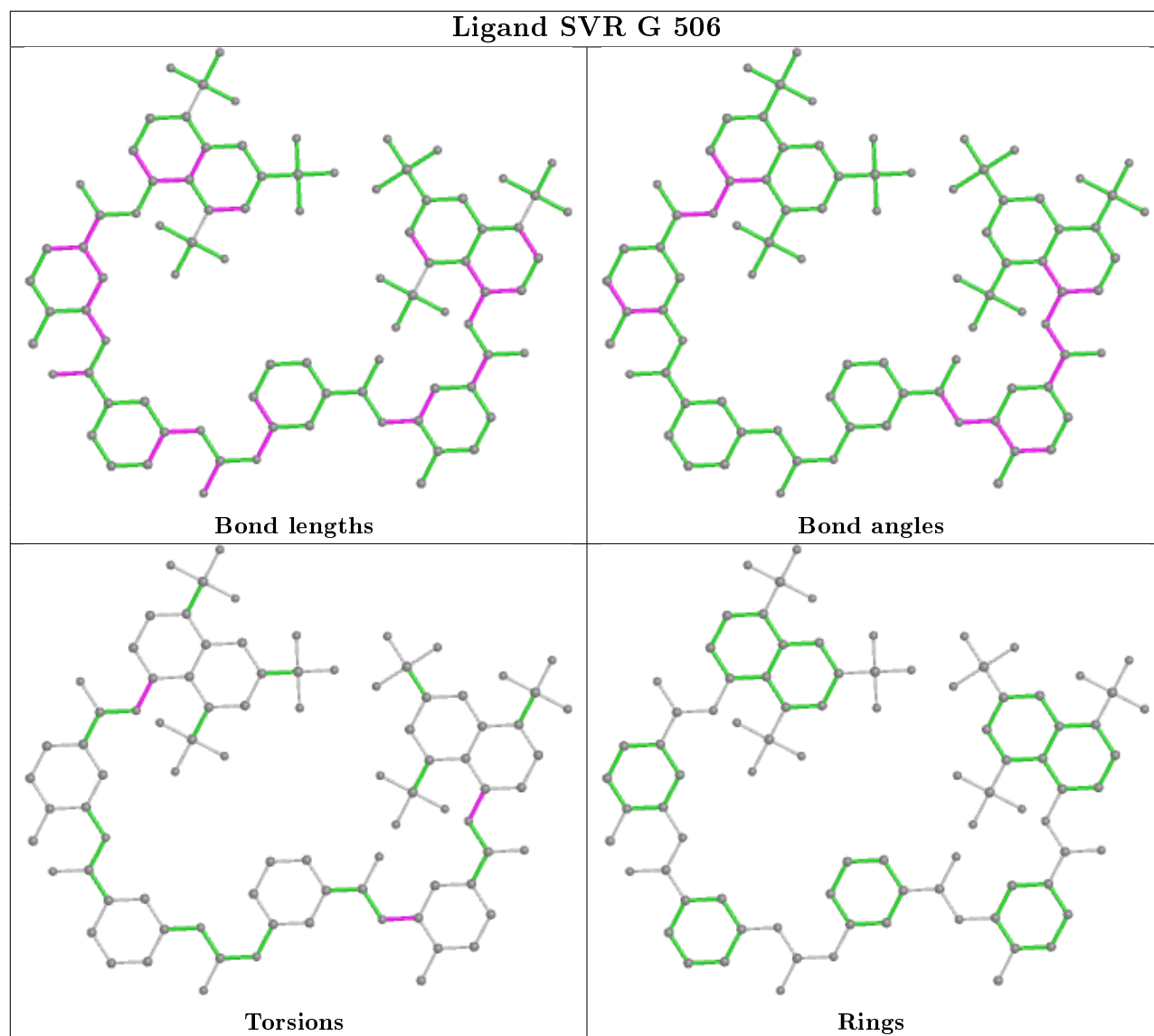
There are no ring outliers.

12 monomers are involved in 61 short contacts:

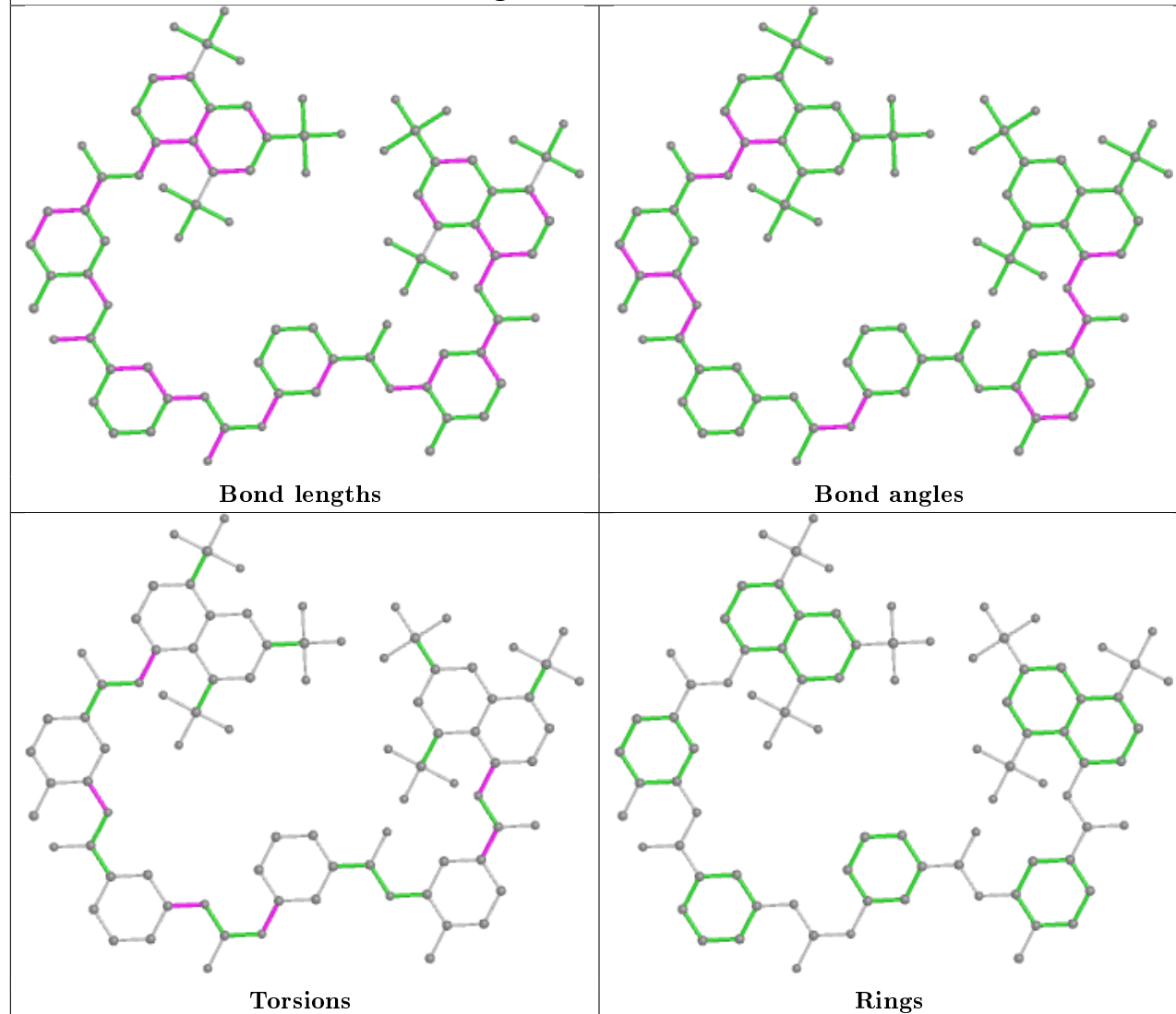
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	506	SVR	3	0
2	C	507	SVR	10	0
2	E	510	SVR	3	0
2	H	504	SVR	8	0
2	E	503	SVR	4	0
2	F	509	SVR	5	0
2	H	511	SVR	5	0
2	B	501	SVR	2	0
2	F	502	SVR	8	0
2	B	512	SVR	2	0
2	A	508	SVR	7	0
2	C	505	SVR	13	0

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

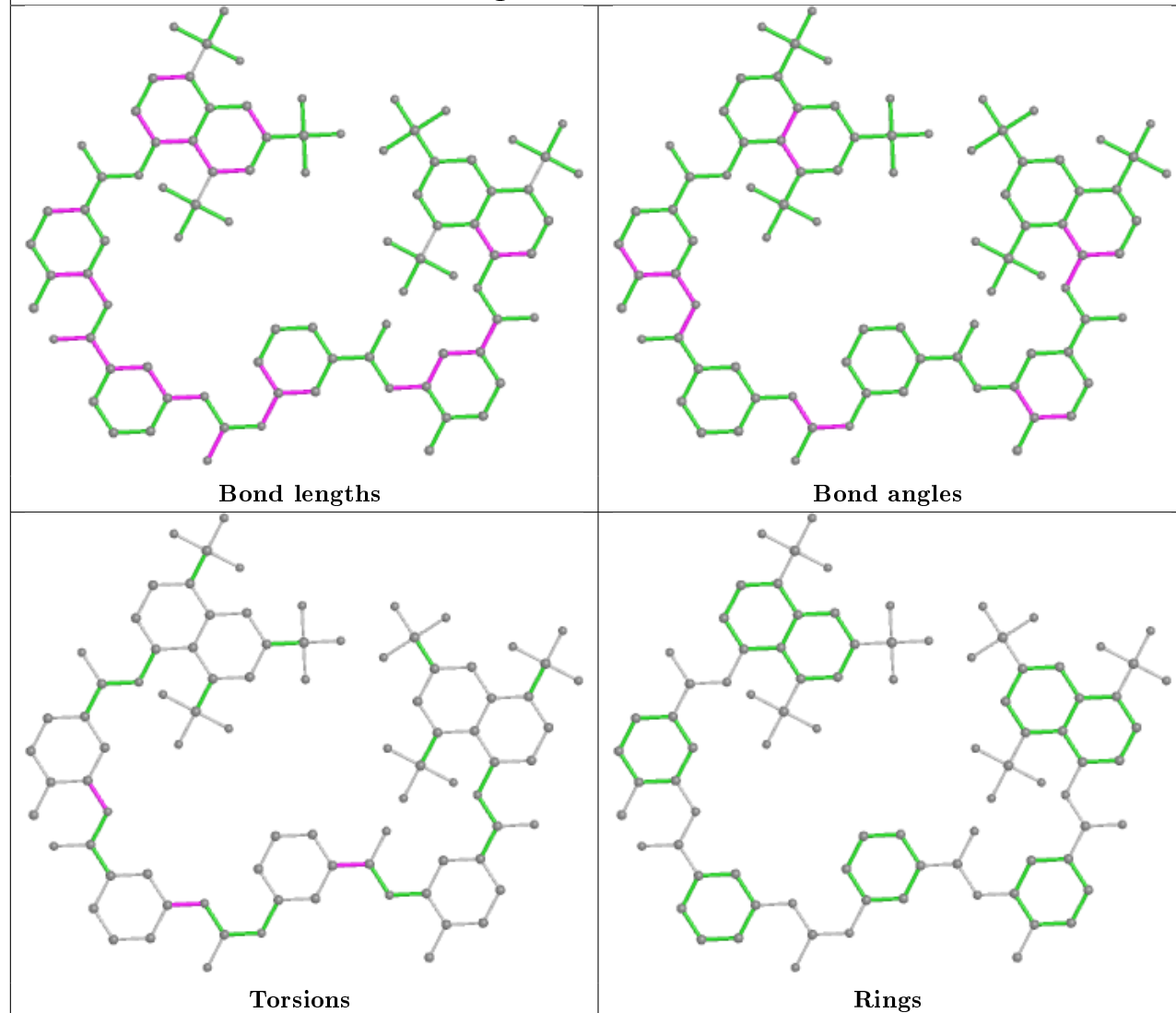
equivalents in the CSD to analyse the geometry.



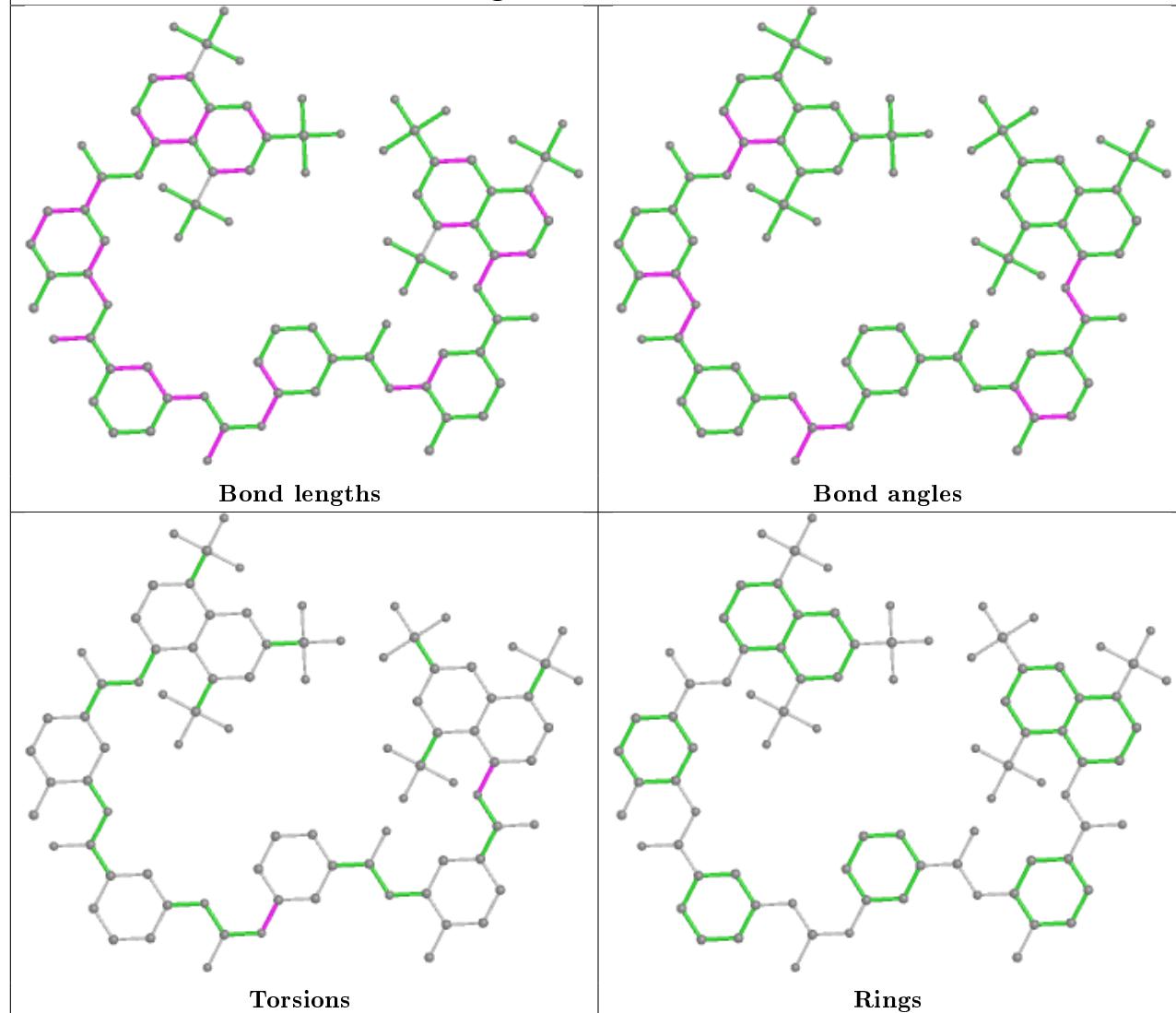
Ligand SVR C 507



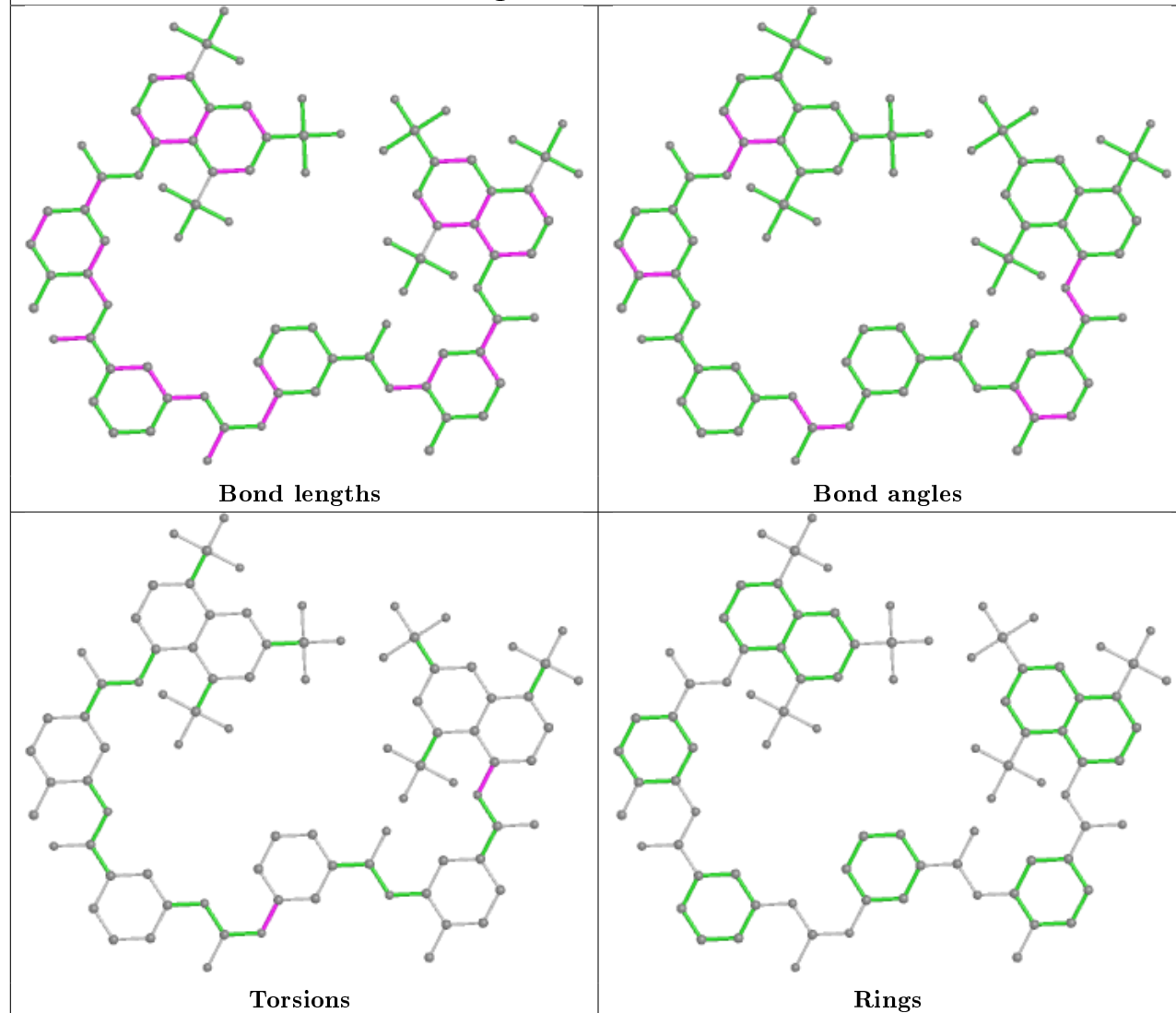
Ligand SVR E 510



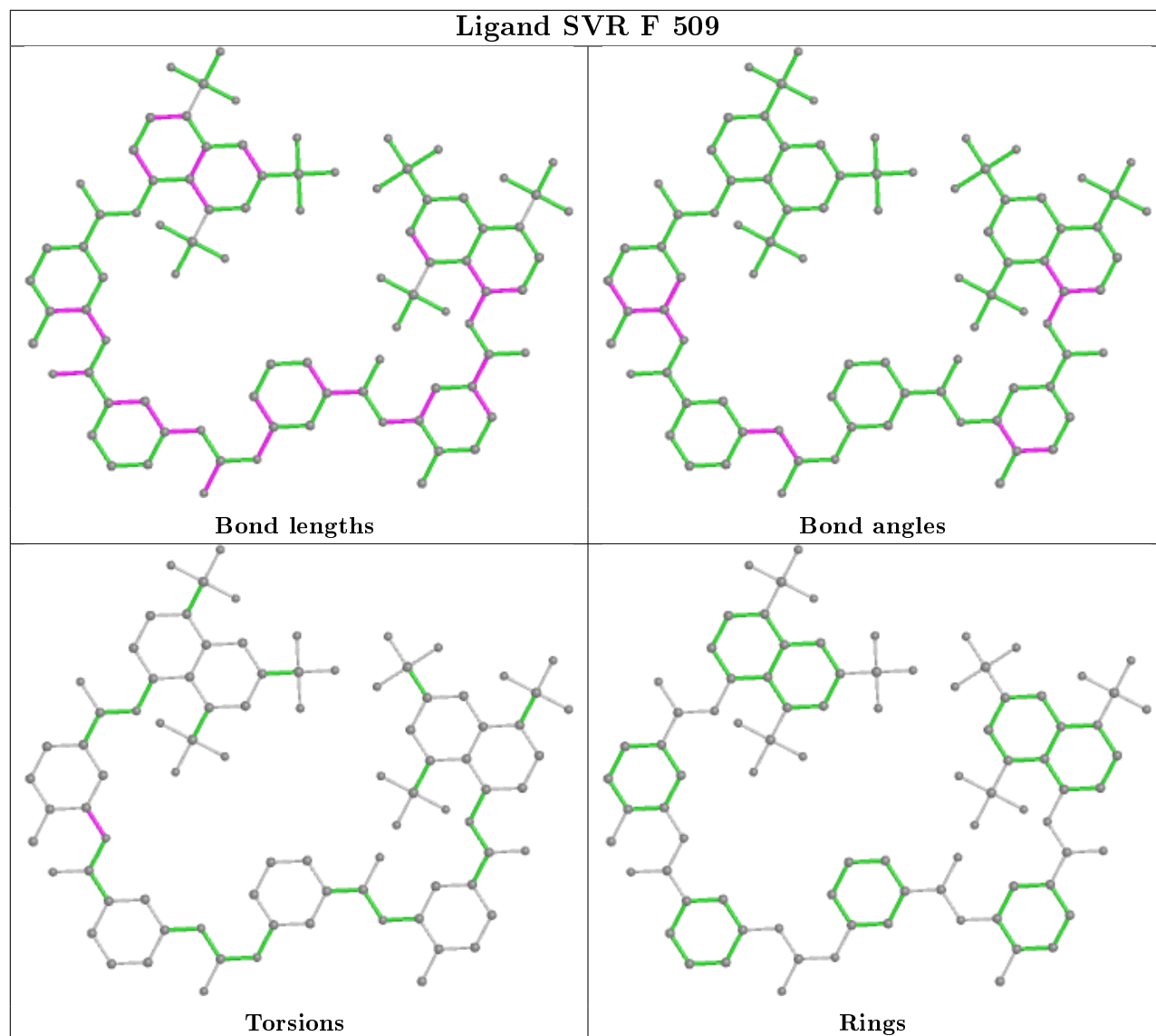
Ligand SVR H 504



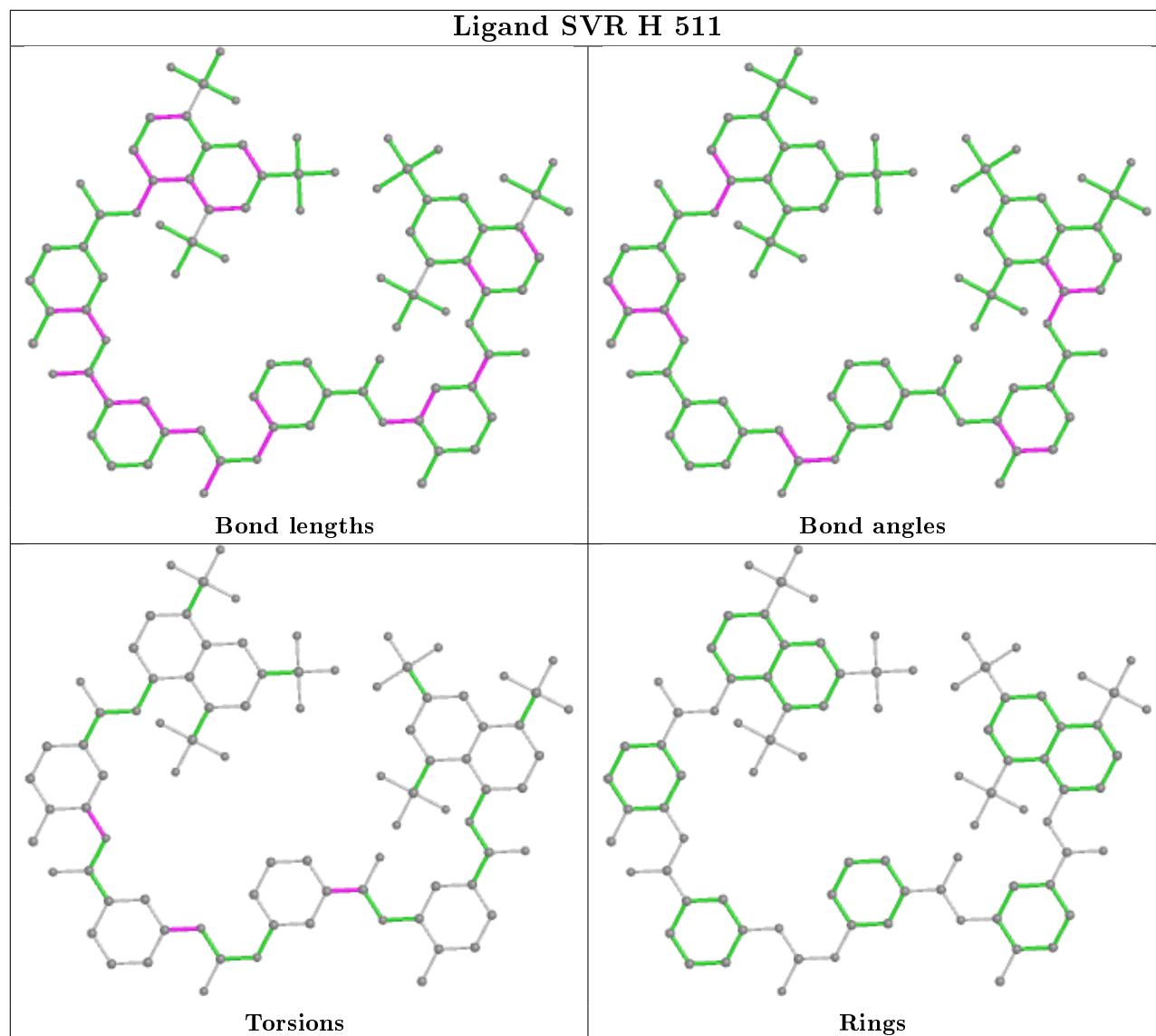
Ligand SVR E 503



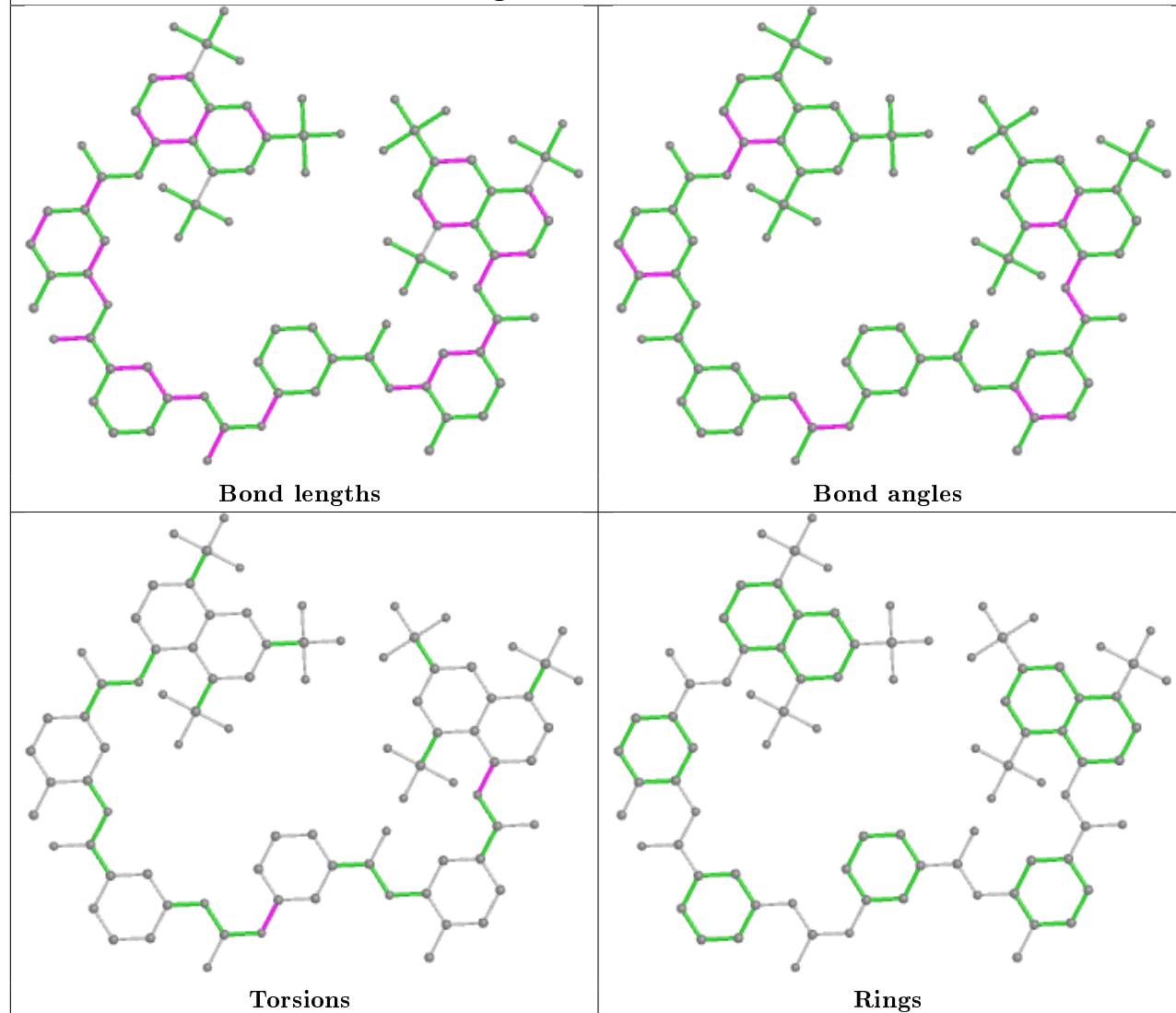
Ligand SVR F 509



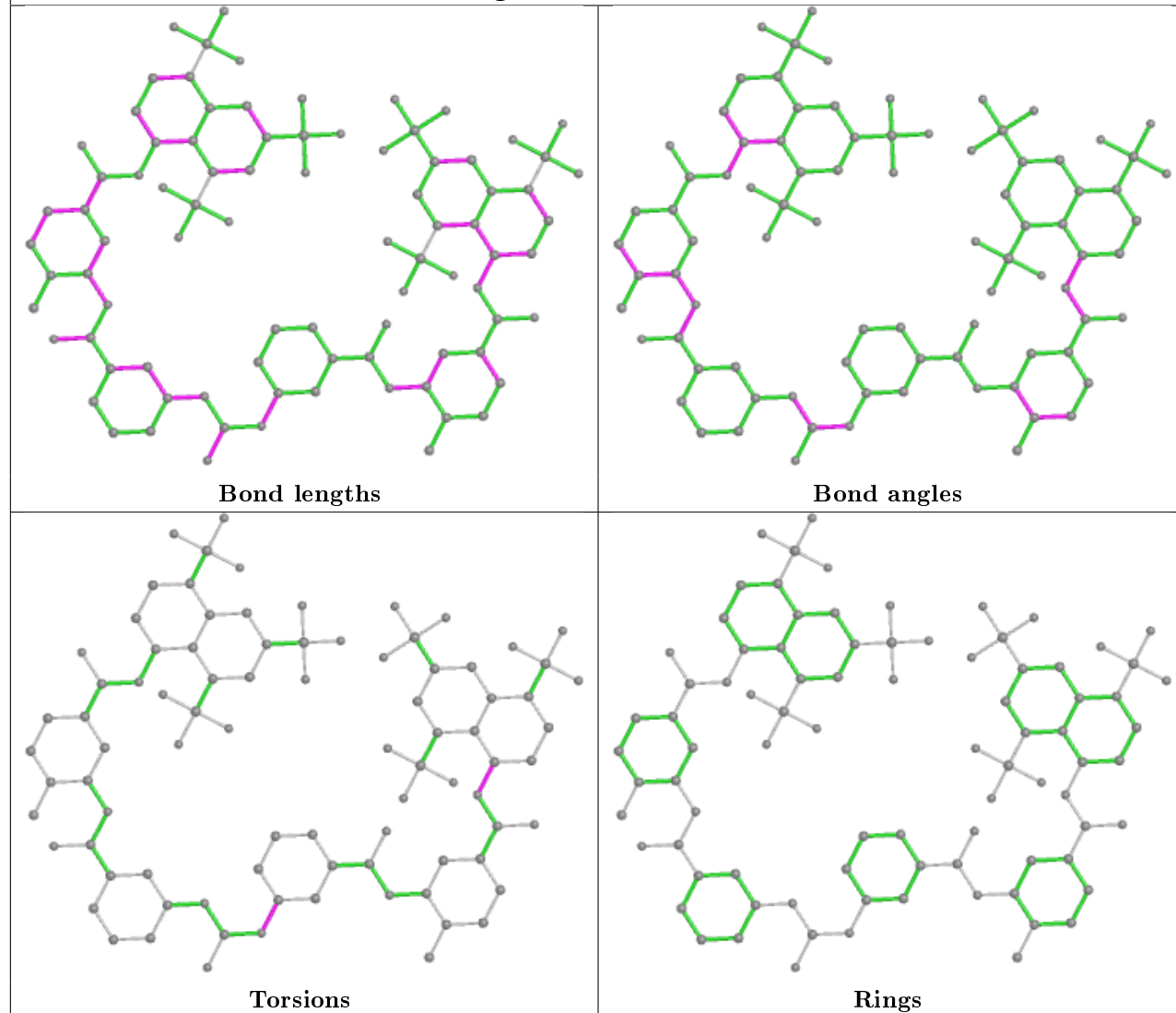
Ligand SVR H 511



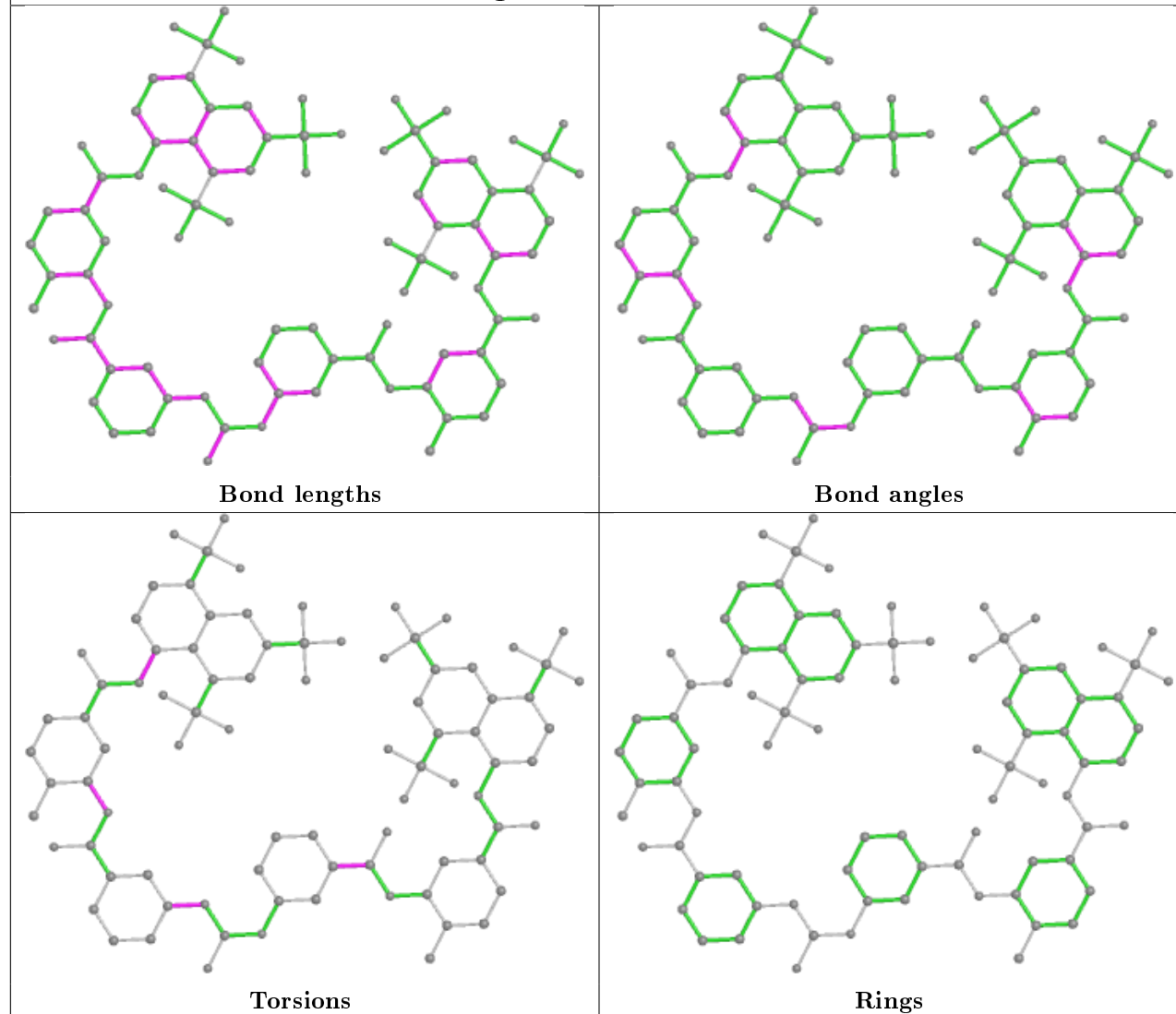
Ligand SVR B 501



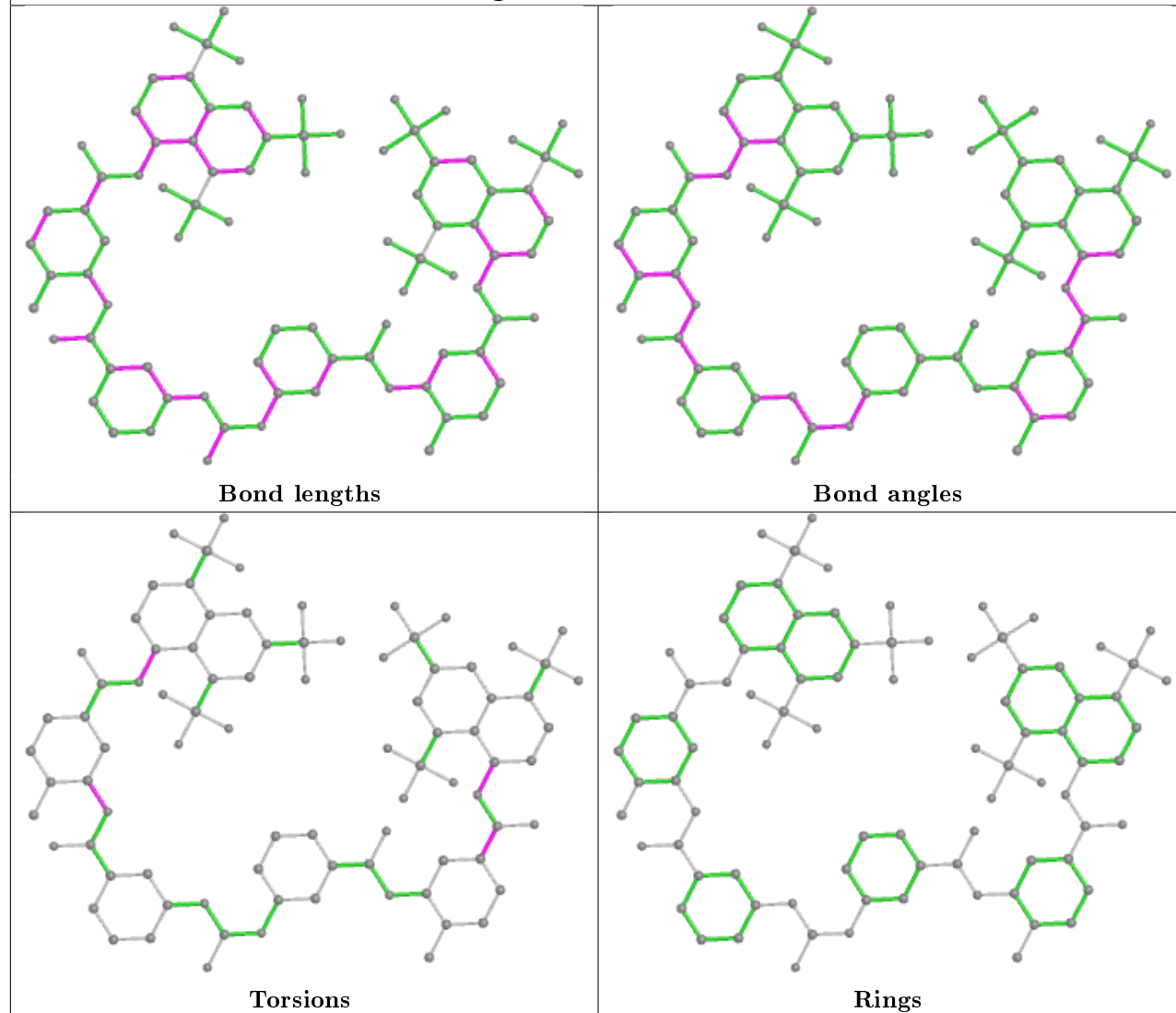
Ligand SVR F 502

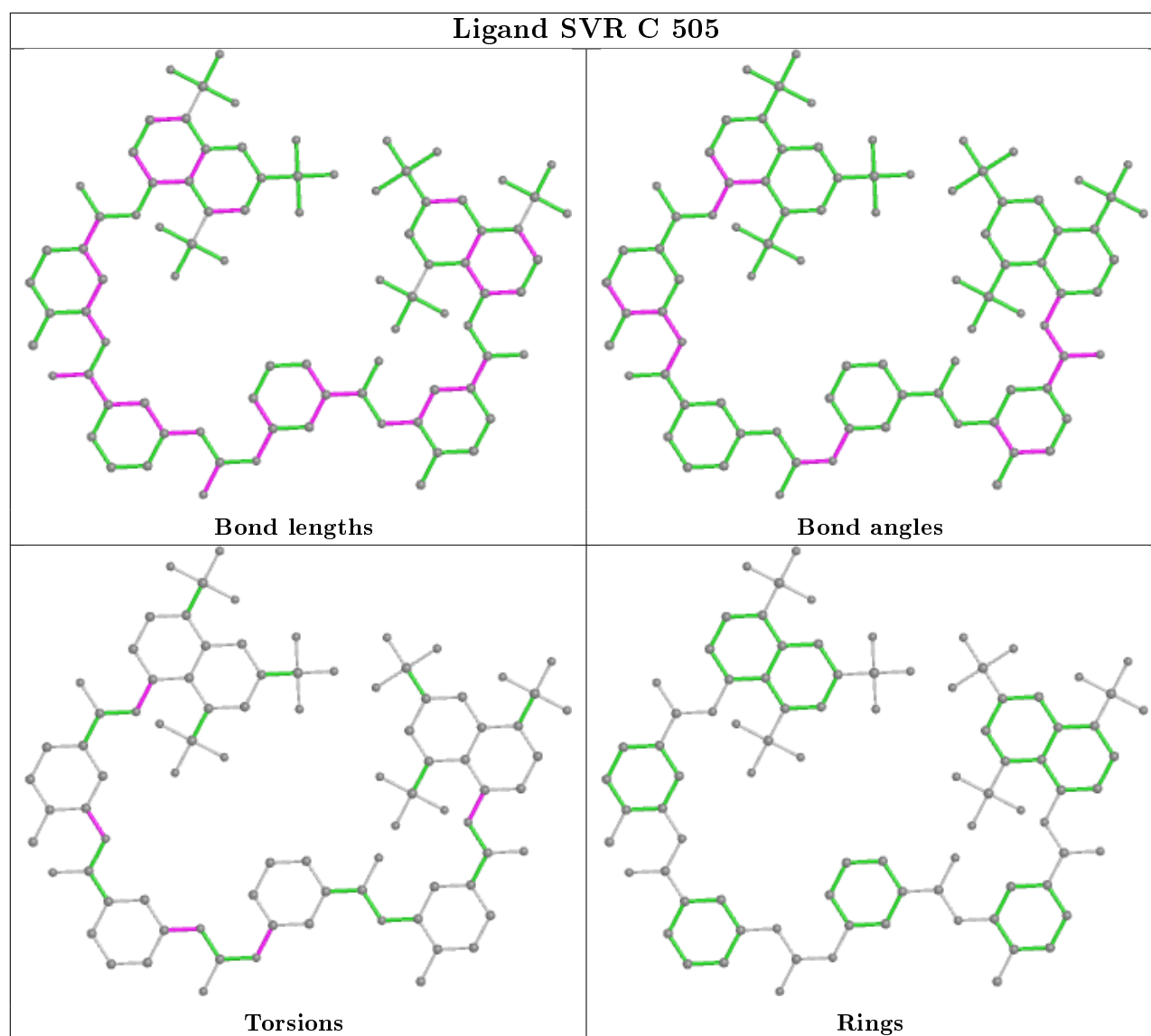


Ligand SVR B 512



Ligand SVR A 508





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	122/122 (100%)	0.34	2 (1%) 72 77	19, 28, 39, 49	0
1	B	122/122 (100%)	0.42	3 (2%) 57 64	18, 29, 44, 60	0
1	C	122/122 (100%)	0.33	3 (2%) 57 64	17, 28, 41, 54	0
1	D	122/122 (100%)	0.41	3 (2%) 57 64	21, 29, 47, 50	0
1	E	122/122 (100%)	1.09	24 (19%) 1 1	22, 40, 68, 73	0
1	F	122/122 (100%)	0.73	9 (7%) 14 19	19, 32, 51, 57	0
1	G	122/122 (100%)	0.44	3 (2%) 57 64	22, 31, 48, 61	0
1	H	122/122 (100%)	0.60	6 (4%) 29 36	22, 35, 53, 62	0
All	All	976/976 (100%)	0.54	53 (5%) 25 32	17, 31, 54, 73	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	55	LEU	5.2
1	E	68	PRO	5.0
1	B	119	TYR	4.8
1	F	95	ILE	4.7
1	G	79	ASN	4.3
1	E	1	SER	4.2
1	E	71	ASP	4.0
1	E	67	SER	3.9
1	E	83	ILE	3.6
1	E	56	PRO	3.6
1	F	119	TYR	3.3
1	B	116	LYS	3.3
1	E	91	CYS	3.2
1	E	133	CYS	3.1
1	F	91	CYS	3.0
1	E	94	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	33	GLU	2.9
1	E	53	ASP	2.7
1	E	59	ASP	2.7
1	A	120	TYR	2.7
1	C	127	LYS	2.6
1	G	1	SER	2.6
1	H	78	GLU	2.6
1	F	133	CYS	2.6
1	A	1	SER	2.6
1	E	119	TYR	2.6
1	E	130	ILE	2.5
1	F	55	LEU	2.5
1	E	122	ASN	2.5
1	E	70	THR	2.4
1	H	49	SER	2.4
1	C	120	TYR	2.4
1	H	77	ARG	2.3
1	E	82	ILE	2.3
1	E	80	GLY	2.3
1	D	84	CYS	2.3
1	G	78	GLU	2.3
1	F	72	ARG	2.3
1	H	82	ILE	2.3
1	F	130	ILE	2.2
1	E	54	THR	2.2
1	D	51	CYS	2.2
1	H	83	ILE	2.2
1	D	76	LYS	2.1
1	E	84	CYS	2.1
1	E	86	ASN	2.1
1	H	119	TYR	2.1
1	B	31	GLY	2.1
1	E	116	LYS	2.1
1	F	88	THR	2.1
1	F	68	PRO	2.1
1	C	1	SER	2.1
1	E	126	CYS	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

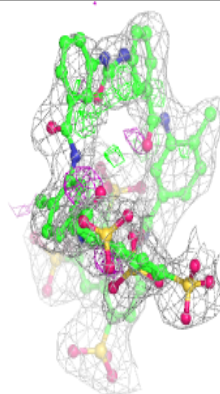
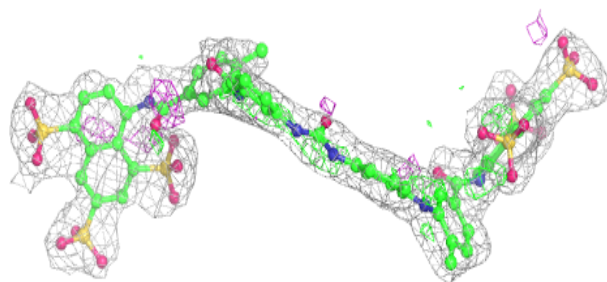
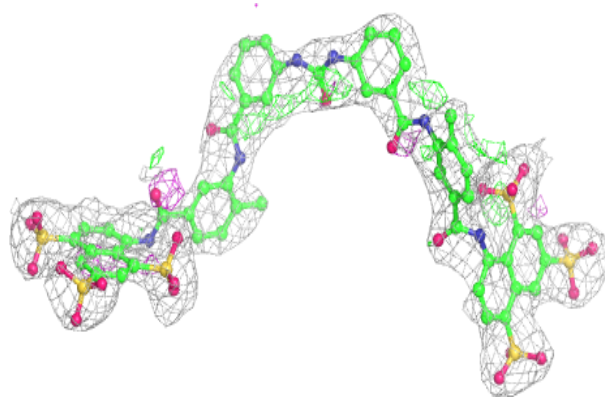
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SVR	A	508	86/86	0.86	0.22	32,45,63,66	0
2	SVR	C	507	86/86	0.89	0.20	32,40,50,52	0
2	SVR	C	505	86/86	0.90	0.20	33,41,48,53	0
2	SVR	E	510	86/86	0.92	0.18	27,44,55,59	0
2	SVR	F	509	86/86	0.93	0.18	20,29,50,56	0
2	SVR	H	511	86/86	0.93	0.19	20,35,55,57	0
2	SVR	G	506	86/86	0.94	0.16	21,33,40,48	0
2	SVR	B	512	86/86	0.94	0.19	19,35,54,56	0
2	SVR	F	502	86/86	0.96	0.16	19,24,35,37	0
2	SVR	H	504	86/86	0.96	0.16	20,30,42,47	0
2	SVR	E	503	86/86	0.96	0.15	21,32,43,46	0
2	SVR	B	501	86/86	0.96	0.16	16,27,37,41	0

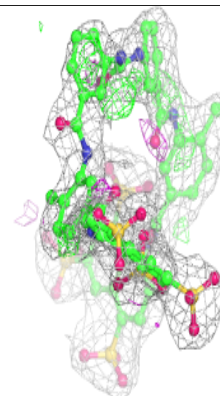
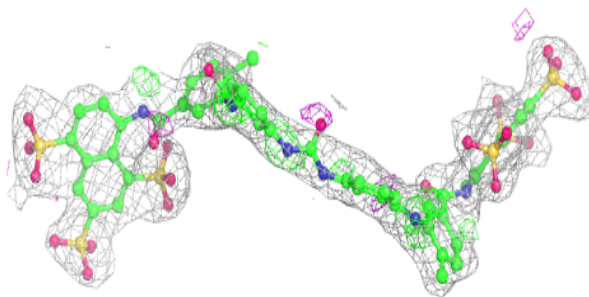
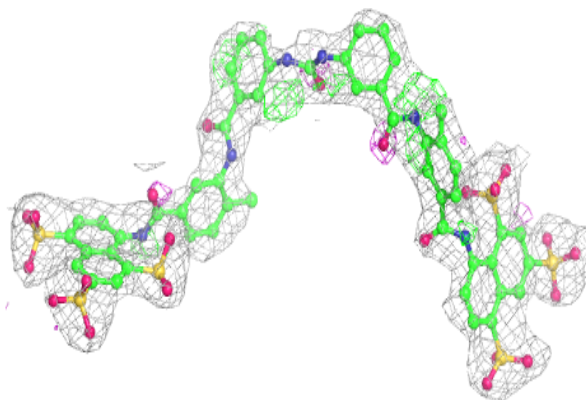
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SVR A 508:

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

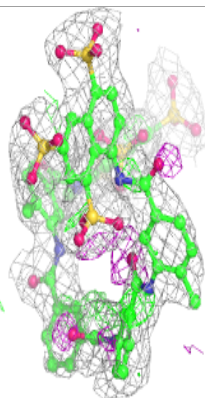
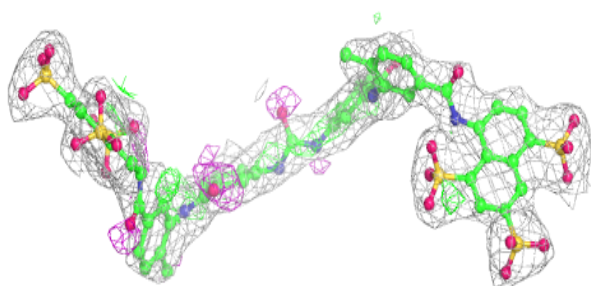
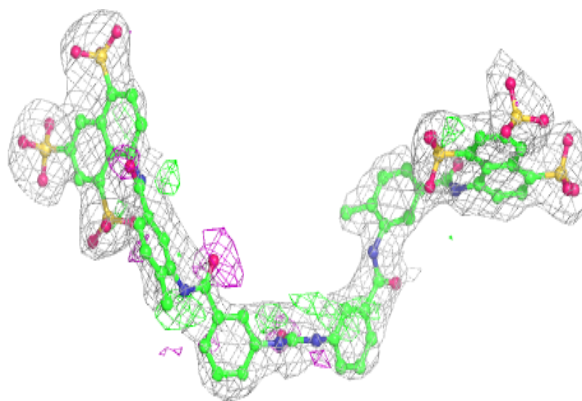
**Electron density around SVR C 507:**

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

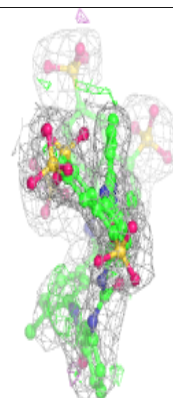
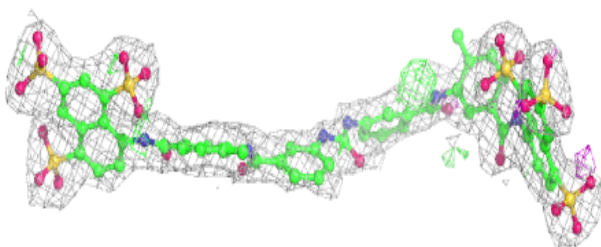
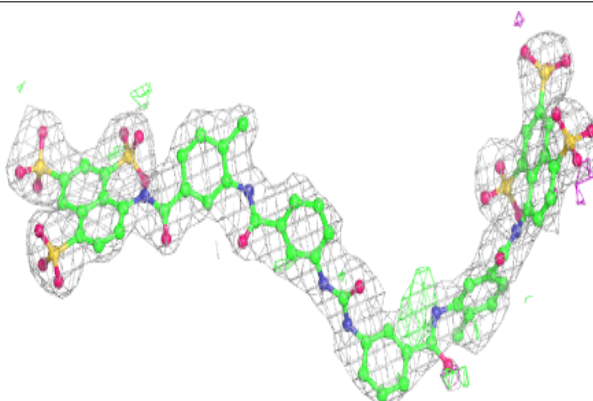


Electron density around SVR C 505:

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

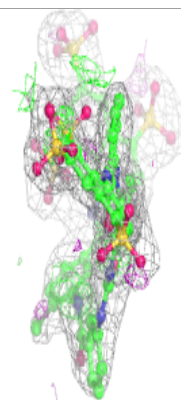
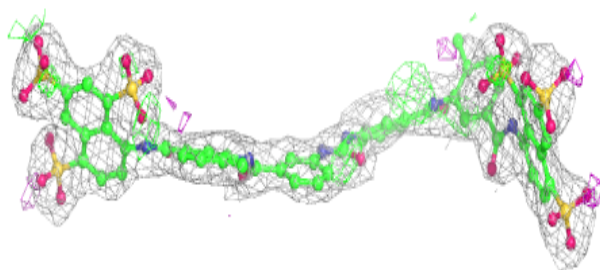
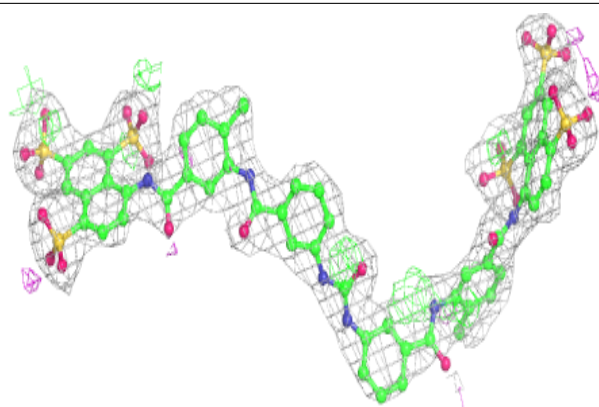
**Electron density around SVR E 510:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

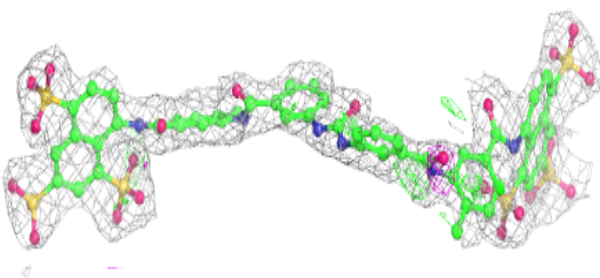
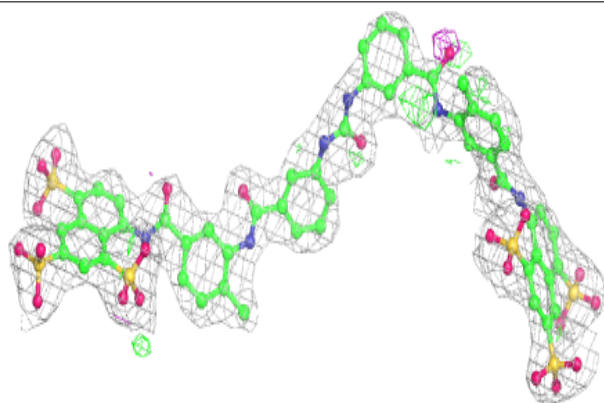


Electron density around SVR F 509:

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

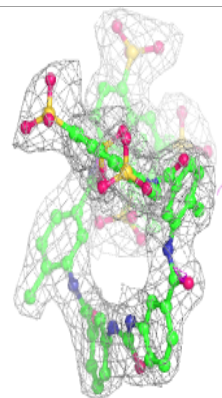
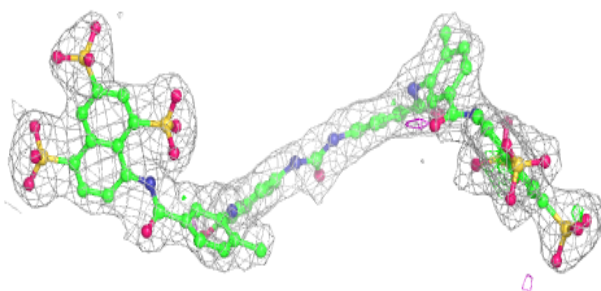
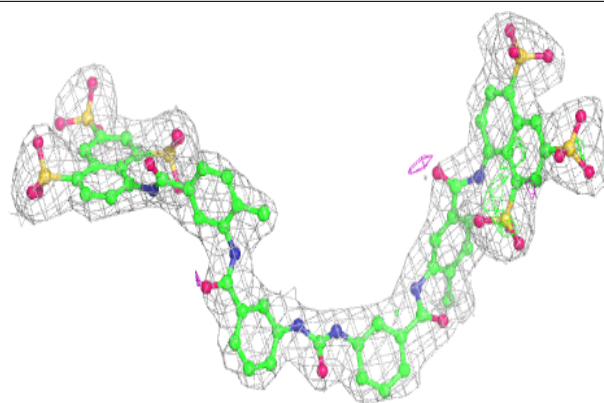
**Electron density around SVR H 511:**

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and green (positive)

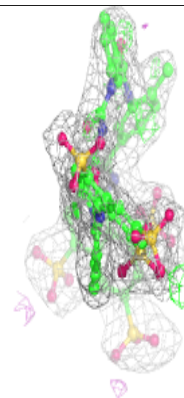
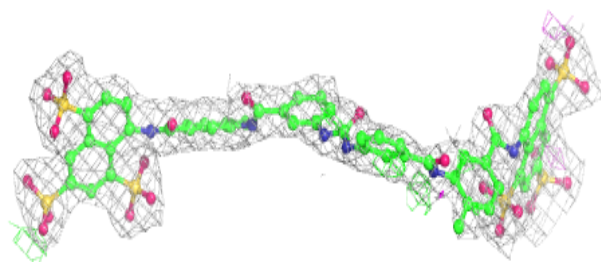
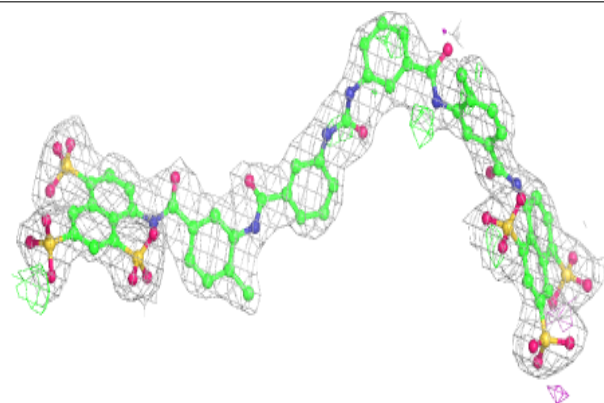


Electron density around SVR G 506:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

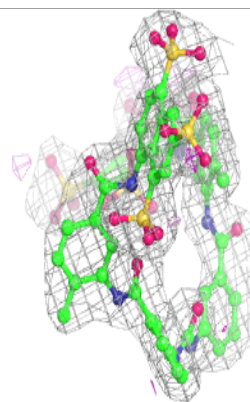
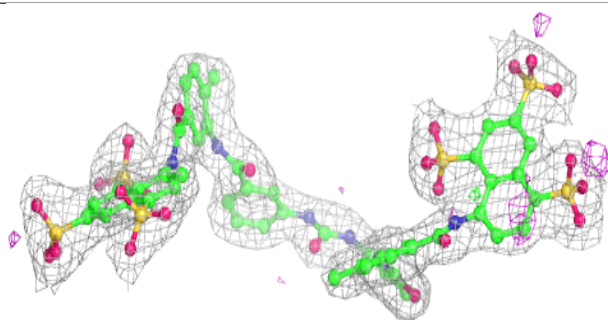
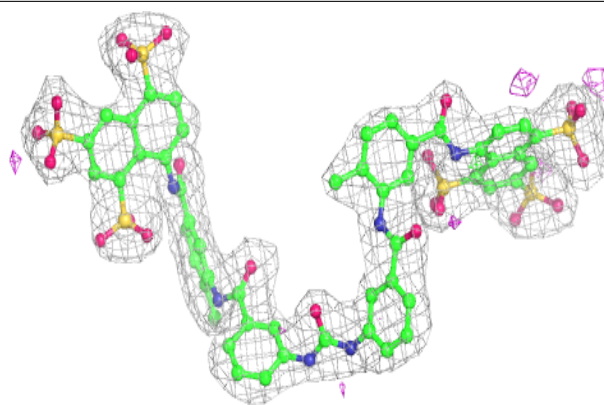
**Electron density around SVR B 512:**

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

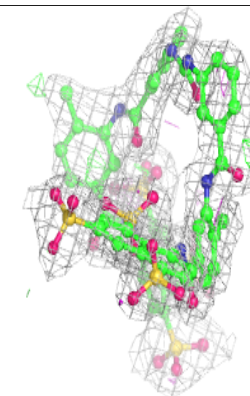
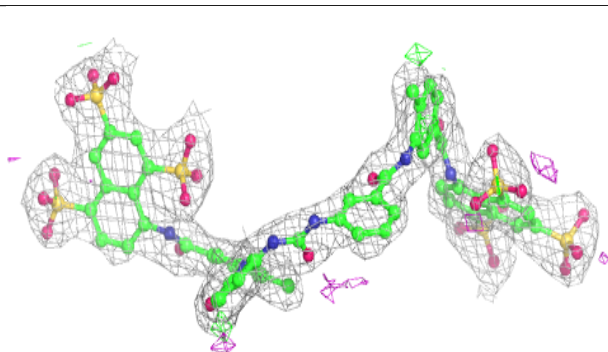
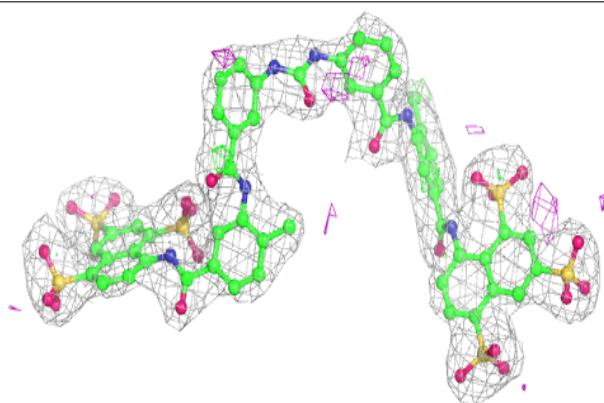


Electron density around SVR F 502:

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

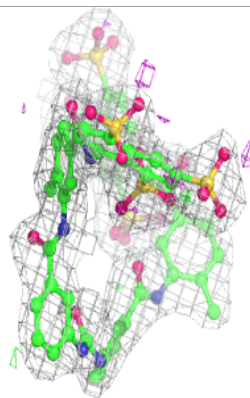
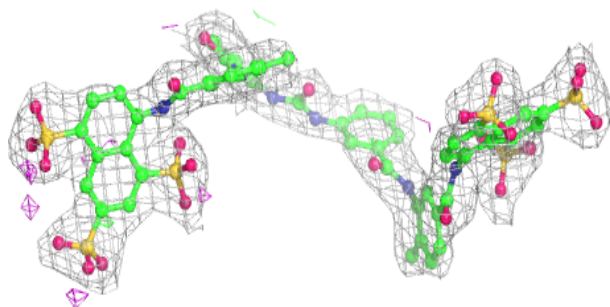
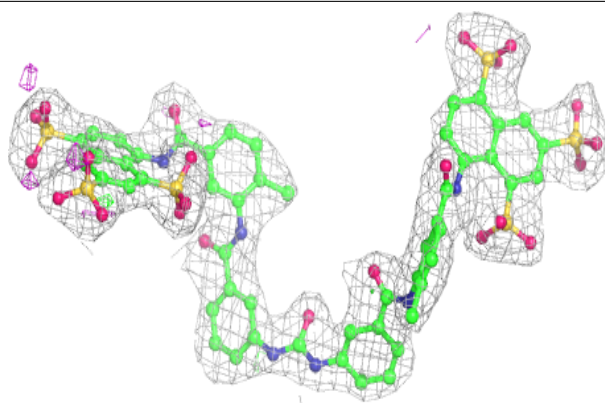
**Electron density around SVR H 504:**

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

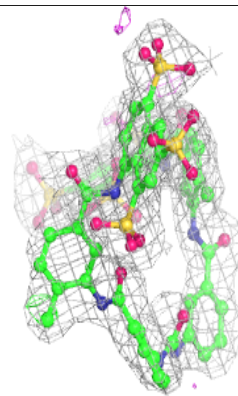
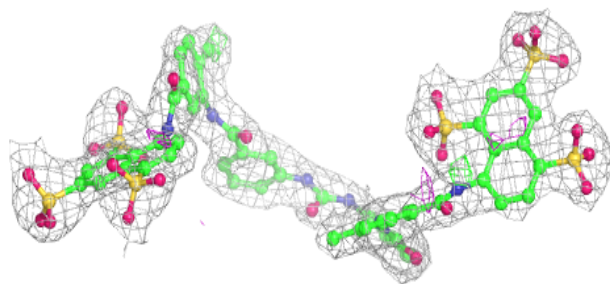
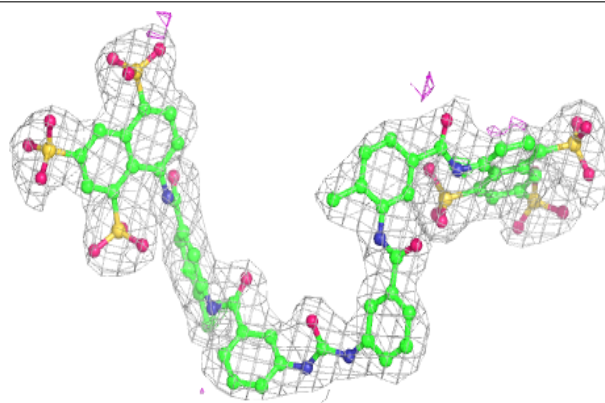


Electron density around SVR E 503:

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

**Electron density around SVR B 501:**

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



6.5 Other polymers

There are no such residues in this entry.