



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:39 AM UTC

PDB ID : 2VAV / pdb_00002vav
Title : Crystal structure of deacetylcephalosporin C acetyltransferase (DAC-Soak)
Authors : Lejon, S.; Ellis, J.; Valegard, K.
Deposited on : 2007-09-04
Resolution : 2.50 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

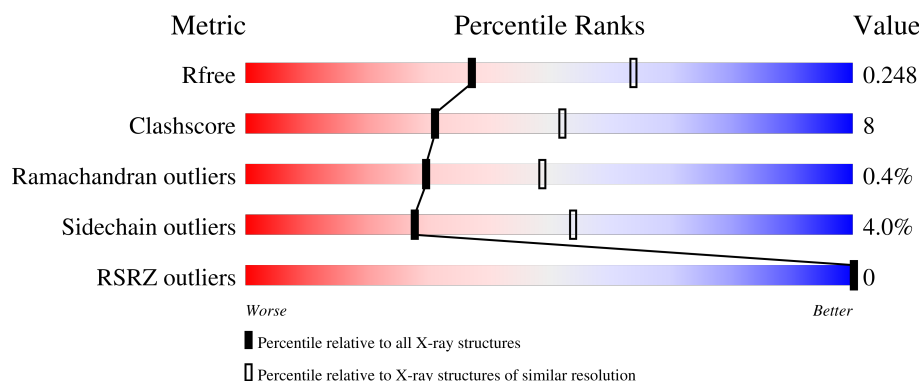
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	

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Mol	Chain	Length	Quality of chain
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	
1	K	444	
1	L	444	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	OAS	A	149[A]	-	X	-	-
1	OAS	B	149[A]	-	X	-	-
1	OAS	C	149[A]	-	X	-	-
1	OAS	D	149[A]	-	X	-	-
1	OAS	E	149[A]	-	X	-	-
1	OAS	F	149[A]	-	X	X	-
1	OAS	G	149[A]	-	X	-	-
1	OAS	H	149[A]	-	X	-	-
1	OAS	I	149[A]	-	X	-	-
1	OAS	J	149[A]	-	X	-	-
1	OAS	K	149[A]	-	X	-	-
1	OAS	L	149[A]	-	X	-	-
2	CSC	A	1383[B]	-	-	X	-
2	CSC	F	1383[A]	-	-	X	-
3	ACT	A	1384	-	-	X	-
3	ACT	C	1384	-	-	X	-
3	ACT	E	1384	-	-	X	-
3	ACT	H	1384	-	-	X	-

2 Entry composition

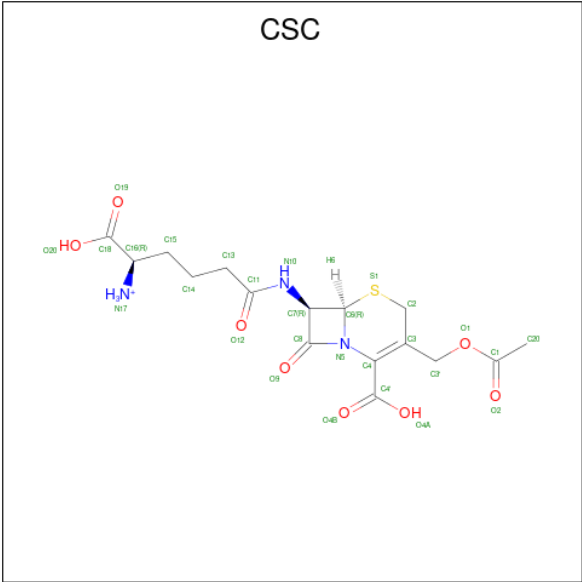
There are 4 unique types of molecules in this entry. The entry contains 33548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE.

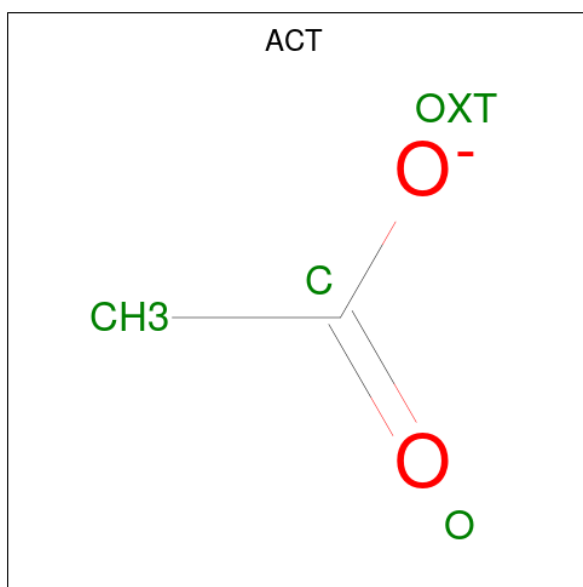
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	2	0
			2743	1730	483	511	19			
1	B	350	Total	C	N	O	S	0	3	0
			2754	1736	486	513	19			
1	C	347	Total	C	N	O	S	0	4	0
			2758	1739	489	511	19			
1	D	345	Total	C	N	O	S	0	4	0
			2745	1732	487	507	19			
1	E	346	Total	C	N	O	S	0	3	0
			2723	1719	478	507	19			
1	F	341	Total	C	N	O	S	0	2	0
			2696	1702	473	502	19			
1	G	342	Total	C	N	O	S	0	3	0
			2707	1708	477	503	19			
1	H	343	Total	C	N	O	S	0	4	0
			2714	1713	478	504	19			
1	I	348	Total	C	N	O	S	0	3	1
			2735	1725	483	508	19			
1	J	344	Total	C	N	O	S	0	2	0
			2714	1713	476	506	19			
1	K	341	Total	C	N	O	S	0	2	0
			2694	1701	473	501	19			
1	L	340	Total	C	N	O	S	0	3	0
			2691	1699	472	501	19			

- Molecule 2 is 4-(3-ACETOXYMETHYL-2-CARBOXY-8-OXO-5-THIA-1-AZA-BICYCL O[4.2.0]OCT-2-EN-7-YLCARBAMOYL)-1-CARBOXY-BUTYL-AMMONIUM (CCD ID: CSC) (formula: C₁₆H₂₂N₃O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	B	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	C	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	D	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	E	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	F	1	Total	C	N	O	S	0	1
			30	17	3	9	1		
2	G	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	H	1	Total	C	N	O	S	0	1
			30	17	3	9	1		
2	I	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	J	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	K	1	Total	C	N	O	S	0	1
			25	14	3	7	1		
2	L	1	Total	C	N	O	S	0	1
			30	17	3	9	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	C	O	0	0
			4	2	2		

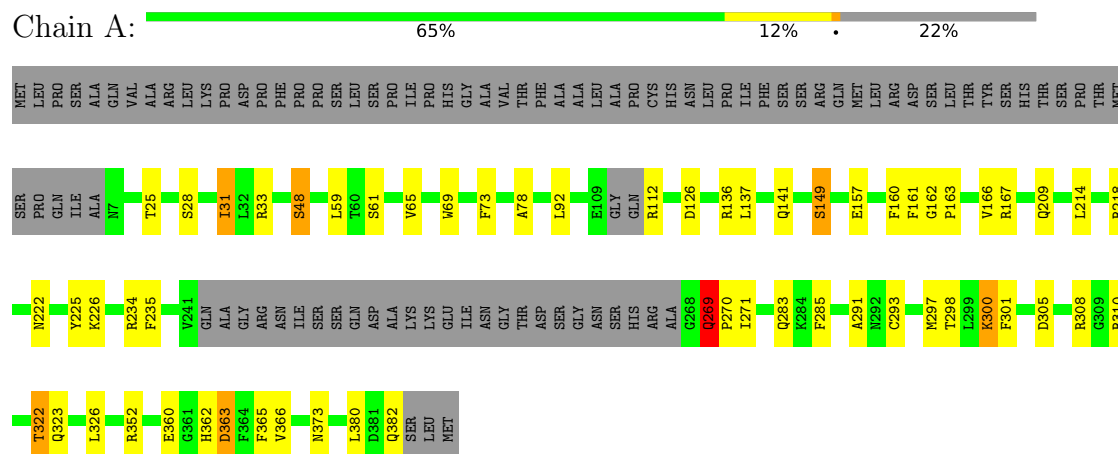
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	51	Total	O	0	0
			51	51		
4	C	43	Total	O	0	0
			43	43		
4	D	49	Total	O	0	0
			49	49		
4	E	46	Total	O	0	0
			46	46		
4	F	41	Total	O	0	0
			41	41		
4	G	52	Total	O	0	0
			52	52		
4	H	48	Total	O	0	0
			48	48		
4	I	56	Total	O	0	0
			56	56		
4	J	17	Total	O	0	0
			17	17		
4	K	11	Total	O	0	0
			11	11		
4	L	37	Total	O	0	0
			37	37		

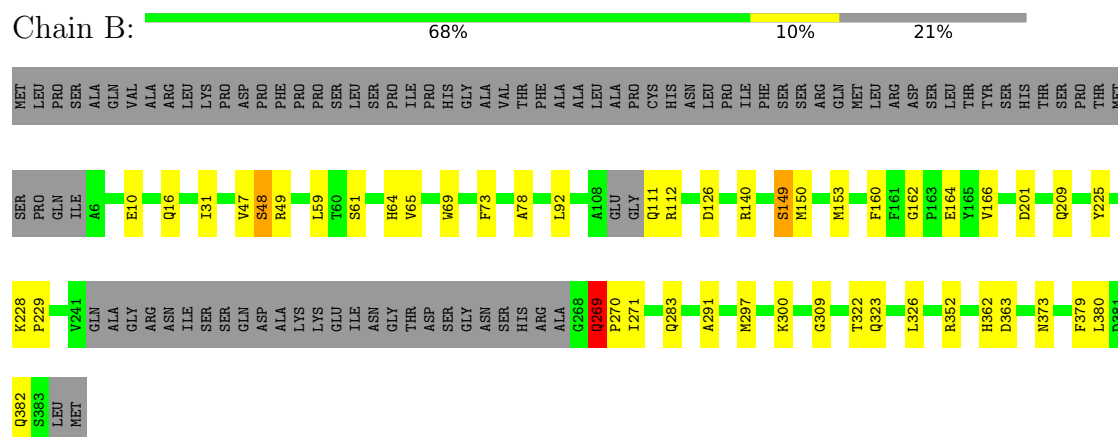
3 Residue-property plots

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

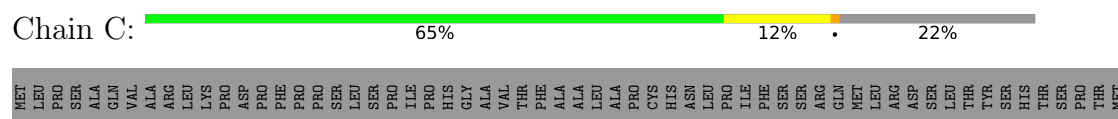
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

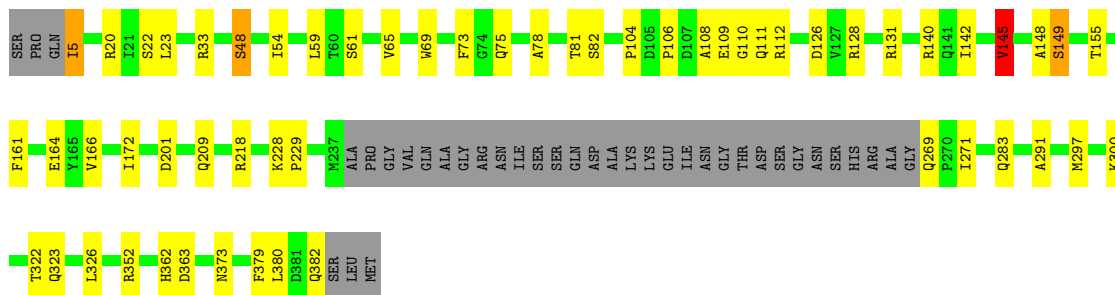


• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

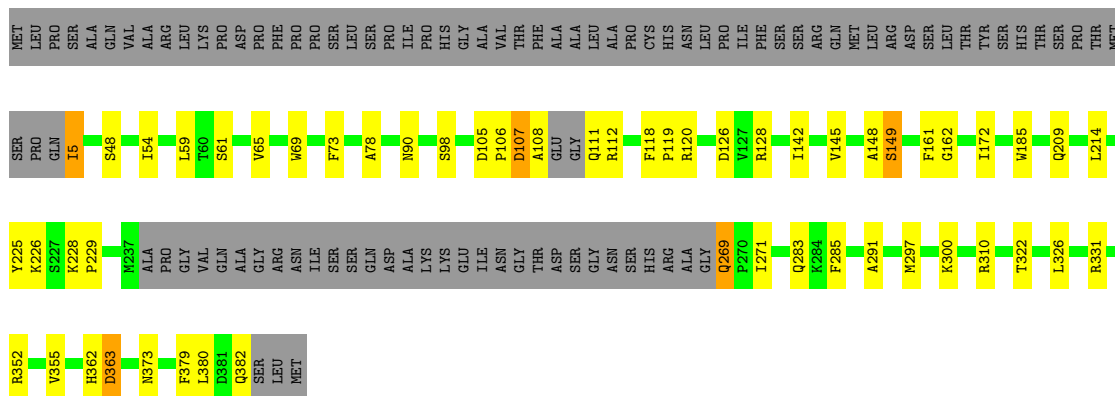


• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

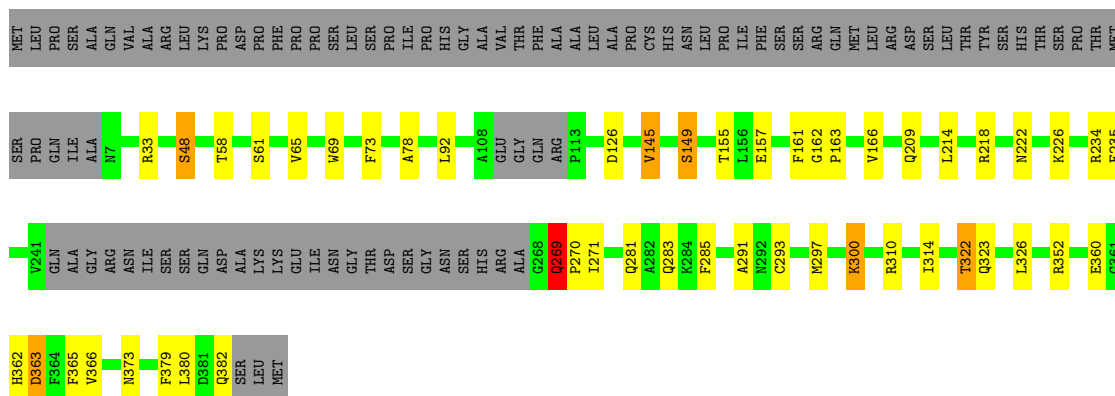




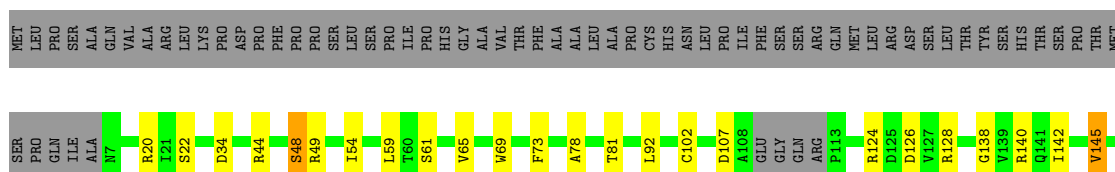
- Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

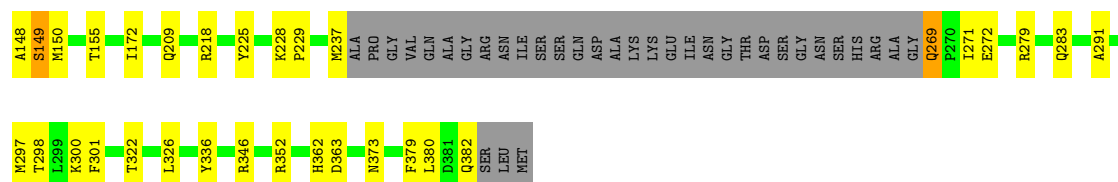


- Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE



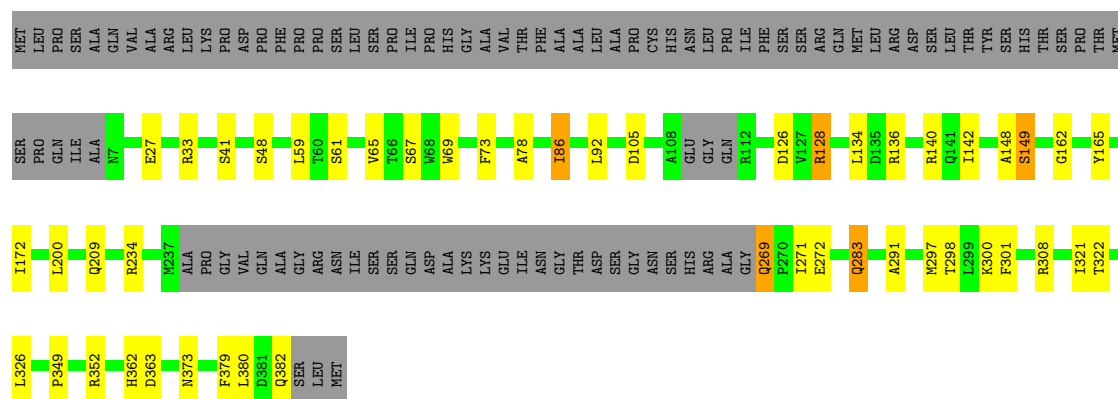
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE





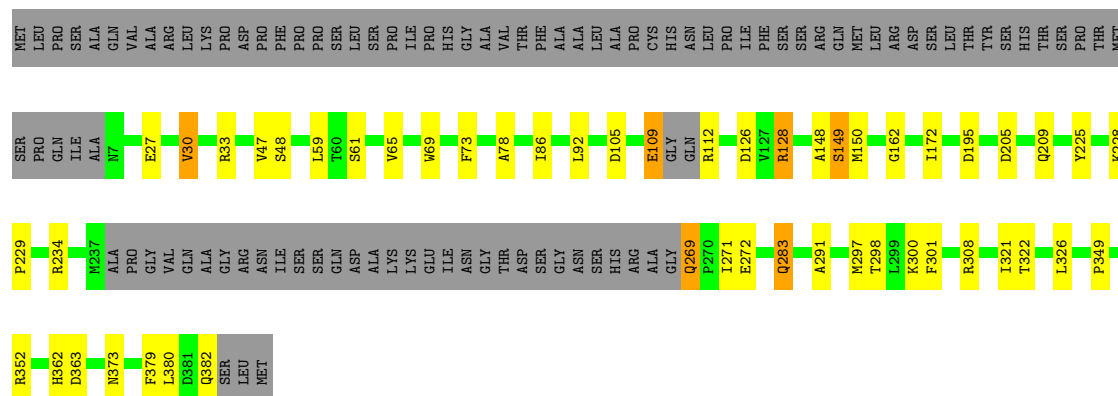
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain G: 66% 10% 23%



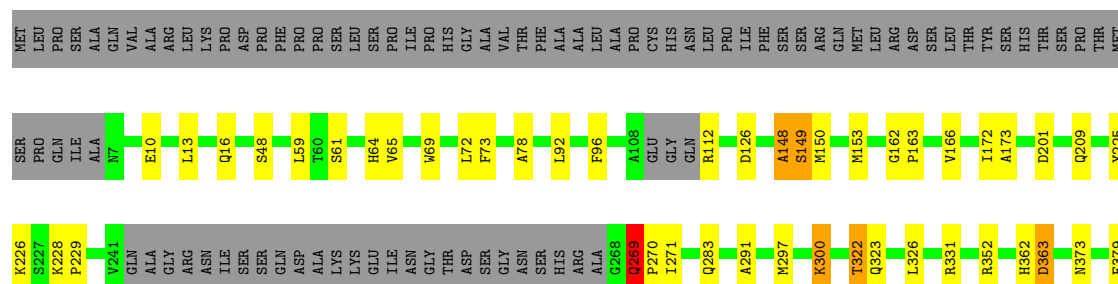
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

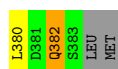
Chain H: 66% 10% 23%



• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

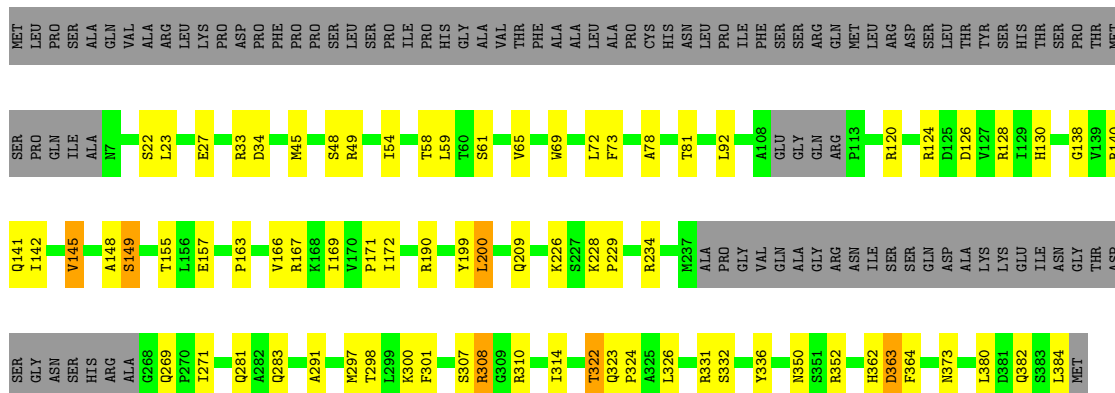
Chain I: 67% 9% 22%





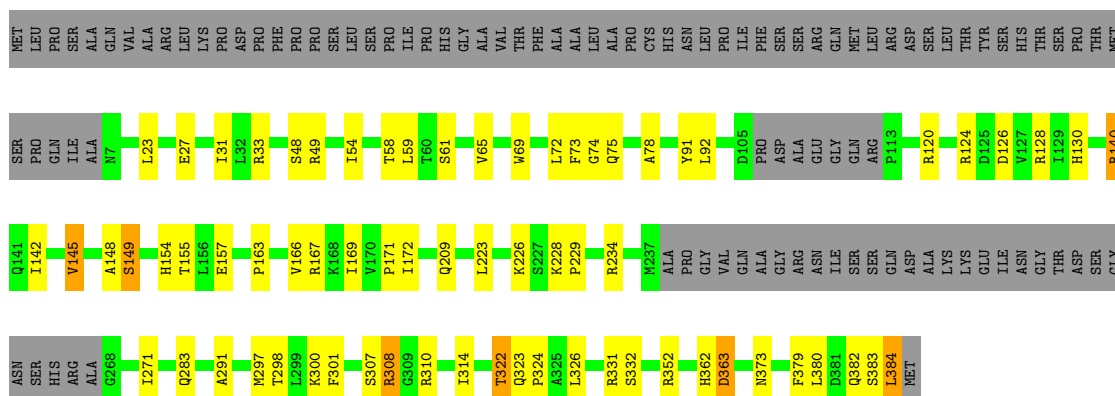
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain J: 60% 16% 23%



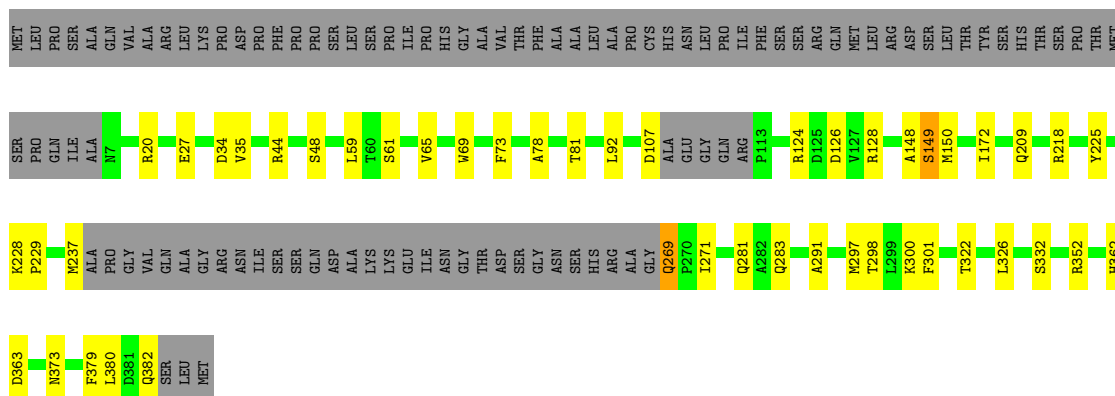
• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain K: 61% 14% 23%



• Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain L: 66% 10% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.06Å 108.86Å 195.79Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	103.70 – 2.50 103.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (103.70-2.50) 99.7 (103.70-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.255 0.214 , 0.248	Depositor DCC
R_{free} test set	3419 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33548	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAS, CSC, ACT

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	0.87	1/2796 (0.0%)	0.98	5/3789 (0.1%)
1	B	0.87	0/2807	0.96	6/3804 (0.2%)
1	C	0.86	0/2817	0.97	3/3816 (0.1%)
1	D	0.85	0/2803	1.00	7/3796 (0.2%)
1	E	0.87	1/2776 (0.0%)	0.97	5/3762 (0.1%)
1	F	0.87	0/2748	0.97	3/3723 (0.1%)
1	G	0.85	0/2759	0.93	4/3738 (0.1%)
1	H	0.84	0/2766	0.95	5/3747 (0.1%)
1	I	0.87	1/2788 (0.0%)	0.98	7/3779 (0.2%)
1	J	0.96	1/2766 (0.0%)	0.99	0/3747
1	K	0.97	2/2745 (0.1%)	0.99	1/3717 (0.0%)
1	L	0.85	0/2743	0.97	3/3716 (0.1%)
All	All	0.88	6/33314 (0.0%)	0.97	49/45134 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	314	ILE	CA-CB	10.95	1.60	1.54
1	K	314	ILE	CA-CB	9.81	1.59	1.54
1	I	382	GLN	C-N	-6.44	1.24	1.33
1	A	31	ILE	CA-CB	5.57	1.60	1.54
1	E	314	ILE	CA-CB	5.33	1.57	1.54
1	K	31	ILE	CA-CB	5.14	1.60	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	112	ARG	CA-C-N	9.78	129.71	120.03
1	I	112	ARG	C-N-CA	9.78	129.71	120.03
1	B	112	ARG	CA-C-N	9.23	129.17	120.03
1	B	112	ARG	C-N-CA	9.23	129.17	120.03
1	D	310	ARG	NE-CZ-NH2	8.46	126.82	119.20
1	A	360	GLU	N-CA-C	8.00	122.86	113.18
1	D	310	ARG	NE-CZ-NH1	-7.76	113.74	121.50
1	E	360	GLU	N-CA-C	7.30	122.01	113.18
1	K	140	ARG	N-CA-C	-6.88	105.03	113.50
1	B	269	GLN	CA-C-N	-6.87	113.23	120.03
1	B	269	GLN	C-N-CA	-6.87	113.23	120.03
1	I	269	GLN	CA-C-N	-6.81	113.28	120.03
1	I	269	GLN	C-N-CA	-6.81	113.28	120.03
1	D	269	GLN	CA-C-N	-6.65	113.80	120.31
1	D	269	GLN	C-N-CA	-6.65	113.80	120.31
1	A	112	ARG	CA-C-N	6.56	126.52	120.03
1	A	112	ARG	C-N-CA	6.56	126.52	120.03
1	A	162	GLY	CA-C-N	6.55	126.18	119.56
1	A	162	GLY	C-N-CA	6.55	126.18	119.56
1	I	162	GLY	CA-C-N	6.55	126.68	119.87
1	I	162	GLY	C-N-CA	6.55	126.68	119.87
1	B	162	GLY	CA-C-N	6.47	126.60	119.87
1	B	162	GLY	C-N-CA	6.47	126.60	119.87
1	F	269	GLN	CA-C-N	-6.42	114.02	120.31
1	F	269	GLN	C-N-CA	-6.42	114.02	120.31
1	D	310	ARG	CD-NE-CZ	6.41	133.38	124.40
1	G	105	ASP	CA-C-N	-6.40	113.10	119.56
1	G	105	ASP	C-N-CA	-6.40	113.10	119.56
1	H	162	GLY	CA-C-N	6.22	126.34	119.87
1	H	162	GLY	C-N-CA	6.22	126.34	119.87
1	L	269	GLN	CA-C-N	-6.20	114.23	120.31
1	L	269	GLN	C-N-CA	-6.20	114.23	120.31
1	C	145	VAL	CB-CA-C	6.05	119.59	110.63
1	F	218	ARG	N-CA-C	6.04	117.94	111.36
1	G	162	GLY	CA-C-N	5.96	126.07	119.87
1	G	162	GLY	C-N-CA	5.96	126.07	119.87
1	I	382	GLN	O-C-N	-5.76	113.78	123.00
1	E	269	GLN	CA-C-N	-5.50	114.04	119.92
1	E	269	GLN	C-N-CA	-5.50	114.04	119.92
1	E	162	GLY	CA-C-N	5.45	125.54	119.87
1	E	162	GLY	C-N-CA	5.45	125.54	119.87
1	L	35	VAL	N-CA-C	5.41	112.49	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	30	VAL	N-CA-CB	5.38	117.63	110.26
1	H	105	ASP	CA-C-N	-5.38	114.13	119.56
1	H	105	ASP	C-N-CA	-5.38	114.13	119.56
1	D	162	GLY	CA-C-N	5.31	125.40	119.87
1	D	162	GLY	C-N-CA	5.31	125.40	119.87
1	C	112	ARG	CA-C-N	5.07	125.28	120.31
1	C	112	ARG	C-N-CA	5.07	125.28	120.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	148	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2743	0	2645	48	0
1	B	2754	0	2656	38	0
1	C	2758	0	2673	44	0
1	D	2745	0	2661	49	0
1	E	2723	0	2624	39	0
1	F	2696	0	2600	64	0
1	G	2707	0	2610	31	1
1	H	2714	0	2613	45	1
1	I	2735	0	2638	43	0
1	J	2714	0	2618	57	1
1	K	2694	0	2602	50	1
1	L	2691	0	2592	38	0
2	A	25	0	16	9	0
2	B	25	0	17	1	0
2	C	25	0	17	2	0
2	D	25	0	16	1	0
2	E	25	0	16	6	0
2	F	30	0	6	14	0
2	G	25	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	30	0	4	5	0
2	I	25	0	17	2	0
2	J	25	0	15	3	0
2	K	25	0	15	3	0
2	L	30	0	6	5	0
3	A	8	0	6	2	0
3	B	8	0	6	1	0
3	C	4	0	3	2	0
3	D	4	0	3	1	0
3	E	8	0	6	4	0
3	F	4	0	3	1	0
3	G	4	0	3	1	0
3	H	4	0	3	2	0
3	I	12	0	9	0	0
3	L	4	0	3	0	0
4	A	48	0	0	1	0
4	B	51	0	0	3	0
4	C	43	0	0	5	0
4	D	49	0	0	1	0
4	E	46	0	0	2	0
4	F	41	0	0	5	0
4	G	52	0	0	3	0
4	H	48	0	0	4	0
4	I	56	0	0	1	0
4	J	17	0	0	1	0
4	K	11	0	0	0	0
4	L	37	0	0	3	0
All	All	33548	0	31738	529	2

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 8.

All (529) 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:F:149[A]:OAS:HB2	2:F:1383[A]:CSC:C20	1.24	1.54
1:F:149[A]:OAS:CB	2:F:1383[A]:CSC:C20	1.89	1.48
1:F:149[A]:OAS:CB	2:F:1383[A]:CSC:H201	1.57	1.27
1:F:149[A]:OAS:OG	2:F:1383[A]:CSC:H202	1.40	1.21
1:F:149[A]:OAS:CB	2:F:1383[A]:CSC:H202	1.65	1.11
1:J:140:ARG:NH1	4:J:2002:HOH:O	1.79	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120[B]:ARG:HG3	1:D:120[B]:ARG:HH11	1.17	1.09
1:E:234:ARG:HH22	2:E:1383[B]:CSC:C18	1.67	1.08
1:D:331:ARG:HH21	1:I:382:GLN:HE21	1.05	1.02
1:H:234:ARG:HD3	4:H:2032:HOH:O	1.62	0.98
2:J:1385[B]:CSC:O1	2:J:1385[B]:CSC:O4A	1.81	0.98
2:K:1385[B]:CSC:O4B	2:K:1385[B]:CSC:O1	1.86	0.93
1:F:150:MET:H	2:F:1383[A]:CSC:H201	1.33	0.93
2:J:1385[B]:CSC:O1	2:J:1385[B]:CSC:C4'	2.15	0.93
1:I:10:GLU:O	1:L:44:ARG:NH1	2.04	0.91
1:C:352:ARG:NH2	1:C:382:GLN:HE22	1.69	0.89
1:D:352:ARG:NH2	1:D:382:GLN:HE22	1.71	0.89
1:E:234:ARG:NH2	2:E:1383[B]:CSC:O20	2.06	0.89
1:B:10:GLU:O	1:F:44:ARG:NH1	2.07	0.88
1:E:222:ASN:HB3	4:E:2030:HOH:O	1.74	0.88
1:D:352:ARG:HH22	1:D:382:GLN:HE22	1.19	0.86
1:H:128[A]:ARG:HH21	1:H:128[A]:ARG:CG	1.90	0.85
1:J:23:LEU:HD23	1:J:33:ARG:HG3	1.59	0.85
1:F:149[A]:OAS:HB2	2:F:1383[A]:CSC:H203	1.54	0.85
2:K:1385[B]:CSC:O1	2:K:1385[B]:CSC:C4'	2.16	0.85
1:I:352:ARG:HH22	1:I:382:GLN:HE22	1.24	0.85
1:A:33:ARG:HH21	1:A:33:ARG:HG3	1.42	0.84
1:L:126:ASP:OD2	1:L:300:LYS:HE3	1.77	0.84
1:J:126:ASP:OD2	1:J:300:LYS:HE3	1.78	0.84
1:C:352:ARG:HH22	1:C:382:GLN:HE22	1.20	0.83
1:D:331:ARG:NH2	1:I:382:GLN:HE21	1.76	0.83
1:F:149[A]:OAS:OG	2:F:1383[A]:CSC:C20	2.11	0.83
1:H:149[B]:OAS:OAC	2:H:1383[B]:CSC:O1	1.89	0.83
1:B:352:ARG:HH22	1:B:382:GLN:HE22	1.28	0.82
1:L:126:ASP:OD2	1:L:300:LYS:CE	2.29	0.80
1:A:48:SER:HB2	4:A:2006:HOH:O	1.83	0.79
1:D:111:GLN:HA	1:D:111:GLN:OE1	1.80	0.79
1:F:346:ARG:NH2	4:F:2038:HOH:O	2.15	0.78
1:F:149[A]:OAS:HB2	2:F:1383[A]:CSC:H201	0.78	0.78
1:K:126:ASP:OD2	1:K:300:LYS:CE	2.32	0.78
1:D:120[B]:ARG:HH11	1:D:120[B]:ARG:CG	1.97	0.77
1:G:126:ASP:OD2	1:G:300:LYS:HE3	1.83	0.77
1:J:126:ASP:OD2	1:J:300:LYS:CE	2.32	0.77
1:J:49:ARG:NH2	1:J:140:ARG:HH21	1.83	0.76
1:D:331:ARG:HH21	1:I:382:GLN:NE2	1.83	0.76
1:K:126:ASP:OD2	1:K:300:LYS:HE3	1.84	0.76
1:E:48:SER:HB2	4:E:2007:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:49:ARG:HH22	1:K:140:ARG:HH21	1.34	0.76
1:G:126:ASP:OD2	1:G:300:LYS:CE	2.33	0.75
1:F:126:ASP:OD2	1:F:300:LYS:CE	2.35	0.74
1:K:92:LEU:O	1:K:300:LYS:NZ	2.20	0.73
1:E:78:ALA:H	1:E:373:ASN:HD21	1.34	0.73
2:E:1383[B]:CSC:H3'1	2:E:1383[B]:CSC:O4B	1.87	0.73
1:D:126:ASP:OD2	1:D:300:LYS:HE3	1.88	0.73
1:A:78:ALA:H	1:A:373:ASN:HD21	1.35	0.73
1:L:149[A]:OAS:OG	1:L:362:HIS:NE2	2.18	0.73
1:E:161:PHE:CZ	3:E:1384:ACT:H3	2.24	0.72
1:D:126:ASP:OD2	1:D:300:LYS:CE	2.37	0.72
1:K:49:ARG:NH2	1:K:140:ARG:HH21	1.85	0.72
1:C:75:GLN:HG3	1:F:140:ARG:HA	1.70	0.72
1:J:209:GLN:HE22	1:J:291:ALA:H	1.36	0.72
1:B:209:GLN:HE22	1:B:291:ALA:H	1.38	0.72
1:H:126:ASP:OD2	1:H:300:LYS:HE3	1.88	0.72
1:H:126:ASP:OD2	1:H:300:LYS:CE	2.38	0.71
1:B:47:VAL:HG23	4:B:2003:HOH:O	1.89	0.71
1:D:355:VAL:O	1:I:382:GLN:HA	1.89	0.71
1:A:234:ARG:NH2	2:A:1383[B]:CSC:O19	2.18	0.71
1:H:47:VAL:HG23	4:H:2003:HOH:O	1.91	0.70
1:H:128[A]:ARG:HH21	1:H:128[A]:ARG:HG3	1.56	0.70
1:F:92:LEU:O	1:F:300:LYS:NZ	2.24	0.70
1:F:126:ASP:OD2	1:F:300:LYS:HE3	1.92	0.70
1:I:149[A]:OAS:OG	1:I:362:HIS:NE2	2.20	0.70
1:C:126:ASP:OD2	1:C:300:LYS:HE3	1.92	0.70
1:K:27:GLU:HB3	1:K:128[A]:ARG:HH22	1.57	0.70
1:E:234:ARG:NH2	2:E:1383[B]:CSC:C18	2.49	0.70
1:K:209:GLN:HE22	1:K:291:ALA:H	1.39	0.70
1:E:78:ALA:H	1:E:373:ASN:ND2	1.89	0.70
1:B:10:GLU:HG2	1:F:44:ARG:HH12	1.56	0.69
1:F:352:ARG:HH22	1:F:382:GLN:HE22	1.37	0.69
1:K:23:LEU:HD23	1:K:33:ARG:HG3	1.74	0.69
1:C:23:LEU:HD23	1:C:33:ARG:HG2	1.74	0.69
1:A:78:ALA:H	1:A:373:ASN:ND2	1.90	0.69
1:I:352:ARG:NH2	1:I:382:GLN:HE22	1.90	0.69
1:D:209:GLN:HE22	1:D:291:ALA:H	1.40	0.69
1:L:92:LEU:O	1:L:300:LYS:NZ	2.26	0.68
1:B:149[A]:OAS:OG	1:B:362:HIS:NE2	2.23	0.68
1:C:209:GLN:HE22	1:C:291:ALA:H	1.41	0.68
1:C:161:PHE:CZ	3:C:1384:ACT:H3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1383[B]:CSC:O4B	2:G:1383[B]:CSC:H3'1	1.92	0.68
1:C:126:ASP:OD2	1:C:300:LYS:CE	2.42	0.68
1:H:352:ARG:HH22	1:H:382:GLN:HE22	1.41	0.67
1:I:209:GLN:HE22	1:I:291:ALA:H	1.42	0.67
1:F:150:MET:N	2:F:1383[A]:CSC:H201	2.07	0.67
1:F:352:ARG:NH1	4:F:2039:HOH:O	2.27	0.67
1:B:126:ASP:OD2	1:B:300:LYS:HE2	1.95	0.67
1:B:352:ARG:NH2	1:B:382:GLN:HE22	1.93	0.66
1:H:205:ASP:HB2	4:H:2028:HOH:O	1.95	0.66
1:I:78:ALA:H	1:I:373:ASN:HD21	1.43	0.66
1:L:352:ARG:HH22	1:L:382:GLN:HE22	1.41	0.66
1:I:92:LEU:O	1:I:300:LYS:NZ	2.28	0.66
1:B:126:ASP:OD2	1:B:300:LYS:CE	2.43	0.66
1:D:352:ARG:HH22	1:D:382:GLN:NE2	1.94	0.66
1:I:64:HIS:HD2	4:I:2002:HOH:O	1.80	0.65
1:I:126:ASP:OD2	1:I:300:LYS:HE2	1.96	0.65
1:A:352:ARG:HH22	1:A:382:GLN:HE22	1.43	0.65
1:G:128[A]:ARG:HH21	3:G:1384:ACT:H1	1.61	0.65
1:H:149[A]:OAS:OG	1:H:362:HIS:NE2	2.22	0.64
1:F:149[A]:OAS:OG	1:F:362:HIS:NE2	2.21	0.64
1:I:126:ASP:OD2	1:I:300:LYS:CE	2.45	0.64
1:A:92:LEU:O	1:A:300:LYS:NZ	2.31	0.64
1:J:92:LEU:O	1:J:300:LYS:NZ	2.29	0.64
1:C:352:ARG:HH22	1:C:382:GLN:NE2	1.93	0.63
1:J:49:ARG:HH22	1:J:140:ARG:HH21	1.45	0.63
1:A:33:ARG:HG3	1:A:33:ARG:NH2	2.10	0.63
1:K:149[A]:OAS:OG	1:K:362:HIS:NE2	2.26	0.63
1:L:209:GLN:HE22	1:L:291:ALA:H	1.46	0.63
1:B:92:LEU:O	1:B:300:LYS:NZ	2.31	0.63
1:K:297:MET:O	1:K:300:LYS:HB2	1.99	0.63
1:E:269:GLN:H	1:E:270:PRO:HD2	1.64	0.63
1:A:149[A]:OAS:OG	1:A:362:HIS:NE2	2.26	0.62
1:B:78:ALA:H	1:B:373:ASN:HD21	1.45	0.62
1:D:120[B]:ARG:HG3	1:D:120[B]:ARG:NH1	1.98	0.62
1:G:149[A]:OAS:OG	1:G:362:HIS:NE2	2.24	0.62
1:I:10:GLU:HG2	1:L:44:ARG:HH12	1.62	0.62
1:E:92:LEU:O	1:E:300:LYS:NZ	2.32	0.62
1:G:352:ARG:HH22	1:G:382:GLN:HE22	1.46	0.62
1:I:149[B]:OAS:HB3	1:I:362:HIS:HE2	1.63	0.62
1:J:149[A]:OAS:OG	1:J:362:HIS:NE2	2.28	0.62
1:H:352:ARG:NH2	1:H:382:GLN:HE22	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128[A]:ARG:HG3	1:H:128[A]:ARG:NH2	2.15	0.62
1:E:209:GLN:HE22	1:E:291:ALA:H	1.47	0.61
1:L:44:ARG:NH2	4:L:2003:HOH:O	2.33	0.61
1:A:209:GLN:HE22	1:A:291:ALA:H	1.48	0.61
1:J:331:ARG:HG2	1:J:331:ARG:HH11	1.66	0.61
1:E:126:ASP:OD2	1:E:300:LYS:CE	2.49	0.61
1:F:209:GLN:HE22	1:F:291:ALA:H	1.48	0.61
1:I:78:ALA:H	1:I:373:ASN:ND2	1.99	0.61
1:A:126:ASP:OD2	1:A:300:LYS:CE	2.49	0.60
1:F:44:ARG:NH2	4:F:2004:HOH:O	2.34	0.60
1:A:65:VAL:HG12	1:A:73:PHE:HE1	1.67	0.60
1:F:65:VAL:HG12	1:F:73:PHE:HE1	1.66	0.60
1:H:109:GLU:HG2	1:H:112:ARG:HB2	1.81	0.60
1:K:126:ASP:OD2	1:K:300:LYS:HE2	1.99	0.60
1:G:352:ARG:NH2	1:G:382:GLN:HE22	1.99	0.60
1:E:352:ARG:HH22	1:E:382:GLN:HE22	1.49	0.60
1:F:124:ARG:O	1:F:128[A]:ARG:HG3	2.02	0.60
1:C:78:ALA:H	1:C:373:ASN:ND2	2.00	0.60
1:L:78:ALA:H	1:L:373:ASN:HD21	1.47	0.60
1:D:5:ILE:HG13	1:D:111:GLN:O	2.01	0.59
1:D:78:ALA:H	1:D:373:ASN:ND2	1.99	0.59
1:F:78:ALA:H	1:F:373:ASN:HD21	1.48	0.59
1:I:16:GLN:HG2	1:L:44:ARG:HH21	1.67	0.59
1:A:297:MET:O	1:A:300:LYS:HB2	2.02	0.59
1:A:160:PHE:O	1:B:31:ILE:HD13	2.02	0.59
1:F:54:ILE:HB	1:F:145:VAL:HB	1.85	0.59
1:J:163:PRO:HG3	1:J:322:THR:CG2	2.33	0.59
1:L:65:VAL:HG12	1:L:73:PHE:HE1	1.67	0.59
1:F:126:ASP:OD2	1:F:300:LYS:HE2	2.02	0.59
1:D:78:ALA:H	1:D:373:ASN:HD21	1.49	0.58
1:D:225:TYR:CZ	2:D:1383[B]:CSC:H3'1	2.39	0.58
1:E:149[A]:OAS:OG	1:E:362:HIS:NE2	2.31	0.58
1:E:297:MET:O	1:E:300:LYS:HB2	2.03	0.58
1:K:163:PRO:HG3	1:K:322:THR:CG2	2.33	0.58
1:B:16:GLN:HG2	1:F:44:ARG:HH21	1.69	0.58
1:J:27:GLU:CD	1:J:308:ARG:HH12	2.12	0.58
1:C:23:LEU:CD2	1:C:33:ARG:HG2	2.34	0.58
1:E:126:ASP:OD2	1:E:300:LYS:HE2	2.04	0.58
1:B:64:HIS:HD2	4:B:2002:HOH:O	1.86	0.57
1:G:92:LEU:O	1:G:300:LYS:NZ	2.35	0.57
1:A:126:ASP:OD2	1:A:300:LYS:HE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:PHE:CZ	3:A:1384:ACT:H2	2.39	0.57
1:B:164:GLU:HB2	4:B:2024:HOH:O	2.04	0.57
1:C:5:ILE:HG13	1:C:111:GLN:O	2.05	0.57
1:C:48:SER:O	1:C:140:ARG:NH2	2.38	0.57
1:H:128[A]:ARG:HH22	3:H:1384:ACT:H1	1.69	0.57
1:E:65:VAL:HG12	1:E:73:PHE:HE1	1.70	0.57
1:E:145:VAL:HG22	1:E:155:THR:HG23	1.85	0.57
1:J:297:MET:O	1:J:300:LYS:HB2	2.04	0.57
1:K:234:ARG:NH2	2:K:1385[B]:CSC:O19	2.37	0.57
1:C:149[A]:OAS:OG	1:C:362:HIS:NE2	2.30	0.57
1:F:225:TYR:CZ	2:F:1383[A]:CSC:H3'1	2.40	0.57
1:C:78:ALA:H	1:C:373:ASN:HD21	1.52	0.57
1:A:25:THR:HG21	3:B:1385:ACT:H2	1.87	0.57
1:L:20:ARG:HD3	1:L:34:ASP:OD1	2.04	0.57
2:E:1383[B]:CSC:O4B	2:E:1383[B]:CSC:C3'	2.53	0.56
1:F:352:ARG:NH2	1:F:382:GLN:HE22	2.02	0.56
1:H:209:GLN:HE22	1:H:291:ALA:H	1.53	0.56
1:H:269:GLN:CA	1:H:269:GLN:HE21	2.18	0.56
1:E:161:PHE:CZ	3:E:1384:ACT:CH3	2.88	0.56
1:G:209:GLN:HE22	1:G:291:ALA:H	1.53	0.56
1:J:234:ARG:NH2	2:J:1385[B]:CSC:O20	2.35	0.56
1:D:149[A]:OAS:OG	1:D:362:HIS:NE2	2.30	0.56
1:B:78:ALA:H	1:B:373:ASN:ND2	2.03	0.56
1:D:297:MET:O	1:D:300:LYS:HB2	2.05	0.56
1:H:78:ALA:H	1:H:373:ASN:HD21	1.52	0.56
1:E:226:LYS:NZ	1:E:363:ASP:OD2	2.38	0.56
1:F:48:SER:HB2	4:F:2007:HOH:O	2.06	0.55
1:L:126:ASP:OD2	1:L:300:LYS:HE2	2.07	0.55
1:C:297:MET:O	1:C:300:LYS:HB2	2.06	0.55
1:D:111:GLN:OE1	1:D:111:GLN:CA	2.54	0.55
1:J:126:ASP:OD2	1:J:300:LYS:HE2	2.05	0.55
1:L:225:TYR:CZ	2:L:1383[A]:CSC:H3'1	2.42	0.55
1:A:269:GLN:H	1:A:270:PRO:HD2	1.70	0.55
1:C:54:ILE:CD1	1:C:142:ILE:HD13	2.36	0.55
1:G:78:ALA:H	1:G:373:ASN:HD21	1.53	0.55
1:A:149[B]:OAS:OAC	2:A:1383[B]:CSC:O1	2.20	0.55
1:D:326:LEU:HD22	1:D:379:PHE:HB2	1.88	0.54
1:F:297:MET:O	1:F:300:LYS:HB2	2.07	0.54
1:L:27:GLU:HB3	1:L:128[A]:ARG:HH12	1.72	0.54
1:L:297:MET:O	1:L:300:LYS:HB2	2.08	0.54
1:D:54:ILE:CD1	1:D:142:ILE:HD13	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:269:GLN:H	1:I:270:PRO:HD2	1.71	0.54
1:J:65:VAL:HG12	1:J:73:PHE:HE1	1.71	0.54
1:C:326:LEU:HD22	1:C:379:PHE:HB2	1.89	0.54
1:I:149[B]:OAS:HB3	1:I:362:HIS:NE2	2.22	0.54
1:A:352:ARG:NH2	1:A:382:GLN:HE22	2.05	0.54
1:D:120[B]:ARG:CG	1:D:120[B]:ARG:NH1	2.63	0.54
1:K:331:ARG:HH11	1:K:331:ARG:HG2	1.72	0.54
1:K:124:ARG:O	1:K:128[A]:ARG:HG3	2.08	0.54
1:G:126:ASP:OD2	1:G:300:LYS:HE2	2.06	0.54
1:J:163:PRO:HG3	1:J:322:THR:HG21	1.90	0.54
1:K:27:GLU:CD	1:K:308:ARG:HH12	2.15	0.54
1:K:163:PRO:HG3	1:K:322:THR:HG21	1.89	0.54
1:B:10:GLU:HG2	1:F:44:ARG:NH1	2.22	0.54
1:D:59:LEU:HD12	1:D:297:MET:HB3	1.90	0.54
1:D:331:ARG:NH2	1:I:382:GLN:NE2	2.51	0.54
1:H:59:LEU:CD1	1:H:297:MET:HB3	2.37	0.53
1:H:92:LEU:O	1:H:300:LYS:NZ	2.40	0.53
1:J:307:SER:O	1:J:308:ARG:C	2.51	0.53
1:A:305:ASP:HB3	1:A:308:ARG:HG2	1.90	0.53
1:D:228:LYS:HB3	1:D:229:PRO:HD3	1.90	0.53
1:G:59:LEU:CD1	1:G:297:MET:HB3	2.37	0.53
1:H:148:ALA:HA	1:H:172:ILE:O	2.09	0.53
1:G:27:GLU:CD	1:G:308:ARG:HH12	2.15	0.53
1:D:108:ALA:C	1:D:111:GLN:HB2	2.33	0.53
1:C:228:LYS:HB3	1:C:229:PRO:HD3	1.91	0.53
1:C:104:PRO:HB3	1:C:110:GLY:HA2	1.91	0.52
2:A:1383[B]:CSC:O4B	2:A:1383[B]:CSC:C3'	2.57	0.52
1:K:65:VAL:HG12	1:K:73:PHE:HE1	1.74	0.52
1:H:33[A]:ARG:HG2	1:H:33[A]:ARG:HH21	1.73	0.52
1:G:148:ALA:HA	1:G:172:ILE:O	2.09	0.52
1:I:269:GLN:H	1:I:270:PRO:CD	2.22	0.52
1:A:31:ILE:HD13	1:B:160:PHE:O	2.09	0.52
1:L:225:TYR:OH	2:L:1383[A]:CSC:H3'1	2.10	0.52
1:B:126:ASP:OD2	1:B:300:LYS:HE3	2.10	0.51
1:K:148:ALA:HA	1:K:172:ILE:O	2.10	0.51
1:H:78:ALA:H	1:H:373:ASN:ND2	2.07	0.51
1:H:109:GLU:HB3	1:H:112:ARG:HB3	1.91	0.51
1:B:65:VAL:HG12	1:B:73:PHE:HE1	1.76	0.51
1:C:65:VAL:HG12	1:C:73:PHE:HE1	1.76	0.51
1:I:10:GLU:HG2	1:L:44:ARG:NH1	2.24	0.51
1:E:352:ARG:NH2	1:E:382:GLN:HE22	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:VAL:HG22	1:K:155:THR:HG23	1.93	0.51
1:I:65:VAL:HG12	1:I:73:PHE:HE1	1.76	0.51
1:G:298:THR:O	1:G:301:PHE:HB2	2.11	0.51
1:H:65:VAL:HG12	1:H:73:PHE:HE1	1.76	0.51
1:C:140:ARG:HB2	1:C:140:ARG:HH21	1.77	0.50
1:G:269:GLN:HA	1:G:269:GLN:NE2	2.26	0.50
1:B:269:GLN:H	1:B:270:PRO:CD	2.25	0.50
1:H:126:ASP:OD2	1:H:300:LYS:HE2	2.09	0.50
1:G:78:ALA:H	1:G:373:ASN:ND2	2.08	0.50
1:L:352:ARG:NH1	4:L:2035:HOH:O	2.43	0.50
1:F:65:VAL:HG12	1:F:73:PHE:CE1	2.46	0.50
1:J:148:ALA:HA	1:J:172:ILE:O	2.12	0.49
1:K:307:SER:O	1:K:308:ARG:C	2.54	0.49
1:D:65:VAL:HG12	1:D:73:PHE:HE1	1.77	0.49
1:I:10:GLU:CG	1:L:44:ARG:HH12	2.25	0.49
1:J:145:VAL:HG22	1:J:155:THR:HG23	1.94	0.49
1:K:226:LYS:NZ	1:K:363:ASP:OD2	2.42	0.49
1:L:352:ARG:NH2	1:L:382:GLN:HE22	2.08	0.49
1:B:269:GLN:H	1:B:270:PRO:HD2	1.78	0.49
1:G:272:GLU:CD	1:G:272:GLU:H	2.21	0.49
1:K:166:VAL:O	1:K:323:GLN:HG2	2.13	0.49
1:H:59:LEU:HD12	1:H:297:MET:HB3	1.93	0.49
1:K:78:ALA:H	1:K:373:ASN:ND2	2.10	0.49
1:A:166:VAL:O	1:A:323:GLN:HG2	2.13	0.49
1:C:82:SER:HB3	1:F:140:ARG:HE	1.78	0.49
1:D:106:PRO:C	1:D:108:ALA:H	2.21	0.48
1:D:148:ALA:HA	1:D:172:ILE:O	2.13	0.48
1:F:148:ALA:HA	1:F:172:ILE:O	2.13	0.48
1:F:228:LYS:HB3	1:F:229:PRO:HD3	1.95	0.48
1:F:78:ALA:H	1:F:373:ASN:ND2	2.11	0.48
1:J:190:ARG:HD3	1:J:298:THR:OG1	2.13	0.48
1:J:324:PRO:HG3	1:J:384:LEU:HD22	1.95	0.48
1:K:383:SER:C	1:K:384:LEU:HG	2.38	0.48
1:A:78:ALA:N	1:A:373:ASN:HD21	2.08	0.48
1:C:59:LEU:HD12	1:C:297:MET:HB3	1.96	0.48
1:C:148:ALA:HA	1:C:172:ILE:O	2.13	0.48
1:G:65:VAL:HG12	1:G:73:PHE:HE1	1.78	0.48
1:F:20:ARG:HG2	1:F:34:ASP:OD1	2.13	0.48
1:H:225:TYR:OH	2:H:1383[B]:CSC:H3'1	2.12	0.48
1:H:128[A]:ARG:HH21	1:H:128[A]:ARG:HG2	1.71	0.48
1:L:59:LEU:HD12	1:L:297:MET:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ARG:HH21	1:C:140:ARG:CB	2.27	0.48
1:H:269:GLN:HA	1:H:269:GLN:NE2	2.29	0.48
1:J:49:ARG:HD2	1:J:138:GLY:O	2.12	0.48
1:L:78:ALA:H	1:L:373:ASN:ND2	2.11	0.48
1:A:163:PRO:HG3	1:A:322:THR:CG2	2.43	0.48
1:A:225:TYR:OH	2:A:1383[B]:CSC:H3'1	2.13	0.48
1:C:54:ILE:HD11	1:C:142:ILE:HD13	1.94	0.48
1:F:59:LEU:HD12	1:F:297:MET:HB3	1.96	0.48
1:D:107:ASP:O	1:D:108:ALA:HB2	2.13	0.47
1:I:126:ASP:OD2	1:I:300:LYS:HE3	2.14	0.47
1:K:228:LYS:HB3	1:K:229:PRO:HD3	1.94	0.47
1:E:163:PRO:HG3	1:E:322:THR:CG2	2.43	0.47
1:J:228:LYS:HB3	1:J:229:PRO:HD3	1.96	0.47
1:L:65:VAL:HG12	1:L:73:PHE:CE1	2.47	0.47
1:A:65:VAL:HG12	1:A:73:PHE:CE1	2.47	0.47
1:F:20:ARG:HD3	1:F:34:ASP:OD1	2.14	0.47
1:H:269:GLN:CA	1:H:269:GLN:NE2	2.78	0.47
1:B:10:GLU:CG	1:F:44:ARG:HH12	2.24	0.47
1:H:298:THR:O	1:H:301:PHE:HB2	2.15	0.47
2:C:1383[B]:CSC:C4'	2:C:1383[B]:CSC:O1	2.63	0.47
1:L:218:ARG:NH2	4:L:2021:HOH:O	2.38	0.47
2:C:1383[B]:CSC:O1	2:C:1383[B]:CSC:O4B	2.33	0.47
1:D:226:LYS:NZ	1:D:363:ASP:OD2	2.45	0.47
1:H:326:LEU:HD22	1:H:379:PHE:HB2	1.96	0.47
1:J:23:LEU:CD2	1:J:33:ARG:HG3	2.38	0.47
1:J:166:VAL:O	1:J:323:GLN:HG2	2.15	0.47
1:K:54:ILE:CD1	1:K:142:ILE:HD13	2.44	0.47
1:L:148:ALA:HA	1:L:172:ILE:O	2.15	0.47
1:L:298:THR:O	1:L:301:PHE:HB2	2.15	0.47
1:B:10:GLU:C	1:F:44:ARG:NH1	2.72	0.47
1:G:59:LEU:HD12	1:G:297:MET:HB3	1.96	0.47
1:K:167:ARG:O	1:K:324:PRO:HD2	2.15	0.47
1:J:298:THR:O	1:J:301:PHE:HB2	2.14	0.47
1:K:145:VAL:HG13	1:K:169:ILE:HG22	1.97	0.47
2:A:1383[B]:CSC:O1	2:A:1383[B]:CSC:C4'	2.63	0.47
1:B:228:LYS:HB3	1:B:229:PRO:HD3	1.96	0.47
1:K:126:ASP:O	1:K:130:HIS:CG	2.68	0.47
1:D:54:ILE:HD12	1:D:142:ILE:HD13	1.96	0.46
1:F:225:TYR:OH	2:F:1383[A]:CSC:H3'1	2.15	0.46
1:D:59:LEU:CD1	1:D:297:MET:HB3	2.44	0.46
1:D:149[B]:OAS:HB3	1:D:362:HIS:HE2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:ARG:O	1:J:128[A]:ARG:HG3	2.16	0.46
1:I:149[A]:OAS:HA	1:I:173:ALA:O	2.16	0.46
1:J:126:ASP:O	1:J:130:HIS:CG	2.69	0.46
1:K:149[B]:OAS:HB3	1:K:362:HIS:HE2	1.81	0.46
1:C:382:GLN:CG	4:C:2043:HOH:O	2.64	0.46
1:L:150:MET:H	2:L:1383[A]:CSC:C20	2.28	0.46
1:C:382:GLN:HG3	4:C:2043:HOH:O	2.14	0.46
1:C:33:ARG:HD3	4:C:2003:HOH:O	2.15	0.46
1:K:59:LEU:HD12	1:K:297:MET:HB3	1.97	0.46
1:A:160:PHE:C	1:B:31:ILE:HD13	2.41	0.46
1:F:128[A]:ARG:HG2	3:F:1384:ACT:H3	1.98	0.46
1:F:102:CYS:HB2	4:F:2015:HOH:O	2.15	0.46
1:K:352:ARG:HH22	1:K:382:GLN:HE22	1.64	0.46
1:A:235:PHE:HA	1:A:269:GLN:O	2.16	0.46
1:C:145:VAL:HG22	1:C:155:THR:HG23	1.98	0.46
1:J:72:LEU:HA	1:J:373:ASN:HD22	1.80	0.46
1:E:218:ARG:HG3	1:E:222:ASN:ND2	2.30	0.45
1:D:54:ILE:HD11	1:D:142:ILE:CD1	2.46	0.45
1:E:65:VAL:HG12	1:E:73:PHE:CE1	2.50	0.45
1:G:269:GLN:NE2	1:G:269:GLN:CA	2.79	0.45
1:A:161:PHE:CZ	3:A:1384:ACT:CH3	2.99	0.45
1:B:326:LEU:HD22	1:B:379:PHE:HB2	1.97	0.45
1:C:81:THR:OG1	1:F:138:GLY:HA2	2.17	0.45
1:F:145:VAL:HG22	1:F:155:THR:HG23	1.99	0.45
1:J:45:MET:SD	1:J:49:ARG:HG2	2.56	0.45
1:J:226:LYS:NZ	1:J:363:ASP:OD2	2.45	0.45
1:K:59:LEU:CD1	1:K:297:MET:HB3	2.47	0.45
1:K:298:THR:O	1:K:301:PHE:HB2	2.16	0.45
1:B:166:VAL:O	1:B:323:GLN:HG2	2.16	0.45
1:E:126:ASP:OD2	1:E:300:LYS:HE3	2.16	0.45
1:L:124:ARG:O	1:L:128[A]:ARG:HG3	2.17	0.45
1:J:49:ARG:HH22	1:J:140:ARG:NH2	2.14	0.45
1:C:54:ILE:HD12	1:C:142:ILE:HD13	1.99	0.45
1:C:82:SER:HA	1:F:49:ARG:HD3	1.98	0.45
1:A:33:ARG:NH2	1:A:33:ARG:CG	2.77	0.45
1:C:164:GLU:HB2	4:C:2022:HOH:O	2.16	0.45
1:E:235:PHE:HA	1:E:269:GLN:O	2.16	0.45
1:G:269:GLN:CA	1:G:269:GLN:HE21	2.30	0.45
1:H:128[A]:ARG:NH2	3:H:1384:ACT:H1	2.32	0.45
1:A:136:ARG:HG2	1:C:22:SER:OG	2.17	0.45
1:A:157:GLU:OE1	1:A:310:ARG:NH2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:ARG:NH1	4:G:2020:HOH:O	2.46	0.45
1:H:272:GLU:CD	1:H:272:GLU:H	2.25	0.45
1:I:226:LYS:NZ	1:I:363:ASP:OD2	2.47	0.45
1:C:54:ILE:HD11	1:C:142:ILE:CD1	2.46	0.45
1:J:157:GLU:OE1	1:J:310:ARG:NH2	2.40	0.45
1:E:166:VAL:O	1:E:323:GLN:HG2	2.17	0.44
1:E:326:LEU:HD22	1:E:379:PHE:HB2	1.99	0.44
1:I:166:VAL:O	1:I:323:GLN:HG2	2.17	0.44
1:J:49:ARG:NH2	1:J:140:ARG:NH2	2.61	0.44
1:L:149[B]:OAS:HC22	2:L:1383[B]:CSC:H12	1.64	0.44
1:L:228:LYS:HB3	1:L:229:PRO:HD3	1.99	0.44
2:A:1383[B]:CSC:O4B	2:A:1383[B]:CSC:H3'1	2.17	0.44
1:K:120:ARG:HE	1:K:120:ARG:HB3	1.61	0.44
1:A:298:THR:O	1:A:301:PHE:HB2	2.17	0.44
1:J:33:ARG:CZ	1:J:33:ARG:HB2	2.48	0.44
1:K:78:ALA:H	1:K:373:ASN:HD21	1.65	0.44
1:D:214:LEU:HD22	1:D:285:PHE:HE1	1.82	0.44
1:B:149[B]:OAS:HB3	1:B:362:HIS:HE2	1.83	0.44
1:J:352:ARG:HH22	1:J:382:GLN:HE22	1.66	0.44
1:K:49:ARG:HH22	1:K:140:ARG:NH2	2.09	0.44
1:A:126:ASP:OD2	1:A:300:LYS:HE3	2.18	0.44
1:A:149[B]:OAS:HC22	2:A:1383[B]:CSC:H12	1.69	0.44
1:F:298:THR:O	1:F:301:PHE:HB2	2.18	0.44
1:H:150:MET:H	2:H:1383[A]:CSC:C20	2.31	0.44
1:A:28:SER:O	1:B:309:GLY:HA3	2.18	0.43
1:I:10:GLU:C	1:L:44:ARG:NH1	2.72	0.43
1:I:326:LEU:HD22	1:I:379:PHE:HB2	1.99	0.43
1:G:234:ARG:HH22	2:G:1383[B]:CSC:C18	2.29	0.43
1:H:225:TYR:OH	2:H:1383[A]:CSC:H3'1	2.16	0.43
1:J:120:ARG:HE	1:J:120:ARG:HB3	1.52	0.43
1:B:150:MET:O	1:B:153:MET:HB2	2.18	0.43
1:C:161:PHE:CE2	3:C:1384:ACT:H3	2.53	0.43
1:D:54:ILE:HD11	1:D:142:ILE:HD13	2.01	0.43
1:D:126:ASP:OD2	1:D:300:LYS:HE2	2.17	0.43
1:F:279:ARG:HH12	1:H:195:ASP:CG	2.26	0.43
1:J:54:ILE:CD1	1:J:142:ILE:HD13	2.49	0.43
1:H:109:GLU:HB3	1:H:112:ARG:CB	2.48	0.43
1:A:225:TYR:CZ	2:A:1383[B]:CSC:H3'1	2.53	0.43
1:J:167:ARG:O	1:J:324:PRO:HD2	2.19	0.43
1:E:269:GLN:HE21	1:E:269:GLN:HB3	1.51	0.43
1:J:22:SER:HA	1:J:34:ASP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:321:ILE:O	1:H:349:PRO:HD2	2.19	0.43
1:D:120[A]:ARG:NH1	4:D:2018:HOH:O	2.51	0.43
1:I:150:MET:O	1:I:153:MET:HB2	2.18	0.43
1:I:228:LYS:HB3	1:I:229:PRO:HD3	2.00	0.43
1:A:149[B]:OAS:HB3	1:A:362:HIS:HE2	1.84	0.43
1:E:161:PHE:CE1	3:E:1384:ACT:H3	2.54	0.43
1:I:148:ALA:HB2	1:I:172:ILE:HB	2.01	0.43
1:J:324:PRO:HA	1:J:350:ASN:O	2.19	0.43
1:I:163:PRO:HG3	1:I:322:THR:CG2	2.49	0.42
1:C:166:VAL:O	1:C:323:GLN:HG2	2.18	0.42
1:E:78:ALA:N	1:E:373:ASN:HD21	2.08	0.42
1:E:161:PHE:CE2	3:E:1384:ACT:CH3	3.02	0.42
1:F:59:LEU:CD1	1:F:297:MET:HB3	2.48	0.42
1:J:54:ILE:HB	1:J:145:VAL:HB	2.00	0.42
1:K:54:ILE:HD11	1:K:142:ILE:CD1	2.50	0.42
1:B:269:GLN:HE21	1:B:269:GLN:HB3	1.66	0.42
1:E:214:LEU:HD22	1:E:285:PHE:CE1	2.55	0.42
1:F:20:ARG:CD	1:F:34:ASP:OD1	2.68	0.42
1:I:16:GLN:HG2	1:L:44:ARG:NH2	2.32	0.42
1:J:54:ILE:HD11	1:J:142:ILE:HD13	2.02	0.42
1:L:326:LEU:HD22	1:L:379:PHE:HB2	2.00	0.42
1:A:218:ARG:HG3	1:A:222:ASN:ND2	2.35	0.42
1:E:58:THR:HB	2:E:1383[B]:CSC:O1	2.20	0.42
1:G:326:LEU:HD22	1:G:379:PHE:HB2	2.01	0.42
1:J:65:VAL:HG12	1:J:73:PHE:CE1	2.54	0.42
1:J:141:GLN:OE1	1:J:167:ARG:NH1	2.52	0.42
1:A:59:LEU:CD1	1:A:297:MET:HB3	2.50	0.42
1:E:293:CYS:O	1:E:297:MET:HG2	2.19	0.42
1:J:59:LEU:CD1	1:J:297:MET:HB3	2.50	0.42
1:J:78:ALA:H	1:J:373:ASN:ND2	2.17	0.42
1:L:20:ARG:HH11	1:L:20:ARG:HG3	1.85	0.42
1:A:141:GLN:OE1	1:A:167:ARG:NH1	2.51	0.42
1:C:126:ASP:OD2	1:C:300:LYS:HE2	2.20	0.42
1:H:209:GLN:HE21	1:H:209:GLN:HB3	1.70	0.42
1:C:218:ARG:NH1	4:C:2027:HOH:O	2.51	0.42
4:G:2035:HOH:O	1:L:237:MET:HE1	2.19	0.42
1:J:145:VAL:HG13	1:J:169:ILE:HG22	2.02	0.42
1:A:226:LYS:NZ	1:A:363:ASP:OD2	2.40	0.42
1:F:209:GLN:HE21	1:F:209:GLN:HB3	1.69	0.42
1:F:326:LEU:HD22	1:F:379:PHE:HB2	2.00	0.42
1:K:72:LEU:HA	1:K:373:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HH22	2:A:1383[B]:CSC:C18	2.23	0.42
1:B:48:SER:O	1:B:140:ARG:HD3	2.19	0.42
1:D:106:PRO:C	1:D:108:ALA:N	2.78	0.42
1:D:112:ARG:HH21	1:D:112:ARG:HG3	1.84	0.42
1:J:59:LEU:HD12	1:J:297:MET:HB3	2.01	0.42
1:E:157:GLU:OE1	1:E:310:ARG:NH2	2.41	0.41
1:G:67:SER:HB3	4:G:2008:HOH:O	2.20	0.41
1:I:72:LEU:HA	1:I:373:ASN:HD22	1.85	0.41
1:F:225:TYR:OH	2:F:1383[B]:CSC:H3'1	2.21	0.41
1:I:149[B]:OAS:HC22	2:I:1383[B]:CSC:H12	1.99	0.41
1:J:336:TYR:CD1	1:J:362:HIS:CE1	3.08	0.41
1:D:118:PHE:HA	1:D:119:PRO:HD3	1.95	0.41
1:G:297:MET:O	1:G:300:LYS:HB2	2.20	0.41
1:G:321:ILE:O	1:G:349:PRO:HD2	2.20	0.41
1:H:269:GLN:HE21	1:H:269:GLN:C	2.28	0.41
1:J:58:THR:O	1:J:59:LEU:C	2.64	0.41
1:K:54:ILE:HB	1:K:145:VAL:HB	2.01	0.41
1:I:13:LEU:HD11	1:I:96:PHE:HB3	2.03	0.41
1:K:157:GLU:CD	1:K:310:ARG:HH22	2.26	0.41
1:L:281:GLN:H	1:L:281:GLN:HG2	1.72	0.41
1:A:214:LEU:HD22	1:A:285:PHE:CE1	2.56	0.41
1:E:209:GLN:HE21	1:E:209:GLN:HB3	1.61	0.41
1:I:225:TYR:HA	1:I:362:HIS:HB3	2.03	0.41
1:K:54:ILE:HD11	1:K:142:ILE:HD13	2.03	0.41
1:B:225:TYR:HA	1:B:362:HIS:HB3	2.03	0.41
1:D:185:TRP:CD2	1:K:223:LEU:HD13	2.55	0.41
1:E:281:GLN:H	1:E:281:GLN:HG2	1.74	0.41
1:F:225:TYR:CZ	2:F:1383[B]:CSC:H3'1	2.55	0.41
1:F:237:MET:HE1	4:H:2036:HOH:O	2.21	0.41
1:F:336:TYR:CD1	1:F:362:HIS:CE1	3.08	0.41
1:G:209:GLN:HE21	1:G:209:GLN:HB3	1.70	0.41
1:C:106:PRO:C	1:C:108:ALA:H	2.28	0.41
1:E:365:PHE:CE1	1:E:366:VAL:HG23	2.55	0.41
1:F:22:SER:HA	1:F:34:ASP:HA	2.02	0.41
1:H:27:GLU:CD	1:H:308:ARG:HH11	2.28	0.41
1:I:297:MET:O	1:I:300:LYS:HB2	2.20	0.41
1:D:161:PHE:CZ	3:D:1384:ACT:H2	2.56	0.41
1:A:293:CYS:O	1:A:297:MET:HG2	2.21	0.41
1:A:365:PHE:CE1	1:A:366:VAL:HG23	2.56	0.41
1:B:49:ARG:NH2	1:B:140:ARG:HD2	2.35	0.41
1:G:142:ILE:HD12	1:G:165:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:LEU:H	2:H:1383[A]:CSC:C1	2.34	0.41
1:H:228:LYS:HB3	1:H:229:PRO:HD3	2.03	0.41
1:J:281:GLN:H	1:J:281:GLN:HG2	1.70	0.41
1:K:58:THR:O	1:K:59:LEU:C	2.64	0.41
1:K:326:LEU:HD22	1:K:379:PHE:HB2	2.03	0.41
1:A:137:LEU:HD23	1:C:23:LEU:HD12	2.03	0.41
1:D:105:ASP:HA	1:D:106:PRO:HD2	1.88	0.41
1:I:226:LYS:NZ	2:I:1383[B]:CSC:O19	2.35	0.41
1:G:234:ARG:NH2	2:G:1383[B]:CSC:O19	2.48	0.40
1:K:226:LYS:CE	1:K:363:ASP:OD2	2.68	0.40
1:D:90:ASN:HB3	1:D:98:SER:OG	2.21	0.40
1:G:41:SER:HA	1:G:86:ILE:O	2.21	0.40
1:J:171:PRO:HD2	1:J:326:LEU:O	2.22	0.40
1:J:199:TYR:O	1:J:200:LEU:HB2	2.21	0.40
1:B:59:LEU:HD12	1:B:297:MET:HB3	2.02	0.40
1:H:33[A]:ARG:HG2	1:H:33[A]:ARG:NH2	2.35	0.40
1:J:149[B]:OAS:HB3	1:J:362:HIS:HE2	1.86	0.40
1:J:363:ASP:O	1:J:364:PHE:C	2.62	0.40
1:B:16:GLN:HG2	1:F:44:ARG:NH2	2.34	0.40
2:B:1384[B]:CSC:O1	2:B:1384[B]:CSC:C4'	2.67	0.40
1:F:272:GLU:H	1:F:272:GLU:CD	2.29	0.40
1:I:59:LEU:HD12	1:I:297:MET:HB3	2.02	0.40
1:K:74:GLY:O	1:K:75:GLN:C	2.64	0.40
1:K:91:TYR:CE2	1:K:154:HIS:CD2	3.10	0.40
1:K:171:PRO:HD2	1:K:326:LEU:O	2.21	0.40
1:B:209:GLN:HE21	1:B:209:GLN:HB3	1.69	0.40
1:C:111:GLN:HA	1:C:111:GLN:OE1	2.22	0.40
1:D:107:ASP:O	1:D:108:ALA:CB	2.70	0.40
1:F:54:ILE:CD1	1:F:142:ILE:HD13	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:GLN:OE1	1:K:49:ARG:NH2[2_655]	1.99	0.21
1:G:283:GLN:OE1	1:J:49:ARG:NH2[1_556]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/444 (77%)	328 (96%)	11 (3%)	2 (1%)	21	38
1	B	343/444 (77%)	329 (96%)	12 (4%)	2 (1%)	21	38
1	C	344/444 (78%)	330 (96%)	13 (4%)	1 (0%)	36	55
1	D	340/444 (77%)	329 (97%)	9 (3%)	2 (1%)	21	38
1	E	339/444 (76%)	327 (96%)	10 (3%)	2 (1%)	21	38
1	F	334/444 (75%)	323 (97%)	10 (3%)	1 (0%)	36	55
1	G	335/444 (76%)	323 (96%)	11 (3%)	1 (0%)	36	55
1	H	336/444 (76%)	324 (96%)	11 (3%)	1 (0%)	36	55
1	I	341/444 (77%)	328 (96%)	11 (3%)	2 (1%)	21	38
1	J	337/444 (76%)	322 (96%)	14 (4%)	1 (0%)	36	55
1	K	334/444 (75%)	319 (96%)	14 (4%)	1 (0%)	36	55
1	L	333/444 (75%)	319 (96%)	13 (4%)	1 (0%)	36	55
All	All	4057/5328 (76%)	3901 (96%)	139 (3%)	17 (0%)	30	49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ASP
1	B	363	ASP
1	C	363	ASP
1	D	363	ASP
1	E	363	ASP
1	F	363	ASP
1	G	363	ASP
1	H	363	ASP
1	I	363	ASP
1	J	363	ASP
1	K	363	ASP
1	L	363	ASP

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Mol	Chain	Res	Type
1	D	107	ASP
1	A	269	GLN
1	E	269	GLN
1	I	269	GLN
1	B	269	GLN

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	290/371 (78%)	280 (97%)	10 (3%)	32	60
1	B	291/371 (78%)	281 (97%)	10 (3%)	32	60
1	C	292/371 (79%)	276 (94%)	16 (6%)	19	40
1	D	291/371 (78%)	280 (96%)	11 (4%)	29	56
1	E	288/371 (78%)	277 (96%)	11 (4%)	29	56
1	F	286/371 (77%)	275 (96%)	11 (4%)	29	56
1	G	287/371 (77%)	273 (95%)	14 (5%)	22	45
1	H	287/371 (77%)	275 (96%)	12 (4%)	26	52
1	I	289/371 (78%)	279 (96%)	10 (4%)	32	58
1	J	288/371 (78%)	275 (96%)	13 (4%)	24	49
1	K	286/371 (77%)	275 (96%)	11 (4%)	29	56
1	L	286/371 (77%)	275 (96%)	11 (4%)	29	56
All	All	3461/4452 (78%)	3321 (96%)	140 (4%)	28	54

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

Mol	Chain	Res	Type
1	A	48	SER
1	A	61	SER
1	A	69	TRP
1	A	269	GLN
1	A	271	ILE

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Mol	Chain	Res	Type
1	A	283	GLN
1	A	300	LYS
1	A	322	THR
1	A	326	LEU
1	A	380	LEU
1	B	48	SER
1	B	61	SER
1	B	69	TRP
1	B	111	GLN
1	B	201	ASP
1	B	269	GLN
1	B	271	ILE
1	B	283	GLN
1	B	322	THR
1	B	380	LEU
1	C	5	ILE
1	C	20[A]	ARG
1	C	20[B]	ARG
1	C	48	SER
1	C	61	SER
1	C	69	TRP
1	C	109	GLU
1	C	128[A]	ARG
1	C	131	ARG
1	C	145	VAL
1	C	201	ASP
1	C	269	GLN
1	C	271	ILE
1	C	283	GLN
1	C	322	THR
1	C	380	LEU
1	D	5	ILE
1	D	48	SER
1	D	61	SER
1	D	69	TRP
1	D	128[A]	ARG
1	D	145	VAL
1	D	269	GLN
1	D	271	ILE
1	D	283	GLN
1	D	322	THR
1	D	380	LEU

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Mol	Chain	Res	Type
1	E	33	ARG
1	E	48	SER
1	E	61	SER
1	E	69	TRP
1	E	145	VAL
1	E	269	GLN
1	E	271	ILE
1	E	283	GLN
1	E	300	LYS
1	E	322	THR
1	E	380	LEU
1	F	48	SER
1	F	61	SER
1	F	69	TRP
1	F	81	THR
1	F	107	ASP
1	F	145	VAL
1	F	269	GLN
1	F	271	ILE
1	F	283	GLN
1	F	322	THR
1	F	380	LEU
1	G	33[A]	ARG
1	G	48	SER
1	G	61	SER
1	G	69	TRP
1	G	86	ILE
1	G	128[A]	ARG
1	G	134	LEU
1	G	140	ARG
1	G	200	LEU
1	G	269	GLN
1	G	271	ILE
1	G	283	GLN
1	G	322	THR
1	G	380	LEU
1	H	30	VAL
1	H	48	SER
1	H	61	SER
1	H	69	TRP
1	H	86	ILE
1	H	109	GLU

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Mol	Chain	Res	Type
1	H	128[A]	ARG
1	H	269	GLN
1	H	271	ILE
1	H	283	GLN
1	H	322	THR
1	H	380	LEU
1	I	48	SER
1	I	61	SER
1	I	69	TRP
1	I	201	ASP
1	I	271	ILE
1	I	283	GLN
1	I	300	LYS
1	I	322	THR
1	I	331	ARG
1	I	380	LEU
1	J	48	SER
1	J	61	SER
1	J	69	TRP
1	J	81	THR
1	J	145	VAL
1	J	200	LEU
1	J	269	GLN
1	J	271	ILE
1	J	283	GLN
1	J	308	ARG
1	J	322	THR
1	J	332	SER
1	J	380	LEU
1	K	48	SER
1	K	61	SER
1	K	69	TRP
1	K	145	VAL
1	K	271	ILE
1	K	283	GLN
1	K	308	ARG
1	K	322	THR
1	K	332	SER
1	K	380	LEU
1	K	384	LEU
1	L	48	SER
1	L	61	SER

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Mol	Chain	Res	Type
1	L	69	TRP
1	L	81	THR
1	L	107	ASP
1	L	269	GLN
1	L	271	ILE
1	L	283	GLN
1	L	322	THR
1	L	332	SER
1	L	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	222	ASN
1	A	236	HIS
1	A	269	GLN
1	A	283	GLN
1	A	373	ASN
1	A	382	GLN
1	B	64	HIS
1	B	209	GLN
1	B	236	HIS
1	B	269	GLN
1	B	283	GLN
1	B	373	ASN
1	B	382	GLN
1	C	64	HIS
1	C	209	GLN
1	C	236	HIS
1	C	269	GLN
1	C	283	GLN
1	C	373	ASN
1	C	382	GLN
1	D	209	GLN
1	D	236	HIS
1	D	269	GLN
1	D	283	GLN
1	D	373	ASN
1	D	382	GLN
1	E	209	GLN
1	E	222	ASN

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Mol	Chain	Res	Type
1	E	236	HIS
1	E	269	GLN
1	E	281	GLN
1	E	283	GLN
1	E	373	ASN
1	E	382	GLN
1	F	64	HIS
1	F	209	GLN
1	F	236	HIS
1	F	283	GLN
1	F	373	ASN
1	F	382	GLN
1	G	64	HIS
1	G	209	GLN
1	G	222	ASN
1	G	236	HIS
1	G	269	GLN
1	G	283	GLN
1	G	350	ASN
1	G	373	ASN
1	G	382	GLN
1	H	64	HIS
1	H	209	GLN
1	H	222	ASN
1	H	236	HIS
1	H	269	GLN
1	H	283	GLN
1	H	350	ASN
1	H	373	ASN
1	H	382	GLN
1	I	64	HIS
1	I	209	GLN
1	I	236	HIS
1	I	269	GLN
1	I	283	GLN
1	I	373	ASN
1	I	382	GLN
1	J	209	GLN
1	J	281	GLN
1	J	283	GLN
1	J	292	ASN
1	J	373	ASN

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Mol	Chain	Res	Type
1	J	382	GLN
1	K	90	ASN
1	K	209	GLN
1	K	236	HIS
1	K	281	GLN
1	K	283	GLN
1	K	292	ASN
1	K	373	ASN
1	L	64	HIS
1	L	209	GLN
1	L	236	HIS
1	L	269	GLN
1	L	283	GLN
1	L	373	ASN
1	L	382	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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
1	OAS	F	149[B]	-	7,8,9	1.31	1 (14%)	4,9,11	0.76	0
1	OAS	H	149[B]	-	7,8,9	1.23	1 (14%)	4,9,11	1.07	0
1	OAS	L	149[A]	-	7,5,9	7.54	1 (14%)	4,5,11	8.19	3 (75%)
1	OAS	D	149[A]	-	7,5,9	7.58	1 (14%)	4,5,11	7.85	3 (75%)
1	OAS	E	149[B]	-	7,8,9	1.21	1 (14%)	4,9,11	0.88	0
1	OAS	A	149[B]	-	7,8,9	1.29	1 (14%)	4,9,11	0.67	0
1	OAS	I	149[A]	-	7,5,9	8.61	1 (14%)	4,5,11	9.06	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OAS	K	149[A]	-	7,5,9	8.83	1 (14%)	4,5,11	8.46	3 (75%)
1	OAS	B	149[A]	-	7,5,9	7.98	1 (14%)	4,5,11	8.37	3 (75%)
1	OAS	C	149[A]	-	7,5,9	7.58	1 (14%)	4,5,11	7.83	3 (75%)
1	OAS	G	149[A]	-	7,5,9	7.77	1 (14%)	4,5,11	8.19	3 (75%)
1	OAS	J	149[A]	-	7,5,9	8.54	1 (14%)	4,5,11	8.29	3 (75%)
1	OAS	L	149[B]	-	7,8,9	1.24	1 (14%)	4,9,11	0.51	0
1	OAS	D	149[B]	-	7,8,9	1.31	1 (14%)	4,9,11	0.86	0
1	OAS	I	149[B]	-	7,8,9	1.34	1 (14%)	4,9,11	1.52	1 (25%)
1	OAS	K	149[B]	-	7,8,9	1.27	1 (14%)	4,9,11	1.28	0
1	OAS	F	149[A]	-	7,5,9	7.58	1 (14%)	4,5,11	8.06	3 (75%)
1	OAS	C	149[B]	-	7,8,9	1.36	1 (14%)	4,9,11	0.87	0
1	OAS	B	149[B]	-	7,8,9	1.17	1 (14%)	4,9,11	1.10	0
1	OAS	H	149[A]	-	7,5,9	7.99	1 (14%)	4,5,11	8.37	3 (75%)
1	OAS	E	149[A]	-	7,5,9	7.53	1 (14%)	4,5,11	8.15	3 (75%)
1	OAS	A	149[A]	-	7,5,9	7.59	1 (14%)	4,5,11	8.55	3 (75%)
1	OAS	J	149[B]	-	7,8,9	1.33	1 (14%)	4,9,11	1.08	0
1	OAS	G	149[B]	-	7,8,9	1.25	1 (14%)	4,9,11	0.97	0

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
1	OAS	F	149[B]	-	-	3/5/7/9	-
1	OAS	H	149[B]	-	-	3/5/7/9	-
1	OAS	L	149[A]	-	-	4/5/4/9	-
1	OAS	D	149[A]	-	-	4/5/4/9	-
1	OAS	E	149[B]	-	-	3/5/7/9	-
1	OAS	A	149[B]	-	-	3/5/7/9	-
1	OAS	I	149[A]	-	-	4/5/4/9	-
1	OAS	K	149[A]	-	-	4/5/4/9	-
1	OAS	B	149[A]	-	-	4/5/4/9	-
1	OAS	C	149[A]	-	-	4/5/4/9	-
1	OAS	G	149[A]	-	-	4/5/4/9	-
1	OAS	J	149[A]	-	-	4/5/4/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OAS	L	149[B]	-	-	3/5/7/9	-
1	OAS	D	149[B]	-	-	3/5/7/9	-
1	OAS	I	149[B]	-	-	3/5/7/9	-
1	OAS	K	149[B]	-	-	3/5/7/9	-
1	OAS	F	149[A]	-	-	4/5/4/9	-
1	OAS	C	149[B]	-	-	3/5/7/9	-
1	OAS	B	149[B]	-	-	3/5/7/9	-
1	OAS	H	149[A]	-	-	4/5/4/9	-
1	OAS	E	149[A]	-	-	4/5/4/9	-
1	OAS	A	149[A]	-	-	4/5/4/9	-
1	OAS	J	149[B]	-	-	3/5/7/9	-
1	OAS	G	149[B]	-	-	3/5/7/9	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	149[A]	OAS	OG-C1A	23.32	2.43	1.33
1	I	149[A]	OAS	OG-C1A	22.66	2.40	1.33
1	J	149[A]	OAS	OG-C1A	22.53	2.39	1.33
1	H	149[A]	OAS	OG-C1A	21.09	2.33	1.33
1	B	149[A]	OAS	OG-C1A	21.07	2.32	1.33
1	G	149[A]	OAS	OG-C1A	20.48	2.30	1.33
1	A	149[A]	OAS	OG-C1A	20.01	2.27	1.33
1	D	149[A]	OAS	OG-C1A	19.99	2.27	1.33
1	F	149[A]	OAS	OG-C1A	19.98	2.27	1.33
1	C	149[A]	OAS	OG-C1A	19.97	2.27	1.33
1	L	149[A]	OAS	OG-C1A	19.91	2.27	1.33
1	E	149[A]	OAS	OG-C1A	19.85	2.27	1.33
1	C	149[B]	OAS	OG-C1A	3.13	1.48	1.33
1	D	149[B]	OAS	OG-C1A	3.09	1.48	1.33
1	F	149[B]	OAS	OG-C1A	3.07	1.48	1.33
1	J	149[B]	OAS	OG-C1A	2.98	1.47	1.33
1	K	149[B]	OAS	OG-C1A	2.93	1.47	1.33
1	L	149[B]	OAS	OG-C1A	2.92	1.47	1.33
1	A	149[B]	OAS	OG-C1A	2.90	1.47	1.33
1	H	149[B]	OAS	OG-C1A	2.82	1.46	1.33
1	I	149[B]	OAS	OG-C1A	2.74	1.46	1.33
1	G	149[B]	OAS	OG-C1A	2.71	1.46	1.33
1	E	149[B]	OAS	OG-C1A	2.63	1.46	1.33
1	B	149[B]	OAS	OG-C1A	2.62	1.46	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	149[A]	OAS	CB-OG-C1A	-17.10	74.90	117.08
1	A	149[A]	OAS	CB-OG-C1A	-16.19	77.15	117.08
1	K	149[A]	OAS	CB-OG-C1A	-15.85	77.97	117.08
1	B	149[A]	OAS	CB-OG-C1A	-15.79	78.11	117.08
1	H	149[A]	OAS	CB-OG-C1A	-15.67	78.43	117.08
1	J	149[A]	OAS	CB-OG-C1A	-15.56	78.70	117.08
1	G	149[A]	OAS	CB-OG-C1A	-15.51	78.82	117.08
1	E	149[A]	OAS	CB-OG-C1A	-15.45	78.96	117.08
1	L	149[A]	OAS	CB-OG-C1A	-15.12	79.77	117.08
1	D	149[A]	OAS	CB-OG-C1A	-14.96	80.18	117.08
1	C	149[A]	OAS	CB-OG-C1A	-14.95	80.21	117.08
1	F	149[A]	OAS	CB-OG-C1A	-14.77	80.65	117.08
1	F	149[A]	OAS	OG-C1A-OAC	4.59	144.63	121.59
1	L	149[A]	OAS	OG-C1A-C2A	-4.46	93.44	112.38
1	F	149[A]	OAS	OG-C1A-C2A	-4.44	93.53	112.38
1	L	149[A]	OAS	OG-C1A-OAC	4.36	143.49	121.59
1	I	149[A]	OAS	OG-C1A-C2A	-4.28	94.19	112.38
1	H	149[A]	OAS	OG-C1A-OAC	4.22	142.78	121.59
1	K	149[A]	OAS	OG-C1A-OAC	4.21	142.74	121.59
1	I	149[A]	OAS	OG-C1A-OAC	4.18	142.60	121.59
1	J	149[A]	OAS	OG-C1A-OAC	4.13	142.30	121.59
1	A	149[A]	OAS	OG-C1A-OAC	4.01	141.72	121.59
1	K	149[A]	OAS	OG-C1A-C2A	-4.00	95.41	112.38
1	H	149[A]	OAS	OG-C1A-C2A	-4.00	95.41	112.38
1	B	149[A]	OAS	OG-C1A-C2A	-3.92	95.74	112.38
1	B	149[A]	OAS	OG-C1A-OAC	3.88	141.05	121.59
1	J	149[A]	OAS	OG-C1A-C2A	-3.83	96.14	112.38
1	G	149[A]	OAS	OG-C1A-C2A	-3.80	96.25	112.38
1	E	149[A]	OAS	OG-C1A-OAC	3.68	140.07	121.59
1	A	149[A]	OAS	OG-C1A-C2A	-3.65	96.89	112.38
1	G	149[A]	OAS	OG-C1A-OAC	3.65	139.91	121.59
1	E	149[A]	OAS	OG-C1A-C2A	-3.64	96.93	112.38
1	D	149[A]	OAS	OG-C1A-OAC	3.42	138.76	121.59
1	C	149[A]	OAS	OG-C1A-OAC	3.36	138.46	121.59
1	D	149[A]	OAS	OG-C1A-C2A	-3.24	98.63	112.38
1	C	149[A]	OAS	OG-C1A-C2A	-3.10	99.20	112.38
1	I	149[B]	OAS	CB-OG-C1A	2.17	122.44	117.08

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	149[A]	OAS	C-CA-CB-OG
1	B	149[A]	OAS	C-CA-CB-OG
1	B	149[B]	OAS	C-CA-CB-OG
1	C	149[A]	OAS	C-CA-CB-OG
1	D	149[A]	OAS	C-CA-CB-OG
1	E	149[A]	OAS	C-CA-CB-OG
1	F	149[A]	OAS	C-CA-CB-OG
1	G	149[A]	OAS	C-CA-CB-OG
1	H	149[A]	OAS	C-CA-CB-OG
1	I	149[A]	OAS	N-CA-CB-OG
1	I	149[A]	OAS	C-CA-CB-OG
1	I	149[B]	OAS	C-CA-CB-OG
1	J	149[A]	OAS	C-CA-CB-OG
1	K	149[A]	OAS	C-CA-CB-OG
1	K	149[B]	OAS	C-CA-CB-OG
1	L	149[A]	OAS	C-CA-CB-OG
1	A	149[B]	OAS	OAC-C1A-OG-CB
1	J	149[A]	OAS	C2A-C1A-OG-CB
1	C	149[B]	OAS	OAC-C1A-OG-CB
1	D	149[B]	OAS	OAC-C1A-OG-CB
1	E	149[B]	OAS	OAC-C1A-OG-CB
1	G	149[B]	OAS	OAC-C1A-OG-CB
1	I	149[B]	OAS	OAC-C1A-OG-CB
1	K	149[A]	OAS	OAC-C1A-OG-CB
1	A	149[A]	OAS	C2A-C1A-OG-CB
1	C	149[A]	OAS	C2A-C1A-OG-CB
1	D	149[A]	OAS	C2A-C1A-OG-CB
1	F	149[A]	OAS	C2A-C1A-OG-CB
1	K	149[A]	OAS	C2A-C1A-OG-CB
1	L	149[A]	OAS	C2A-C1A-OG-CB
1	B	149[B]	OAS	OAC-C1A-OG-CB
1	C	149[A]	OAS	OAC-C1A-OG-CB
1	F	149[B]	OAS	OAC-C1A-OG-CB
1	H	149[B]	OAS	OAC-C1A-OG-CB
1	J	149[A]	OAS	OAC-C1A-OG-CB
1	J	149[B]	OAS	OAC-C1A-OG-CB
1	L	149[A]	OAS	OAC-C1A-OG-CB
1	L	149[B]	OAS	OAC-C1A-OG-CB
1	A	149[B]	OAS	C2A-C1A-OG-CB
1	B	149[A]	OAS	C2A-C1A-OG-CB
1	C	149[B]	OAS	C2A-C1A-OG-CB
1	D	149[B]	OAS	C2A-C1A-OG-CB
1	E	149[A]	OAS	C2A-C1A-OG-CB

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Mol	Chain	Res	Type	Atoms
1	E	149[B]	OAS	C2A-C1A-OG-CB
1	F	149[B]	OAS	C2A-C1A-OG-CB
1	G	149[A]	OAS	C2A-C1A-OG-CB
1	G	149[B]	OAS	C2A-C1A-OG-CB
1	H	149[A]	OAS	C2A-C1A-OG-CB
1	H	149[B]	OAS	C2A-C1A-OG-CB
1	L	149[B]	OAS	C2A-C1A-OG-CB
1	F	149[A]	OAS	OAC-C1A-OG-CB
1	K	149[B]	OAS	OAC-C1A-OG-CB
1	B	149[B]	OAS	C2A-C1A-OG-CB
1	I	149[A]	OAS	C2A-C1A-OG-CB
1	I	149[B]	OAS	C2A-C1A-OG-CB
1	J	149[B]	OAS	C2A-C1A-OG-CB
1	D	149[A]	OAS	OAC-C1A-OG-CB
1	A	149[A]	OAS	OAC-C1A-OG-CB
1	B	149[A]	OAS	OAC-C1A-OG-CB
1	H	149[A]	OAS	OAC-C1A-OG-CB
1	K	149[B]	OAS	C2A-C1A-OG-CB
1	E	149[A]	OAS	OAC-C1A-OG-CB
1	G	149[A]	OAS	OAC-C1A-OG-CB
1	I	149[A]	OAS	OAC-C1A-OG-CB
1	A	149[B]	OAS	C-CA-CB-OG
1	C	149[B]	OAS	C-CA-CB-OG
1	D	149[B]	OAS	C-CA-CB-OG
1	E	149[B]	OAS	C-CA-CB-OG
1	F	149[B]	OAS	C-CA-CB-OG
1	G	149[B]	OAS	C-CA-CB-OG
1	H	149[B]	OAS	C-CA-CB-OG
1	J	149[B]	OAS	C-CA-CB-OG
1	L	149[B]	OAS	C-CA-CB-OG
1	A	149[A]	OAS	N-CA-CB-OG
1	B	149[A]	OAS	N-CA-CB-OG
1	C	149[A]	OAS	N-CA-CB-OG
1	D	149[A]	OAS	N-CA-CB-OG
1	E	149[A]	OAS	N-CA-CB-OG
1	F	149[A]	OAS	N-CA-CB-OG
1	G	149[A]	OAS	N-CA-CB-OG
1	H	149[A]	OAS	N-CA-CB-OG
1	J	149[A]	OAS	N-CA-CB-OG
1	K	149[A]	OAS	N-CA-CB-OG
1	L	149[A]	OAS	N-CA-CB-OG

There are no ring outliers.

21 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	149[B]	OAS	1	0
1	H	149[B]	OAS	1	0
1	L	149[A]	OAS	1	0
1	D	149[A]	OAS	1	0
1	A	149[B]	OAS	3	0
1	I	149[A]	OAS	2	0
1	K	149[A]	OAS	1	0
1	B	149[A]	OAS	1	0
1	C	149[A]	OAS	1	0
1	G	149[A]	OAS	1	0
1	J	149[A]	OAS	1	0
1	L	149[B]	OAS	1	0
1	D	149[B]	OAS	1	0
1	I	149[B]	OAS	3	0
1	K	149[B]	OAS	1	0
1	F	149[A]	OAS	9	0
1	B	149[B]	OAS	1	0
1	H	149[A]	OAS	1	0
1	E	149[A]	OAS	1	0
1	A	149[A]	OAS	1	0
1	J	149[B]	OAS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

30 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	CSC	H	1383[A]	-	28,29,29	1.51	6 (21%)	36,41,41	2.12	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	I	1384	-	3,3,3	0.98	0	3,3,3	0.27	0
2	CSC	I	1383[B]	-	24,26,29	1.65	5 (20%)	31,37,41	1.97	5 (16%)
2	CSC	F	1383[A]	-	28,29,29	1.52	5 (17%)	36,41,41	2.32	5 (13%)
3	ACT	D	1384	-	3,3,3	0.87	0	3,3,3	0.88	0
2	CSC	B	1384[B]	-	24,26,29	1.65	5 (20%)	31,37,41	2.14	8 (25%)
3	ACT	H	1384	-	3,3,3	0.79	0	3,3,3	0.95	0
3	ACT	G	1384	-	3,3,3	0.75	0	3,3,3	0.95	0
3	ACT	A	1385	-	3,3,3	0.94	0	3,3,3	0.28	0
2	CSC	H	1383[B]	-	28,26,29	1.74	6 (21%)	36,37,41	2.13	6 (16%)
2	CSC	F	1383[B]	-	28,26,29	1.46	4 (14%)	36,37,41	2.45	6 (16%)
2	CSC	E	1383[B]	-	24,26,29	1.37	5 (20%)	31,37,41	2.28	8 (25%)
3	ACT	I	1386	-	3,3,3	0.89	0	3,3,3	0.80	0
2	CSC	K	1385[B]	-	24,26,29	1.60	4 (16%)	31,37,41	2.46	9 (29%)
2	CSC	A	1383[B]	-	24,26,29	1.47	5 (20%)	31,37,41	2.22	6 (19%)
3	ACT	A	1384	-	3,3,3	0.84	0	3,3,3	1.08	0
3	ACT	E	1384	-	3,3,3	0.81	0	3,3,3	1.23	0
3	ACT	I	1385	-	3,3,3	1.02	0	3,3,3	0.59	0
3	ACT	B	1386	-	3,3,3	0.78	0	3,3,3	1.15	0
3	ACT	B	1385	-	3,3,3	1.03	0	3,3,3	0.25	0
2	CSC	C	1383[B]	-	24,26,29	1.52	6 (25%)	31,37,41	2.17	3 (9%)
3	ACT	E	1385	-	3,3,3	0.81	0	3,3,3	1.19	0
3	ACT	C	1384	-	3,3,3	0.92	0	3,3,3	1.09	0
3	ACT	L	1384	-	3,3,3	0.83	0	3,3,3	0.96	0
3	ACT	F	1384	-	3,3,3	0.88	0	3,3,3	0.59	0
2	CSC	G	1383[B]	-	24,26,29	1.62	5 (20%)	31,37,41	2.29	8 (25%)
2	CSC	J	1385[B]	-	24,26,29	1.65	4 (16%)	31,37,41	2.42	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSC	C	1383[B]	-	-	7/20/49/52	0/2/2/2
2	CSC	H	1383[A]	-	-	10/23/52/52	0/2/2/2
2	CSC	I	1383[B]	-	-	8/20/49/52	0/2/2/2
2	CSC	K	1385[B]	-	-	9/20/49/52	0/2/2/2
2	CSC	G	1383[B]	-	-	5/20/49/52	0/2/2/2
2	CSC	F	1383[A]	-	-	10/23/52/52	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSC	A	1383[B]	-	-	6/20/49/52	0/2/2/2
2	CSC	F	1383[B]	-	-	9/23/49/52	0/2/2/2
2	CSC	H	1383[B]	-	-	11/23/49/52	0/2/2/2
2	CSC	E	1383[B]	-	-	5/20/49/52	0/2/2/2
2	CSC	B	1384[B]	-	-	9/20/49/52	0/2/2/2
2	CSC	J	1385[B]	-	-	8/20/49/52	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1383[B]	CSC	O1-C1	5.20	1.58	1.33
2	K	1385[B]	CSC	C4-N5	-4.73	1.32	1.41
2	J	1385[B]	CSC	C4-N5	-4.48	1.33	1.41
2	I	1383[B]	CSC	C4-N5	-4.46	1.33	1.41
2	B	1384[B]	CSC	C4-N5	-4.36	1.33	1.41
2	F	1383[A]	CSC	C4-N5	-4.17	1.33	1.41
2	F	1383[B]	CSC	C4-N5	-4.17	1.33	1.41
2	C	1383[B]	CSC	C4-N5	-4.10	1.33	1.41
2	G	1383[B]	CSC	C4-N5	-3.99	1.33	1.41
2	H	1383[A]	CSC	C4-N5	-3.85	1.34	1.41
2	H	1383[B]	CSC	C4-N5	-3.85	1.34	1.41
2	A	1383[B]	CSC	C4-N5	-3.60	1.34	1.41
2	G	1383[B]	CSC	C6-S1	-3.43	1.73	1.80
2	B	1384[B]	CSC	C6-S1	-3.42	1.73	1.80
2	K	1385[B]	CSC	C8-N5	-3.34	1.28	1.38
2	J	1385[B]	CSC	C8-N5	-3.30	1.29	1.38
2	H	1383[A]	CSC	C2-S1	-3.22	1.75	1.82
2	H	1383[B]	CSC	C2-S1	-3.22	1.75	1.82
2	A	1383[B]	CSC	C2-S1	-3.09	1.75	1.82
2	J	1385[B]	CSC	C2-S1	-3.02	1.76	1.82
2	I	1383[B]	CSC	C6-S1	-2.98	1.74	1.80
2	C	1383[B]	CSC	C2-S1	-2.96	1.76	1.82
2	F	1383[A]	CSC	C2-S1	-2.95	1.76	1.82
2	F	1383[B]	CSC	C2-S1	-2.95	1.76	1.82
2	B	1384[B]	CSC	C2-S1	-2.79	1.76	1.82
2	E	1383[B]	CSC	C2-S1	-2.77	1.76	1.82
2	B	1384[B]	CSC	C8-N5	-2.72	1.30	1.38
2	K	1385[B]	CSC	C2-S1	-2.68	1.76	1.82
2	I	1383[B]	CSC	C8-N5	-2.67	1.30	1.38
2	I	1383[B]	CSC	C7-C8	-2.65	1.48	1.54
2	H	1383[A]	CSC	O1-C1	2.64	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	1385[B]	CSC	C6-S1	-2.63	1.75	1.80
2	G	1383[B]	CSC	C8-N5	-2.61	1.31	1.38
2	G	1383[B]	CSC	C2-S1	-2.59	1.76	1.82
2	F	1383[A]	CSC	O1-C1	2.59	1.45	1.33
2	G	1383[B]	CSC	O4A-C4'	-2.53	1.23	1.30
2	E	1383[B]	CSC	C6-S1	-2.53	1.75	1.80
2	I	1383[B]	CSC	C2-S1	-2.51	1.77	1.82
2	C	1383[B]	CSC	C8-N5	-2.43	1.31	1.38
2	H	1383[A]	CSC	C8-N5	-2.40	1.31	1.38
2	H	1383[B]	CSC	C8-N5	-2.40	1.31	1.38
2	F	1383[A]	CSC	C8-N5	-2.35	1.31	1.38
2	F	1383[B]	CSC	C8-N5	-2.35	1.31	1.38
2	B	1384[B]	CSC	C7-C8	-2.34	1.49	1.54
2	A	1383[B]	CSC	C6-S1	-2.32	1.75	1.80
2	E	1383[B]	CSC	C4-N5	-2.32	1.37	1.41
2	H	1383[A]	CSC	C6-S1	-2.29	1.75	1.80
2	H	1383[B]	CSC	C6-S1	-2.29	1.75	1.80
2	H	1383[A]	CSC	O4A-C4'	-2.28	1.24	1.30
2	H	1383[B]	CSC	O4A-C4'	-2.28	1.24	1.30
2	A	1383[B]	CSC	C8-N5	-2.25	1.32	1.38
2	A	1383[B]	CSC	O4A-C4'	-2.20	1.24	1.30
2	K	1385[B]	CSC	O4A-C4'	-2.18	1.24	1.30
2	E	1383[B]	CSC	O4A-C4'	-2.18	1.24	1.30
2	C	1383[B]	CSC	C6-S1	-2.12	1.76	1.80
2	C	1383[B]	CSC	O4A-C4'	-2.04	1.25	1.30
2	C	1383[B]	CSC	C7-C8	-2.03	1.49	1.54
2	E	1383[B]	CSC	C8-N5	-2.03	1.32	1.38
2	F	1383[A]	CSC	O4A-C4'	-2.00	1.25	1.30
2	F	1383[B]	CSC	O4A-C4'	-2.00	1.25	1.30

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1383[A]	CSC	C6-C7-N10	-8.85	100.16	118.49
2	F	1383[B]	CSC	C6-C7-N10	-8.85	100.16	118.49
2	G	1383[B]	CSC	S1-C6-N5	-7.85	97.02	110.60
2	B	1384[B]	CSC	S1-C6-N5	-7.38	97.83	110.60
2	J	1385[B]	CSC	S1-C6-N5	-7.29	97.98	110.60
2	E	1383[B]	CSC	S1-C6-N5	-6.96	98.56	110.60
2	H	1383[A]	CSC	C6-C7-N10	-6.94	104.12	118.49
2	H	1383[B]	CSC	C6-C7-N10	-6.94	104.12	118.49
2	K	1385[B]	CSC	C2-S1-C6	6.77	106.77	94.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1385[B]	CSC	C6-C7-N10	-6.75	104.52	118.49
2	A	1383[B]	CSC	C6-C7-N10	-6.66	104.70	118.49
2	C	1383[B]	CSC	S1-C6-N5	-6.57	99.24	110.60
2	K	1385[B]	CSC	S1-C6-N5	-6.41	99.51	110.60
2	F	1383[A]	CSC	S1-C6-N5	-6.40	99.53	110.60
2	F	1383[B]	CSC	S1-C6-N5	-6.40	99.53	110.60
2	C	1383[B]	CSC	C6-C7-N10	-6.39	105.25	118.49
2	A	1383[B]	CSC	C2-S1-C6	6.38	106.05	94.36
2	J	1385[B]	CSC	C2-S1-C6	6.12	105.58	94.36
2	C	1383[B]	CSC	C2-S1-C6	6.11	105.56	94.36
2	I	1383[B]	CSC	S1-C6-N5	-6.07	100.09	110.60
2	E	1383[B]	CSC	C2-S1-C6	6.02	105.39	94.36
2	J	1385[B]	CSC	C6-C7-N10	-6.01	106.05	118.49
2	H	1383[A]	CSC	S1-C6-N5	-5.97	100.27	110.60
2	H	1383[B]	CSC	S1-C6-N5	-5.97	100.27	110.60
2	F	1383[A]	CSC	C2-S1-C6	5.49	104.41	94.36
2	F	1383[B]	CSC	C2-S1-C6	5.49	104.41	94.36
2	G	1383[B]	CSC	C2-S1-C6	5.47	104.38	94.36
2	H	1383[A]	CSC	C2-S1-C6	5.33	104.13	94.36
2	H	1383[B]	CSC	C2-S1-C6	5.33	104.13	94.36
2	F	1383[B]	CSC	C3'-O1-C1	5.24	125.29	116.10
2	A	1383[B]	CSC	S1-C6-N5	-4.72	102.44	110.60
2	B	1384[B]	CSC	C2-S1-C6	4.42	102.46	94.36
2	G	1383[B]	CSC	C6-C7-N10	-4.16	109.88	118.49
2	E	1383[B]	CSC	C6-C7-N10	-3.96	110.28	118.49
2	I	1383[B]	CSC	C7-N10-C11	-3.68	114.53	121.80
2	I	1383[B]	CSC	C2-S1-C6	3.53	100.83	94.36
2	E	1383[B]	CSC	C3-C2-S1	-3.46	109.95	115.36
2	B	1384[B]	CSC	C7-N10-C11	-3.33	115.22	121.80
2	I	1383[B]	CSC	C6-C7-N10	-3.33	111.59	118.49
2	B	1384[B]	CSC	C6-C7-N10	-3.29	111.66	118.49
2	I	1383[B]	CSC	C13-C11-N10	2.96	121.09	115.86
2	G	1383[B]	CSC	C7-N10-C11	-2.94	115.98	121.80
2	E	1383[B]	CSC	C7-N10-C11	2.72	127.17	121.80
2	B	1384[B]	CSC	C13-C11-N10	2.63	120.49	115.86
2	K	1385[B]	CSC	C6-N5-C4	2.62	132.19	125.54
2	J	1385[B]	CSC	C6-N5-C4	2.60	132.15	125.54
2	G	1383[B]	CSC	C3-C2-S1	-2.60	111.29	115.36
2	J	1385[B]	CSC	O12-C11-C13	-2.59	117.32	122.02
2	A	1383[B]	CSC	C3-C2-S1	-2.58	111.31	115.36
2	E	1383[B]	CSC	O12-C11-C13	-2.56	117.39	122.02
2	A	1383[B]	CSC	C7-N10-C11	2.48	126.69	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1385[B]	CSC	C3-C2-S1	-2.42	111.58	115.36
2	E	1383[B]	CSC	C8-C7-N10	2.37	122.00	115.29
2	F	1383[A]	CSC	C3-C2-S1	-2.34	111.70	115.36
2	F	1383[B]	CSC	C3-C2-S1	-2.34	111.70	115.36
2	G	1383[B]	CSC	C13-C11-N10	2.31	119.93	115.86
2	H	1383[B]	CSC	O1-C1-C20	2.31	122.17	112.38
2	H	1383[A]	CSC	C7-C6-N5	-2.30	84.48	87.26
2	H	1383[B]	CSC	C7-C6-N5	-2.30	84.48	87.26
2	K	1385[B]	CSC	O12-C11-C13	-2.29	117.86	122.02
2	G	1383[B]	CSC	C3'-C3-C2	2.29	119.66	113.86
2	H	1383[A]	CSC	C3'-O1-C1	2.28	120.10	116.10
2	B	1384[B]	CSC	C6-N5-C4	2.25	131.26	125.54
2	K	1385[B]	CSC	C7-C6-N5	-2.25	84.55	87.26
2	G	1383[B]	CSC	O4A-C4'-C4	2.22	122.42	116.08
2	E	1383[B]	CSC	O4A-C4'-C4	2.20	122.38	116.08
2	J	1385[B]	CSC	O4A-C4'-O4B	-2.20	118.67	123.90
2	F	1383[A]	CSC	C8-C7-N10	2.19	121.50	115.29
2	F	1383[B]	CSC	C8-C7-N10	2.19	121.50	115.29
2	J	1385[B]	CSC	C7-C6-S1	-2.17	112.88	116.74
2	K	1385[B]	CSC	C8-N5-C4	-2.13	129.17	133.72
2	K	1385[B]	CSC	C14-C13-C11	-2.12	107.32	113.19
2	B	1384[B]	CSC	O4A-C4'-C4	2.05	121.95	116.08
2	H	1383[B]	CSC	C3'-O1-C1	-2.04	112.53	116.10
2	B	1384[B]	CSC	C3-C2-S1	-2.02	112.19	115.36
2	K	1385[B]	CSC	O4A-C4'-O4B	-2.02	119.09	123.90
2	A	1383[B]	CSC	C14-C15-C16	-2.02	106.71	113.22

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1383[B]	CSC	C2-C3-C3'-O1
2	A	1383[B]	CSC	C14-C15-C16-N17
2	A	1383[B]	CSC	C14-C15-C16-C18
2	B	1384[B]	CSC	C2-C3-C3'-O1
2	B	1384[B]	CSC	C4-C3-C3'-O1
2	E	1383[B]	CSC	C2-C3-C3'-O1
2	E	1383[B]	CSC	C14-C15-C16-C18
2	F	1383[A]	CSC	C2-C3-C3'-O1
2	F	1383[A]	CSC	C4-C3-C3'-O1
2	H	1383[A]	CSC	C14-C15-C16-N17
2	H	1383[A]	CSC	C14-C15-C16-C18

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Mol	Chain	Res	Type	Atoms
2	H	1383[B]	CSC	C2-C3-C3'-O1
2	H	1383[B]	CSC	C4-C3-C3'-O1
2	H	1383[B]	CSC	C14-C15-C16-N17
2	H	1383[B]	CSC	C14-C15-C16-C18
2	I	1383[B]	CSC	C2-C3-C3'-O1
2	I	1383[B]	CSC	C4-C3-C3'-O1
2	J	1385[B]	CSC	C4-C3-C3'-O1
2	J	1385[B]	CSC	C14-C15-C16-N17
2	J	1385[B]	CSC	C14-C15-C16-C18
2	K	1385[B]	CSC	C2-C3-C3'-O1
2	K	1385[B]	CSC	C4-C3-C3'-O1
2	K	1385[B]	CSC	C14-C15-C16-N17
2	K	1385[B]	CSC	C14-C15-C16-C18
2	H	1383[A]	CSC	C11-C13-C14-C15
2	H	1383[B]	CSC	C11-C13-C14-C15
2	J	1385[B]	CSC	C11-C13-C14-C15
2	K	1385[B]	CSC	C11-C13-C14-C15
2	E	1383[B]	CSC	C11-C13-C14-C15
2	F	1383[A]	CSC	C11-C13-C14-C15
2	F	1383[B]	CSC	C11-C13-C14-C15
2	F	1383[B]	CSC	O2-C1-O1-C3'
2	F	1383[B]	CSC	C20-C1-O1-C3'
2	H	1383[B]	CSC	O2-C1-O1-C3'
2	H	1383[A]	CSC	O2-C1-O1-C3'
2	F	1383[A]	CSC	O2-C1-O1-C3'
2	F	1383[A]	CSC	C20-C1-O1-C3'
2	B	1384[B]	CSC	N17-C16-C18-O20
2	C	1383[B]	CSC	N17-C16-C18-O20
2	H	1383[A]	CSC	C20-C1-O1-C3'
2	H	1383[B]	CSC	C20-C1-O1-C3'
2	I	1383[B]	CSC	N17-C16-C18-O20
2	A	1383[B]	CSC	C11-C13-C14-C15
2	I	1383[B]	CSC	N10-C11-C13-C14
2	I	1383[B]	CSC	O12-C11-C13-C14
2	E	1383[B]	CSC	C13-C14-C15-C16
2	G	1383[B]	CSC	C13-C14-C15-C16
2	B	1384[B]	CSC	O12-C11-C13-C14
2	C	1383[B]	CSC	C13-C14-C15-C16
2	B	1384[B]	CSC	N10-C11-C13-C14
2	H	1383[A]	CSC	C13-C14-C15-C16
2	H	1383[B]	CSC	C13-C14-C15-C16
2	G	1383[B]	CSC	N17-C16-C18-O20

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Mol	Chain	Res	Type	Atoms
2	B	1384[B]	CSC	N17-C16-C18-O19
2	C	1383[B]	CSC	N17-C16-C18-O19
2	I	1383[B]	CSC	N17-C16-C18-O19
2	B	1384[B]	CSC	C15-C16-C18-O19
2	F	1383[A]	CSC	C13-C14-C15-C16
2	F	1383[B]	CSC	C13-C14-C15-C16
2	J	1385[B]	CSC	C13-C14-C15-C16
2	K	1385[B]	CSC	C13-C14-C15-C16
2	A	1383[B]	CSC	C4-C3-C3'-O1
2	C	1383[B]	CSC	C4-C3-C3'-O1
2	F	1383[B]	CSC	C4-C3-C3'-O1
2	H	1383[A]	CSC	C4-C3-C3'-O1
2	B	1384[B]	CSC	C15-C16-C18-O20
2	F	1383[A]	CSC	C15-C16-C18-O20
2	F	1383[B]	CSC	C15-C16-C18-O20
2	J	1385[B]	CSC	C15-C16-C18-O20
2	F	1383[A]	CSC	C15-C16-C18-O19
2	F	1383[B]	CSC	C15-C16-C18-O19
2	H	1383[A]	CSC	C15-C16-C18-O20
2	H	1383[B]	CSC	C15-C16-C18-O20
2	J	1385[B]	CSC	C15-C16-C18-O19
2	K	1385[B]	CSC	C15-C16-C18-O20
2	I	1383[B]	CSC	C13-C14-C15-C16
2	H	1383[A]	CSC	C15-C16-C18-O19
2	H	1383[B]	CSC	C15-C16-C18-O19
2	K	1385[B]	CSC	C15-C16-C18-O19
2	K	1385[B]	CSC	N5-C4-C4'-O4B
2	G	1383[B]	CSC	N17-C16-C18-O19
2	C	1383[B]	CSC	C3-C4-C4'-O4B
2	J	1385[B]	CSC	C2-C3-C3'-O1
2	I	1383[B]	CSC	N5-C4-C4'-O4B
2	C	1383[B]	CSC	C15-C16-C18-O19
2	G	1383[B]	CSC	N5-C4-C4'-O4B
2	H	1383[A]	CSC	N5-C4-C4'-O4B
2	H	1383[B]	CSC	N5-C4-C4'-O4B
2	F	1383[A]	CSC	C3-C4-C4'-O4A
2	F	1383[B]	CSC	C3-C4-C4'-O4A
2	G	1383[B]	CSC	C6-C7-N10-C11
2	F	1383[A]	CSC	C3-C4-C4'-O4B
2	F	1383[B]	CSC	C3-C4-C4'-O4B
2	A	1383[B]	CSC	N5-C4-C4'-O4B
2	B	1384[B]	CSC	N5-C4-C4'-O4B

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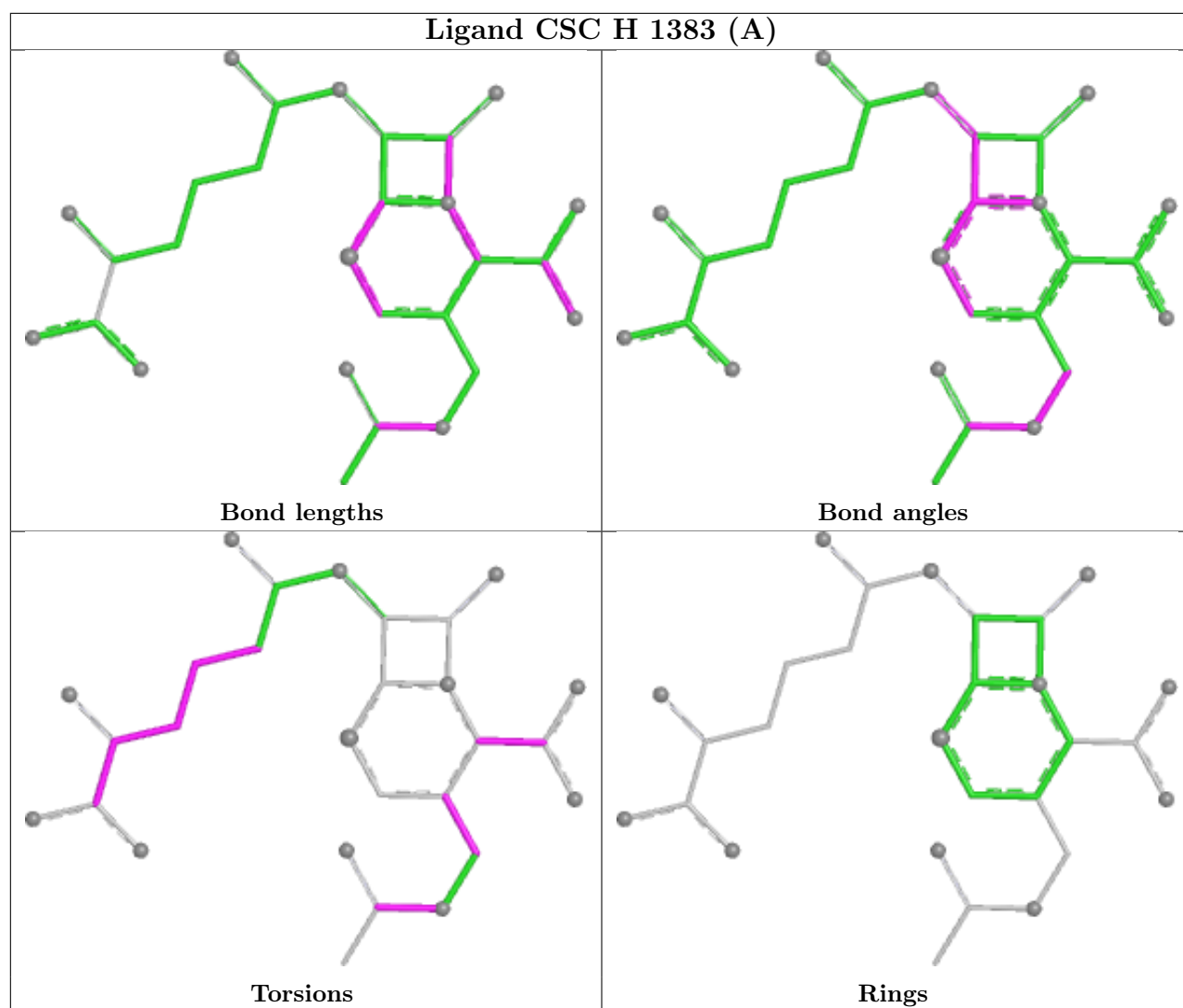
Mol	Chain	Res	Type	Atoms
2	C	1383[B]	CSC	N5-C4-C4'-O4B
2	E	1383[B]	CSC	N5-C4-C4'-O4B

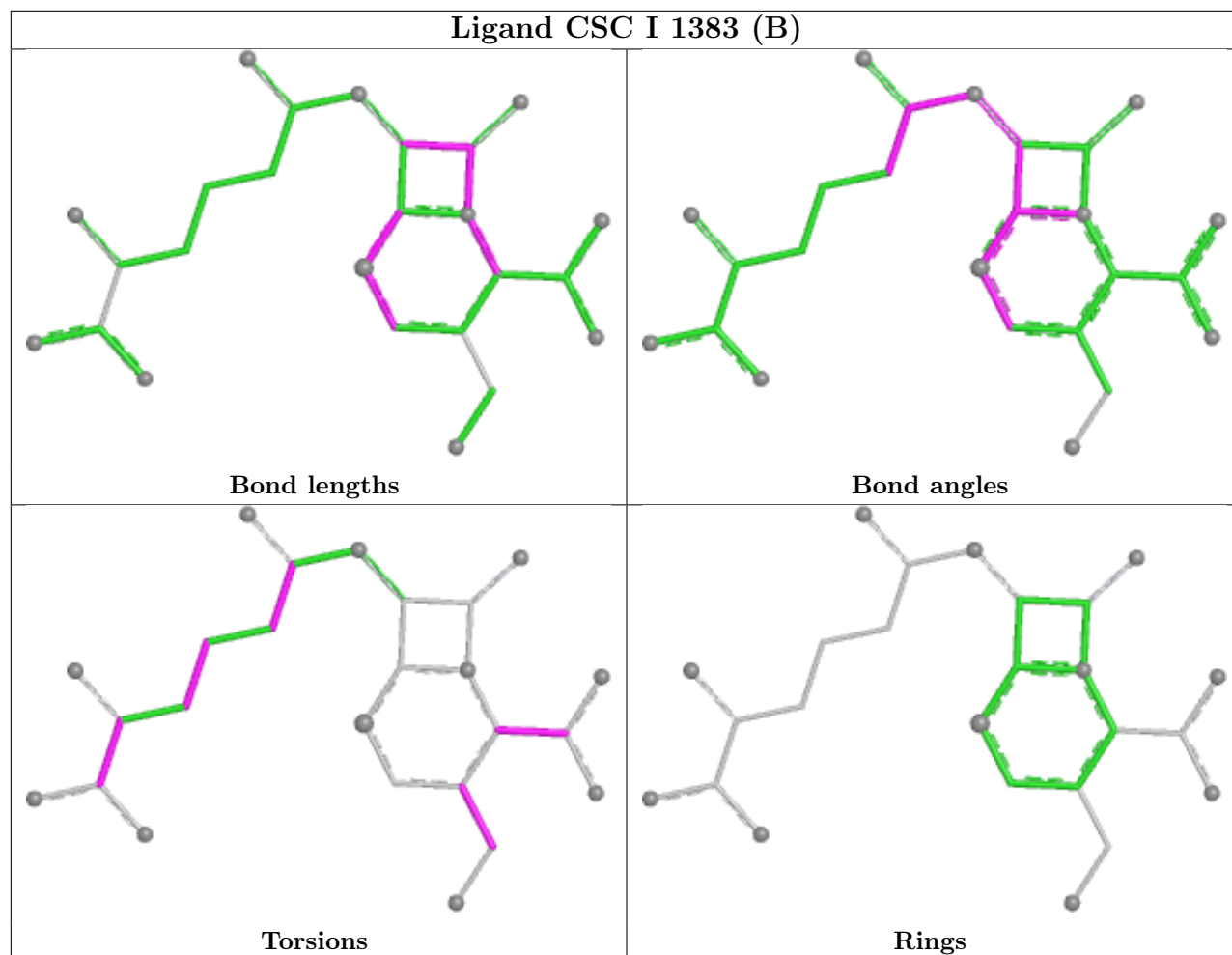
There are no ring outliers.

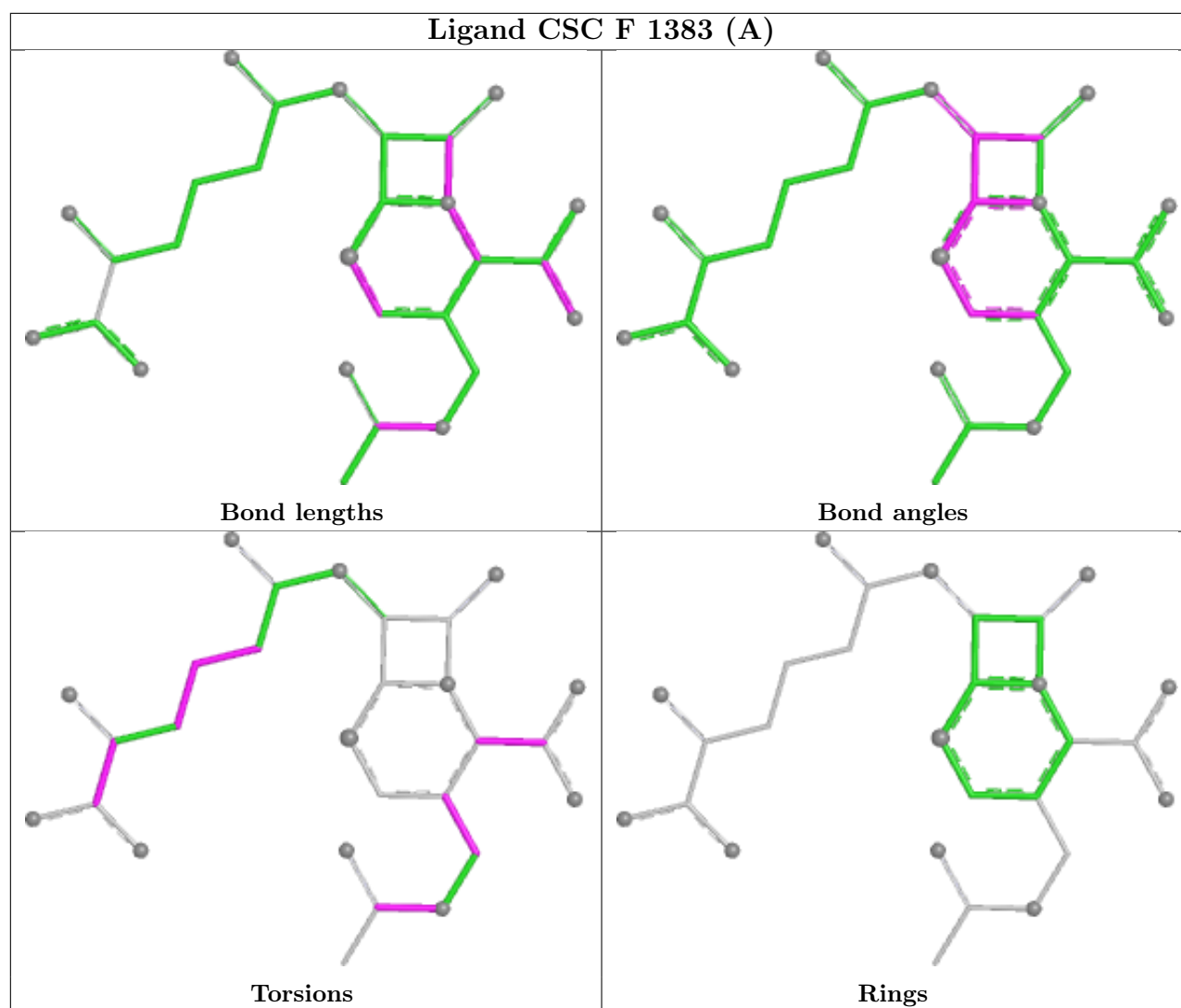
20 monomers are involved in 62 short contacts:

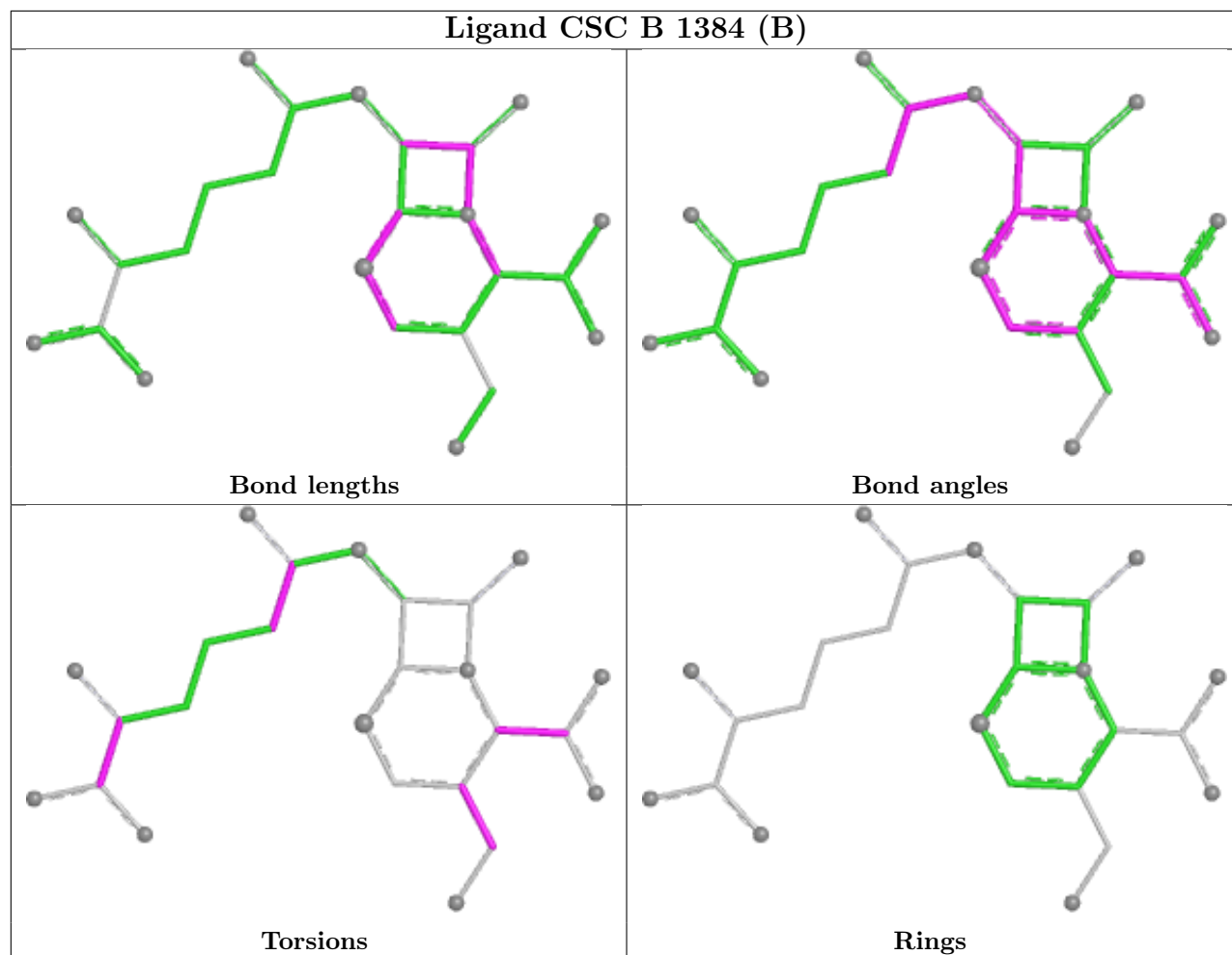
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1383[A]	CSC	3	0
2	I	1383[B]	CSC	2	0
2	F	1383[A]	CSC	12	0
3	D	1384	ACT	1	0
2	B	1384[B]	CSC	1	0
3	H	1384	ACT	2	0
3	G	1384	ACT	1	0
2	H	1383[B]	CSC	2	0
2	F	1383[B]	CSC	2	0
2	E	1383[B]	CSC	6	0
2	K	1385[B]	CSC	3	0
2	A	1383[B]	CSC	9	0
3	A	1384	ACT	2	0
3	E	1384	ACT	4	0
3	B	1385	ACT	1	0
2	C	1383[B]	CSC	2	0
3	C	1384	ACT	2	0
3	F	1384	ACT	1	0
2	G	1383[B]	CSC	3	0
2	J	1385[B]	CSC	3	0

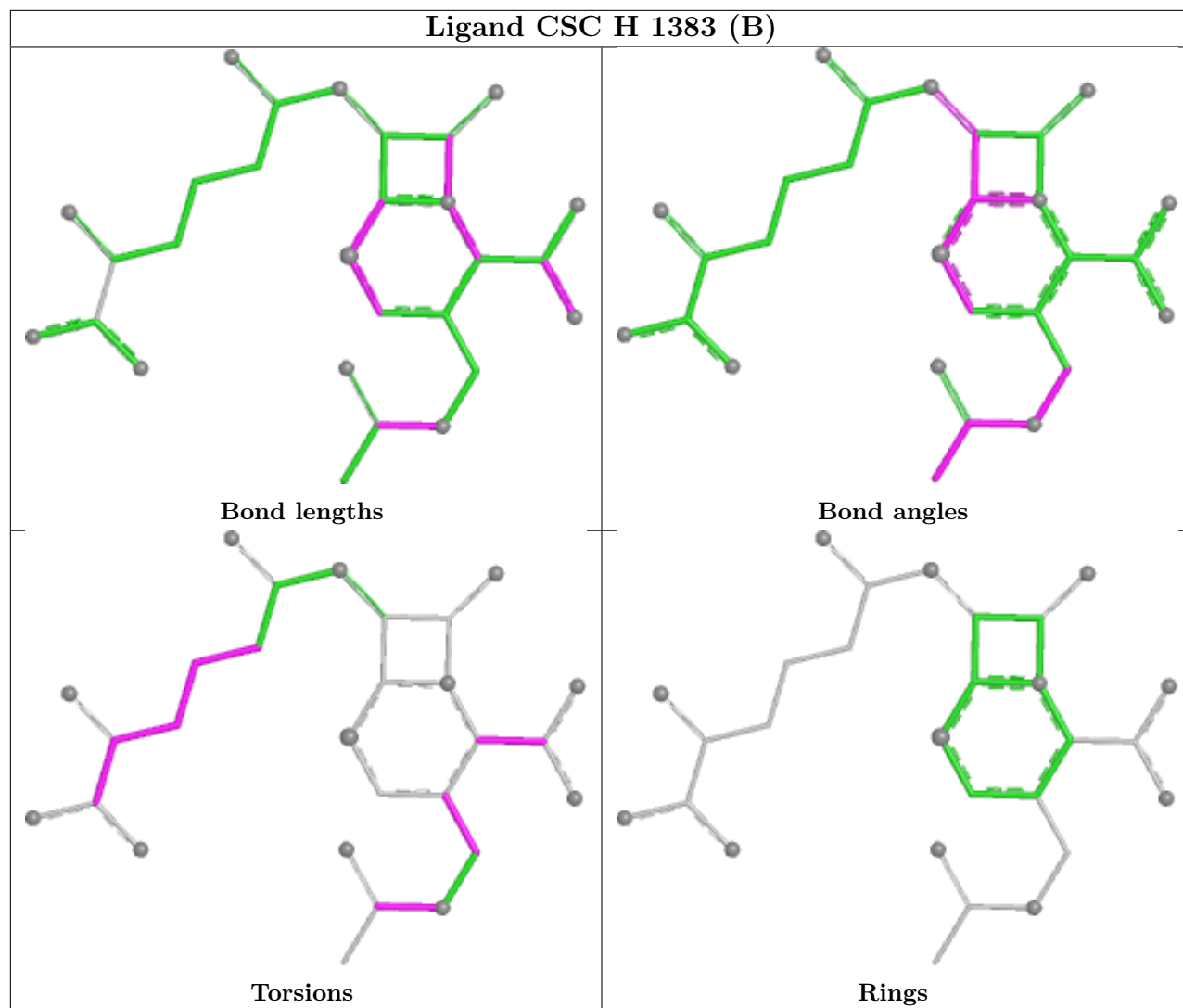
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

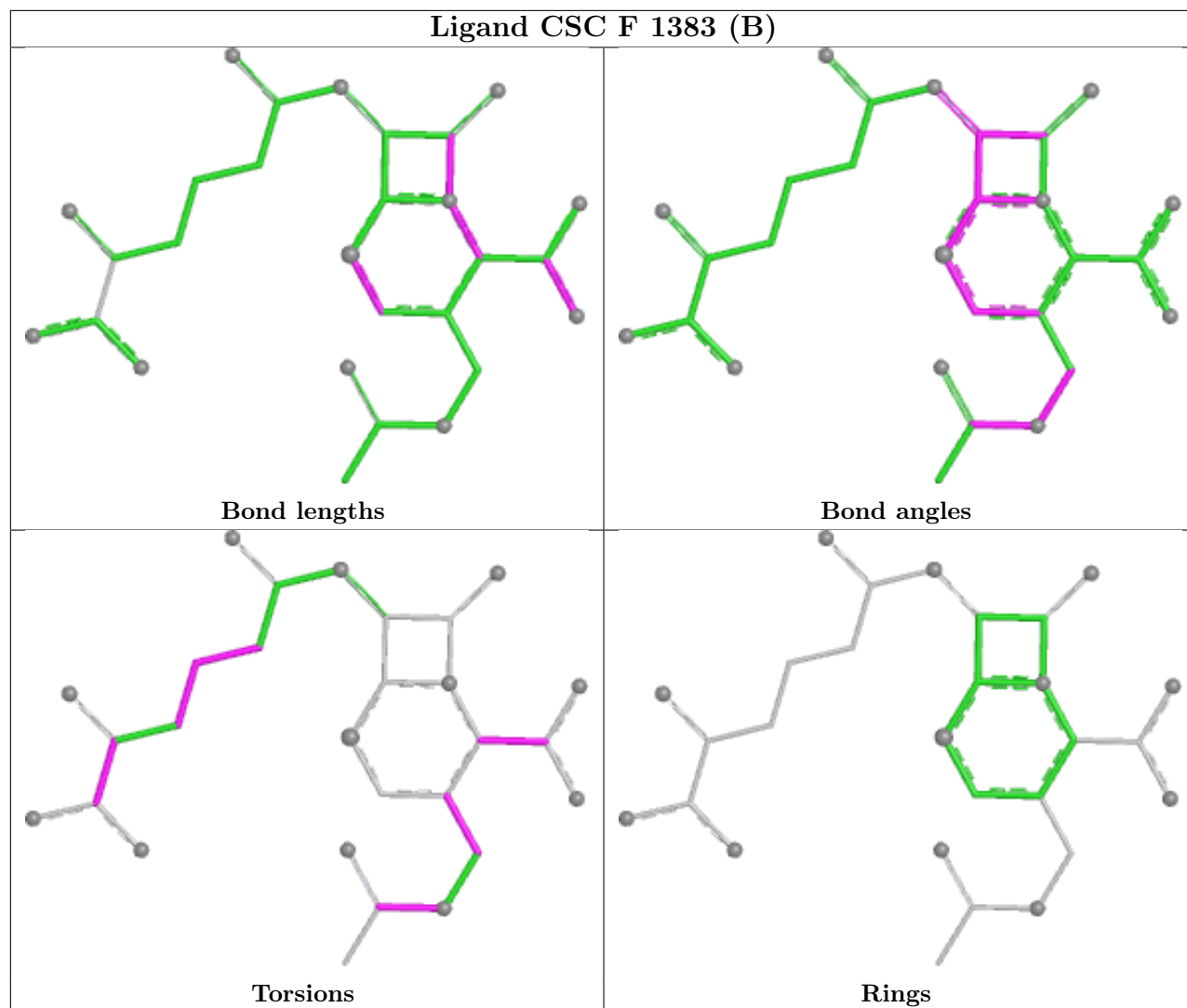


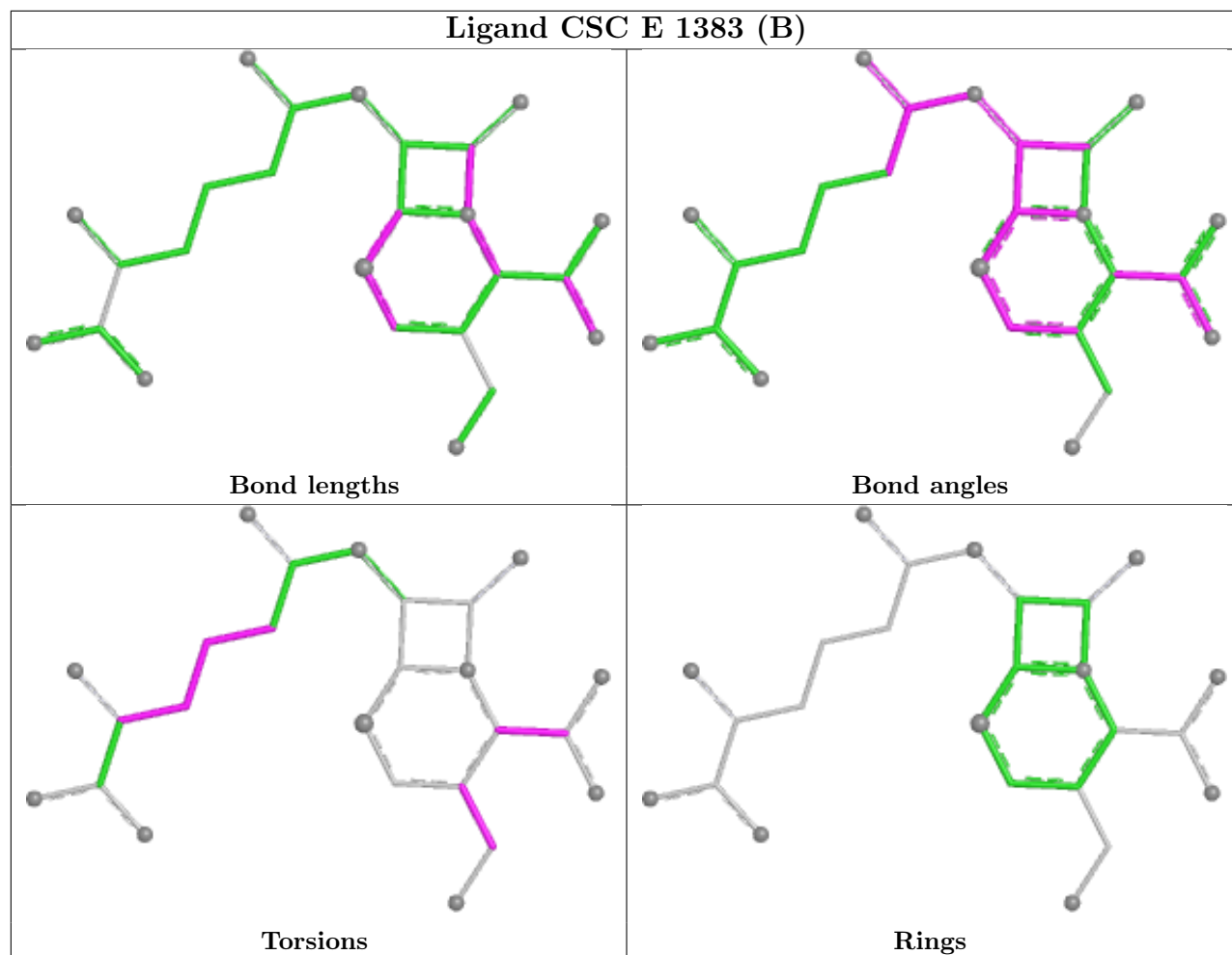


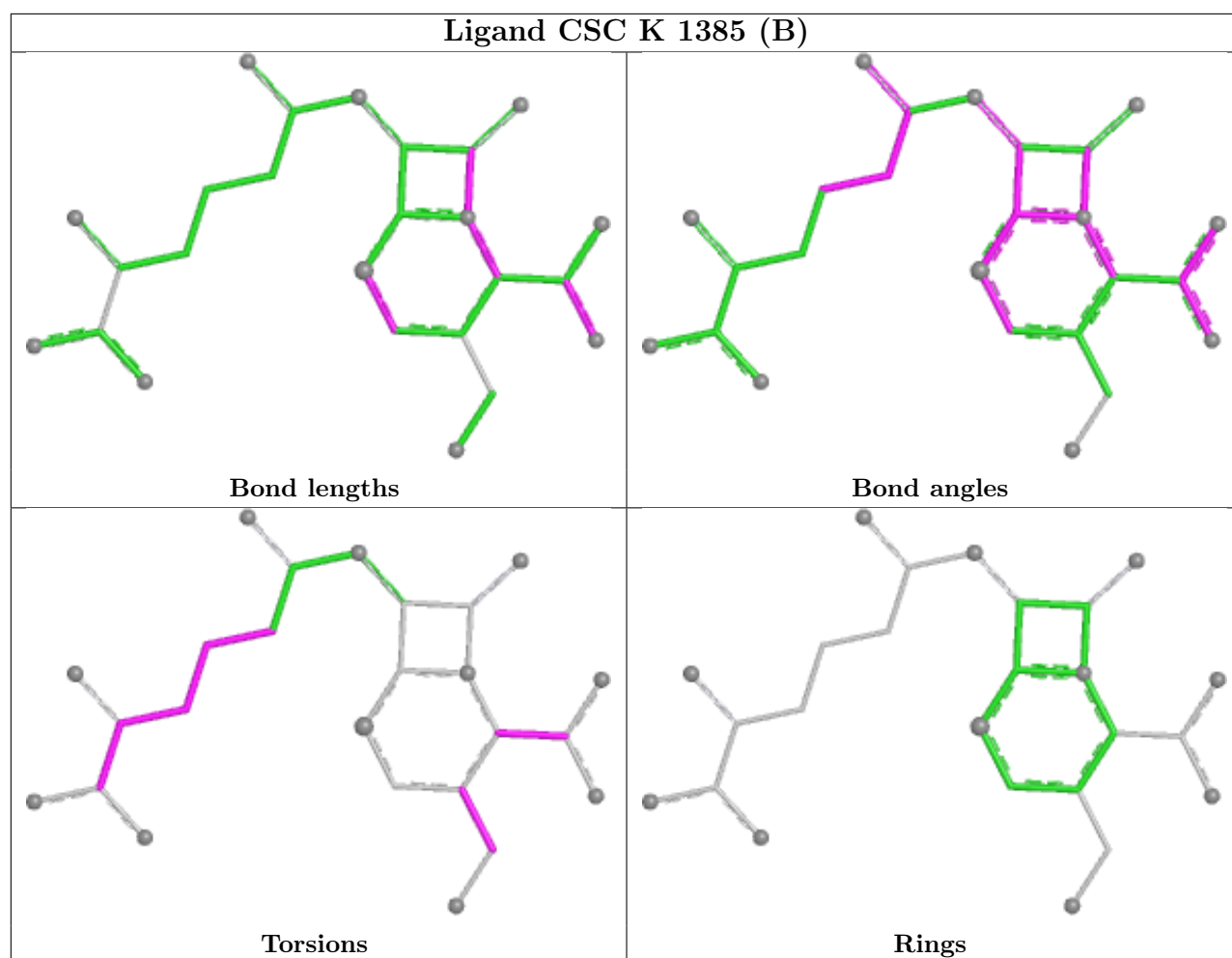


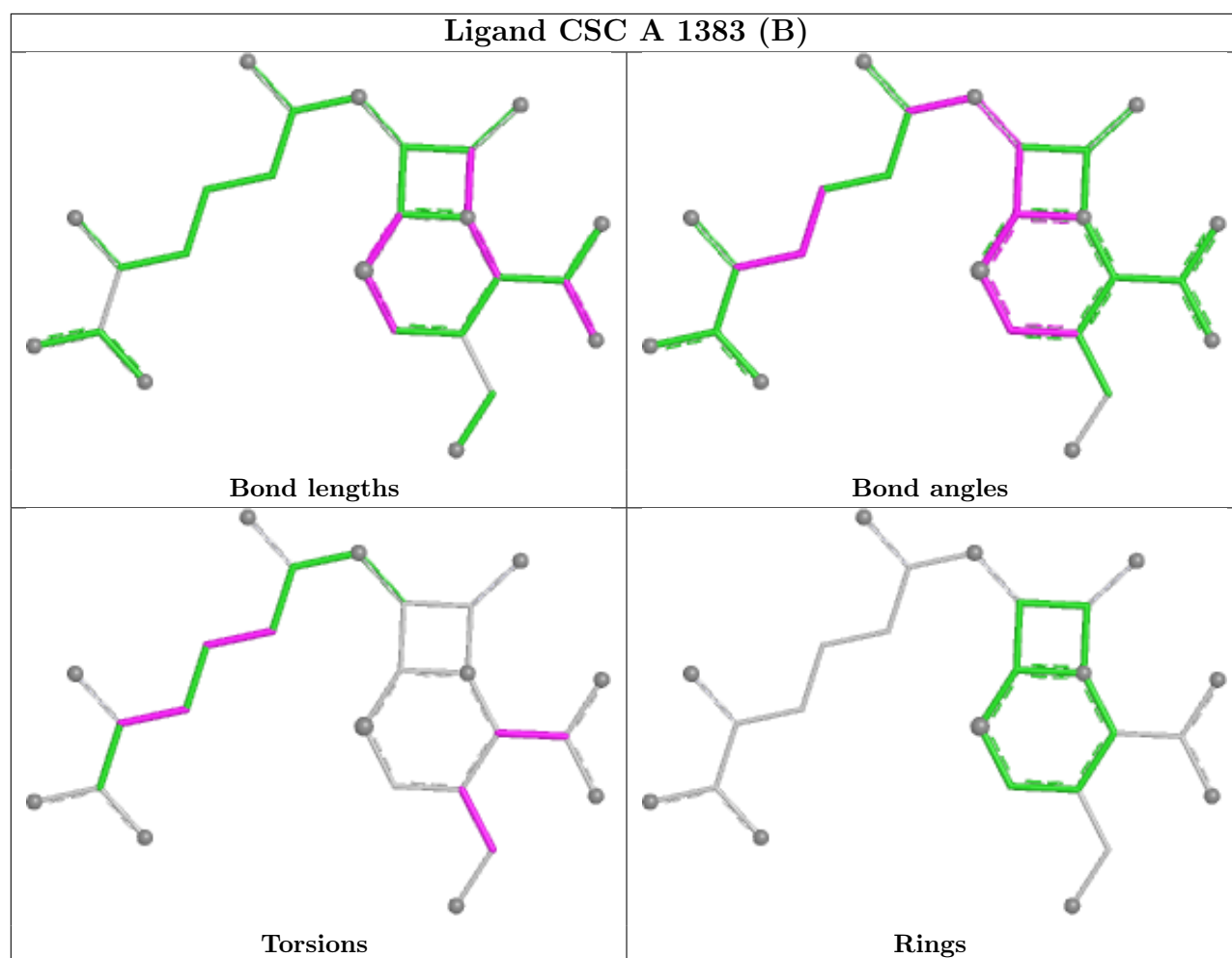


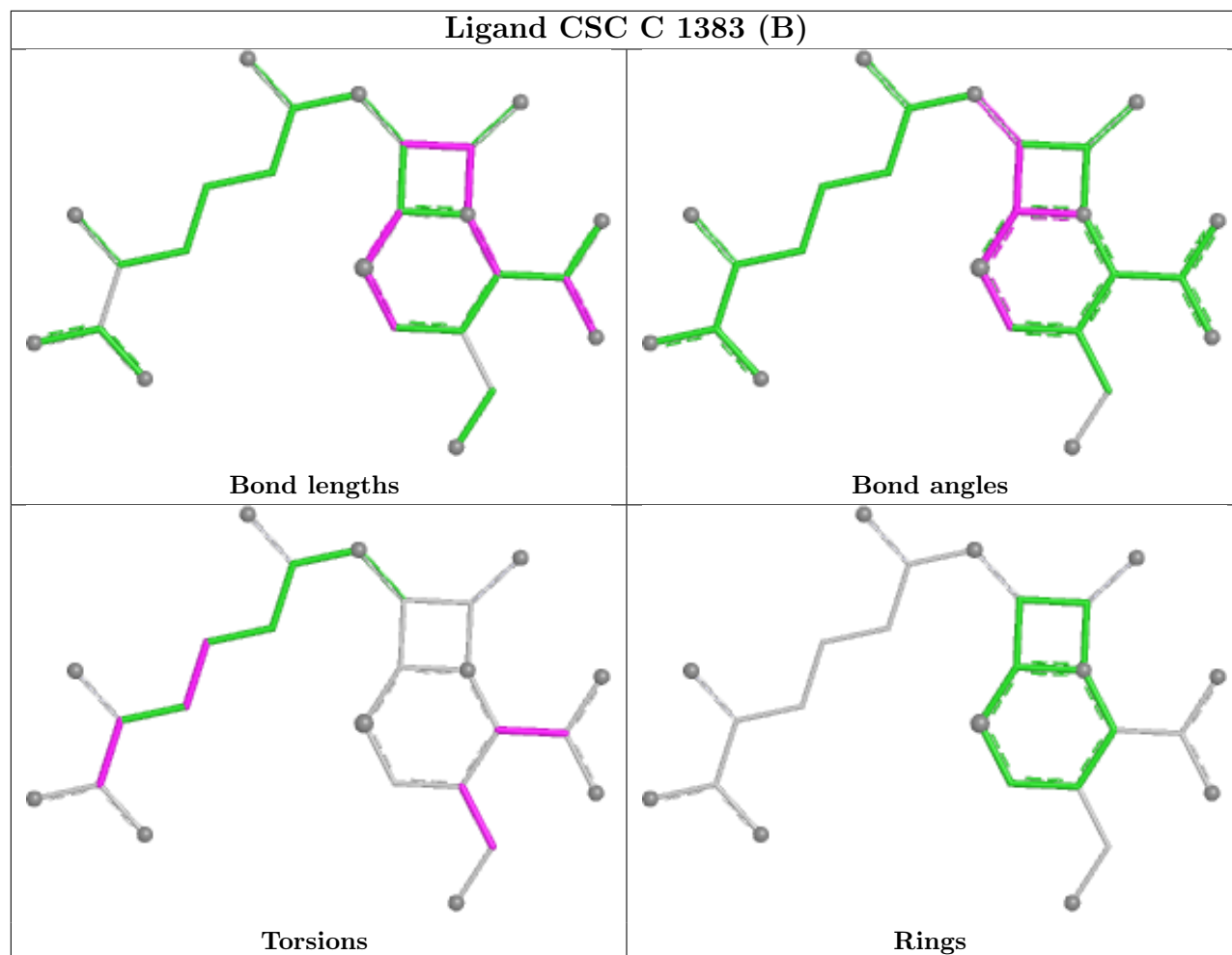


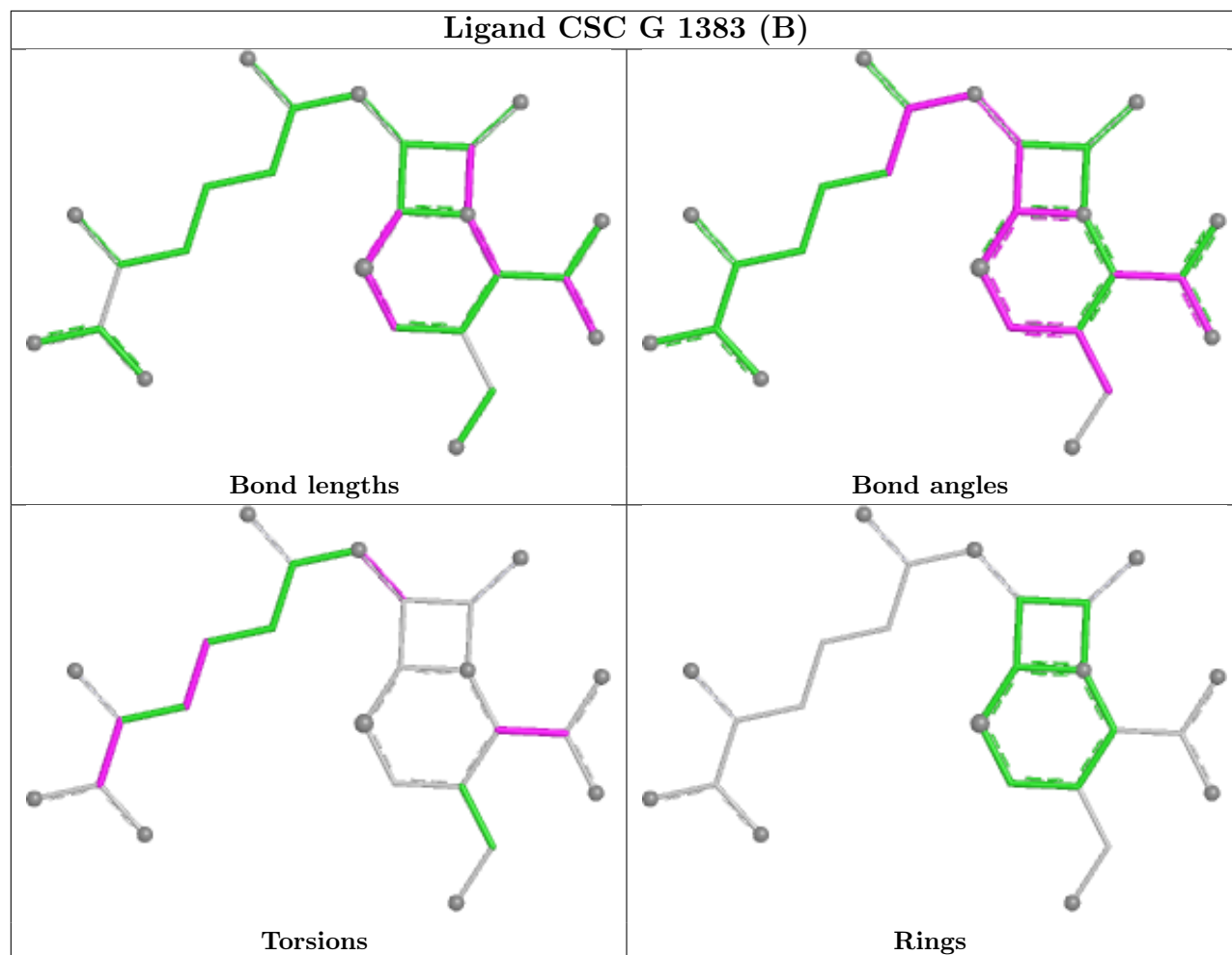


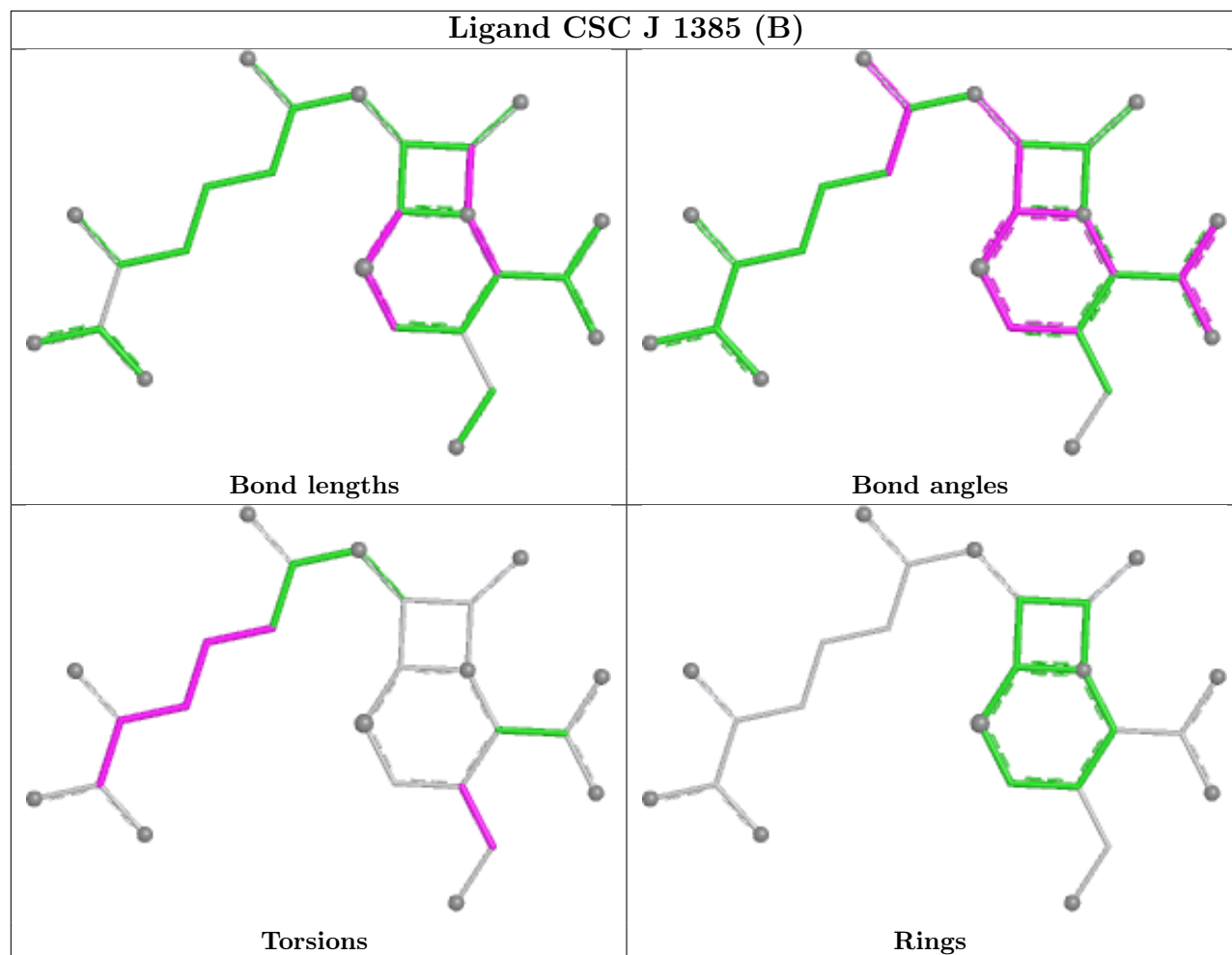












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	347/444 (78%)	-1.46	0 100 100	12, 27, 46, 60	1 (0%)
1	B	349/444 (78%)	-1.45	0 100 100	9, 27, 46, 67	2 (0%)
1	C	346/444 (77%)	-1.44	0 100 100	9, 26, 46, 60	3 (0%)
1	D	344/444 (77%)	-1.43	0 100 100	9, 26, 45, 55	3 (0%)
1	E	345/444 (77%)	-1.44	0 100 100	11, 27, 45, 61	2 (0%)
1	F	340/444 (76%)	-1.43	0 100 100	16, 27, 44, 59	1 (0%)
1	G	341/444 (76%)	-1.43	0 100 100	16, 26, 44, 53	2 (0%)
1	H	342/444 (77%)	-1.48	0 100 100	16, 26, 44, 59	3 (0%)
1	I	347/444 (78%)	-1.47	0 100 100	10, 26, 46, 67	2 (0%)
1	J	343/444 (77%)	-1.32	0 100 100	16, 27, 45, 65	1 (0%)
1	K	340/444 (76%)	-1.30	0 100 100	16, 27, 44, 53	1 (0%)
1	L	339/444 (76%)	-1.43	0 100 100	16, 27, 44, 53	2 (0%)
All	All	4123/5328 (77%)	-1.42	0 100 100	9, 27, 45, 67	23 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OAS	J	149[A]	6/10	0.97	0.06	15,17,17,18	3
1	OAS	J	149[B]	9/10	0.97	0.06	8,16,17,18	6
1	OAS	C	149[A]	6/10	0.99	0.03	15,17,17,18	3

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OAS	C	149[B]	9/10	0.99	0.03	8,16,17,18	6
1	OAS	D	149[A]	6/10	0.99	0.03	15,16,17,18	3
1	OAS	D	149[B]	9/10	0.99	0.03	7,16,17,18	6
1	OAS	E	149[A]	6/10	0.99	0.03	15,17,17,17	3
1	OAS	E	149[B]	9/10	0.99	0.03	7,17,17,17	6
1	OAS	G	149[A]	6/10	0.99	0.05	15,17,17,17	3
1	OAS	G	149[B]	9/10	0.99	0.05	8,16,17,17	6
1	OAS	I	149[A]	6/10	0.99	0.04	15,17,17,18	3
1	OAS	I	149[B]	9/10	0.99	0.04	8,16,17,18	6
1	OAS	B	149[A]	6/10	0.99	0.04	15,17,17,18	3
1	OAS	B	149[B]	9/10	0.99	0.04	8,16,17,18	6
1	OAS	K	149[A]	6/10	0.99	0.04	15,17,17,18	3
1	OAS	K	149[B]	9/10	0.99	0.04	8,16,17,18	6
1	OAS	F	149[A]	6/10	1.00	0.02	15,16,17,17	3
1	OAS	F	149[B]	9/10	1.00	0.02	8,16,17,17	6
1	OAS	A	149[A]	6/10	1.00	0.03	15,16,17,17	3
1	OAS	A	149[B]	9/10	1.00	0.03	8,16,17,17	6
1	OAS	H	149[A]	6/10	1.00	0.02	15,16,17,17	3
1	OAS	H	149[B]	9/10	1.00	0.02	8,16,17,17	6
1	OAS	L	149[A]	6/10	1.00	0.02	15,16,17,17	3
1	OAS	L	149[B]	9/10	1.00	0.02	8,16,17,17	6

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	G	1384	4/4	0.97	0.07	37,37,37,38	0
2	CSC	C	1383[B]	25/28	0.98	0.05	11,22,33,34	25
2	CSC	D	1383[B]	25/28	0.98	0.05	7,18,33,35	25
2	CSC	E	1383[B]	25/28	0.98	0.05	14,27,29,31	25
2	CSC	A	1383[B]	25/28	0.98	0.05	29,43,48,48	25
3	ACT	H	1384	4/4	0.98	0.06	37,37,38,38	0
3	ACT	I	1386	4/4	0.98	0.06	41,42,42,42	0

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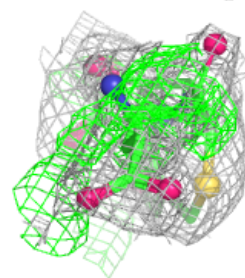
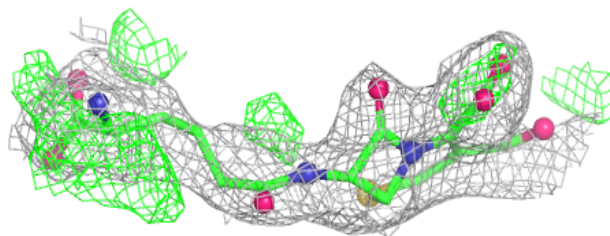
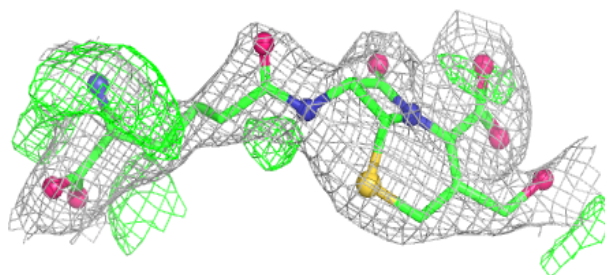
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CSC	G	1383[B]	25/28	0.99	0.05	11,21,36,37	25
2	CSC	H	1383[A]	28/28	0.99	0.05	46,60,84,84	5
2	CSC	H	1383[B]	25/28	0.99	0.05	46,60,84,84	2
2	CSC	I	1383[B]	25/28	0.99	0.04	4,16,29,30	25
2	CSC	J	1385[B]	25/28	0.99	0.04	19,23,30,30	25
2	CSC	K	1385[B]	25/28	0.99	0.05	23,26,30,31	25
2	CSC	L	1383[B]	25/28	0.99	0.04	37,46,55,56	2
2	CSC	L	1383[A]	25/28	0.99	0.04	37,50,55,56	5
3	ACT	A	1384	4/4	0.99	0.03	26,26,27,27	0
3	ACT	A	1385	4/4	0.99	0.06	43,44,44,45	0
3	ACT	B	1385	4/4	0.99	0.03	30,31,31,33	0
3	ACT	B	1386	4/4	0.99	0.07	35,37,37,39	0
3	ACT	D	1384	4/4	0.99	0.03	23,24,24,25	0
3	ACT	E	1384	4/4	0.99	0.04	25,26,26,26	0
3	ACT	E	1385	4/4	0.99	0.04	39,39,40,40	0
3	ACT	F	1384	4/4	0.99	0.06	40,40,40,40	0
2	CSC	B	1384[B]	25/28	0.99	0.04	11,19,28,29	25
2	CSC	F	1383[A]	28/28	0.99	0.04	39,51,61,62	5
3	ACT	I	1384	4/4	0.99	0.03	26,28,28,30	0
3	ACT	I	1385	4/4	0.99	0.04	37,37,38,40	0
2	CSC	F	1383[B]	25/28	0.99	0.04	39,49,61,62	2
3	ACT	L	1384	4/4	0.99	0.05	43,43,43,44	0
3	ACT	C	1384	4/4	1.00	0.05	22,22,22,23	0

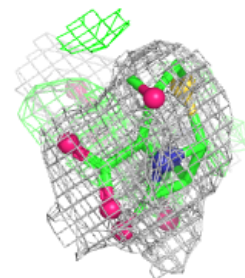
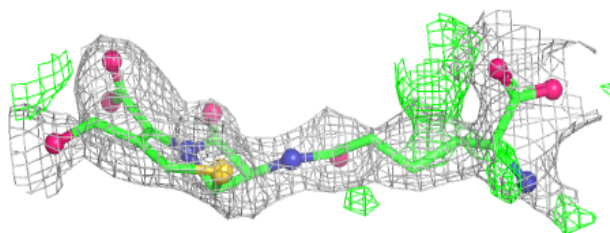
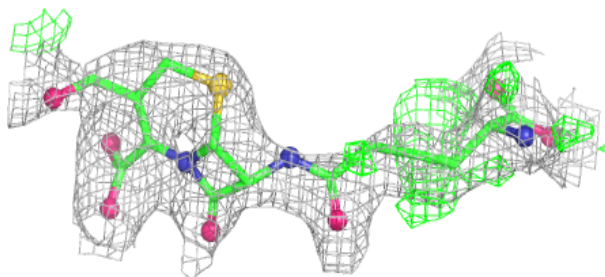
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CSC C 1383 (B):

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

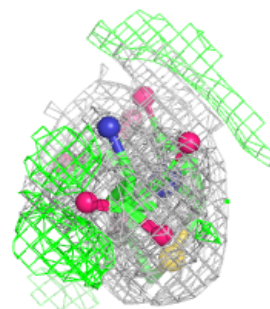
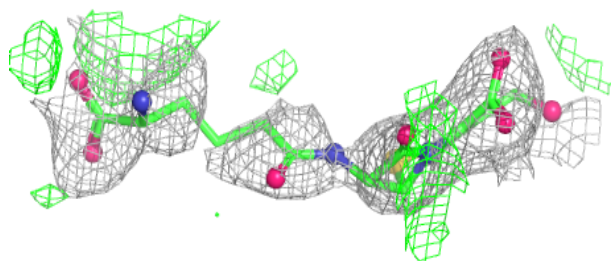
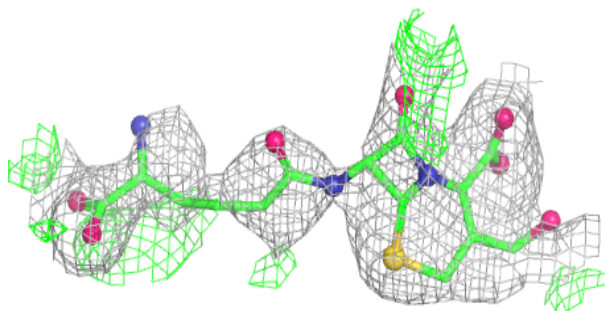
**Electron density around CSC E 1383 (B):**

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

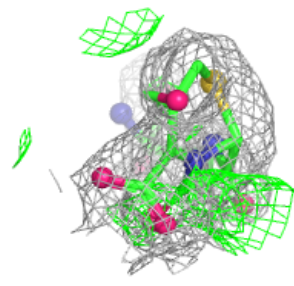
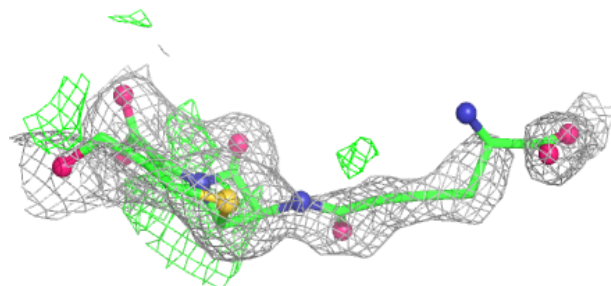
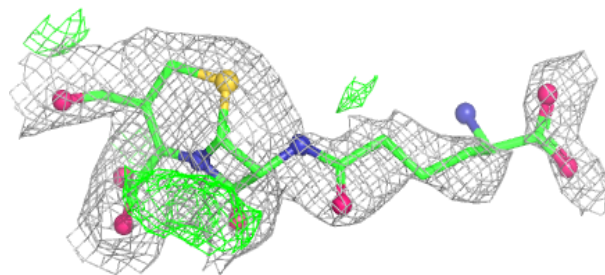


Electron density around CSC A 1383 (B):

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

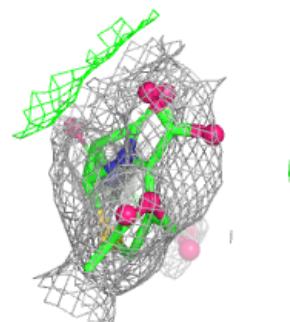
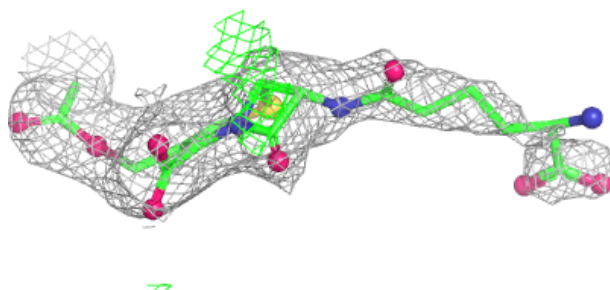
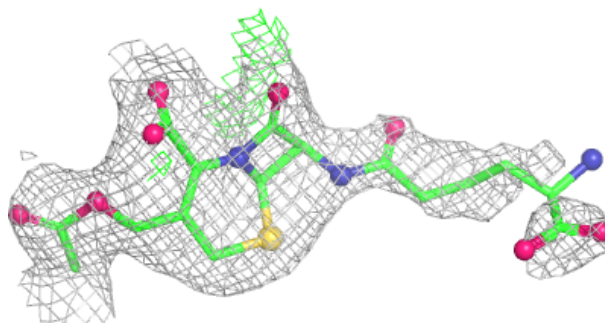
**Electron density around CSC G 1383 (B):**

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

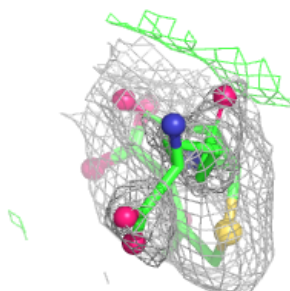
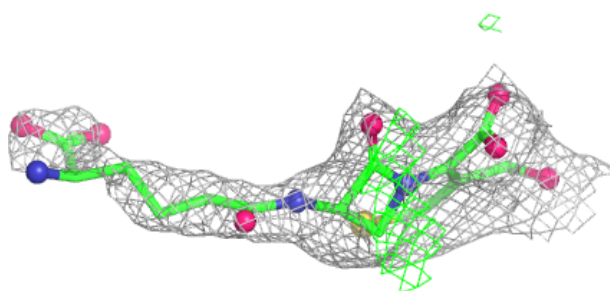
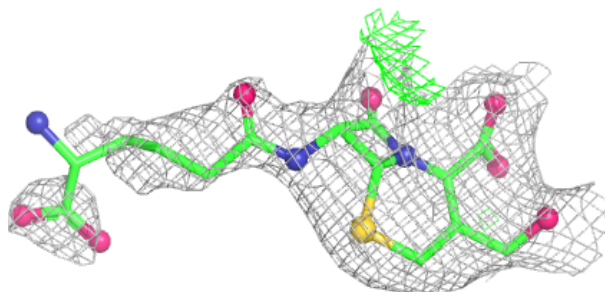


Electron density around CSC H 1383 (A):

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

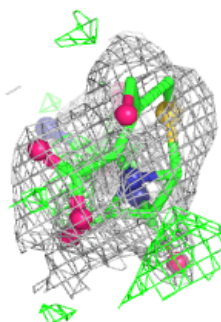
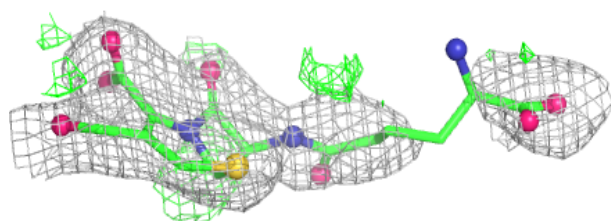
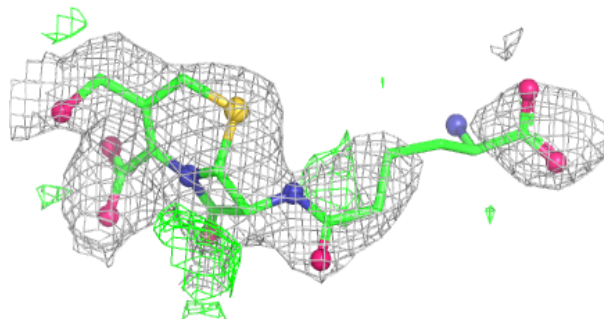
**Electron density around CSC H 1383 (B):**

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

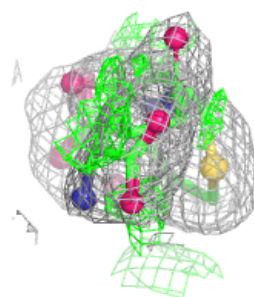
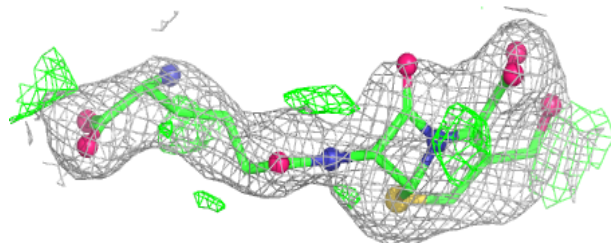
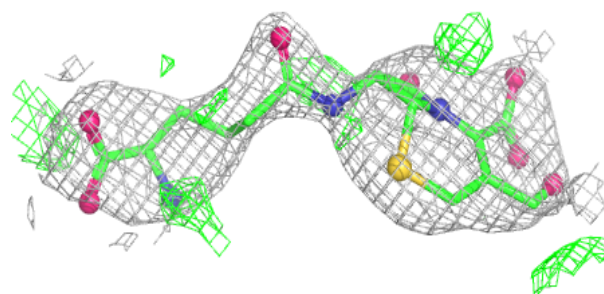


Electron density around CSC I 1383 (B):

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

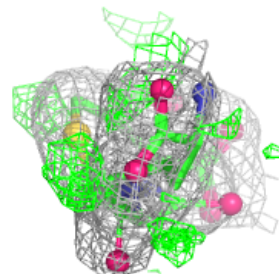
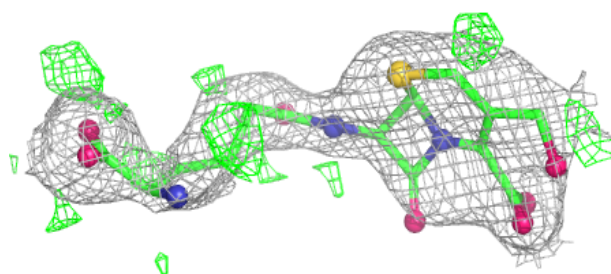
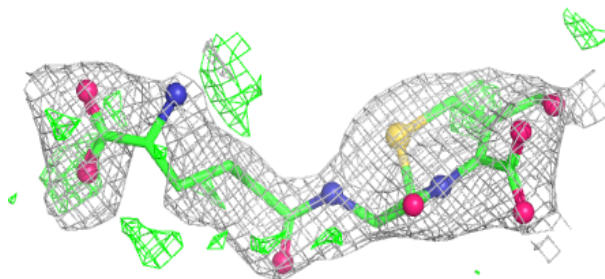
**Electron density around CSC J 1385 (B):**

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and green (positive)

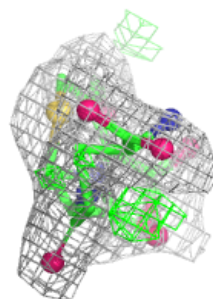
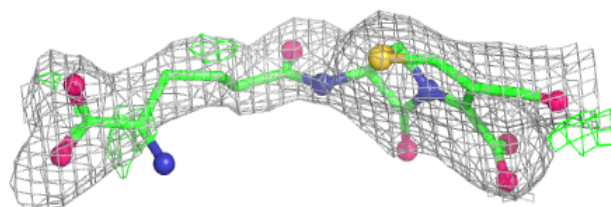
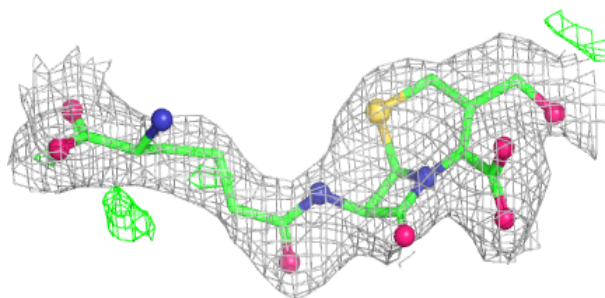


Electron density around CSC K 1385 (B):

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

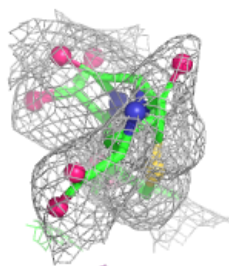
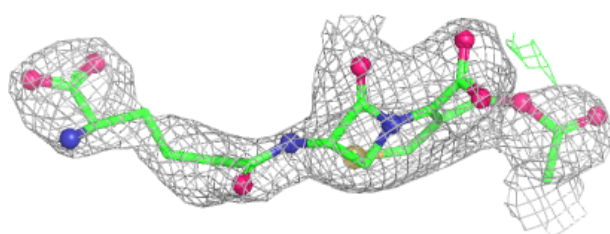
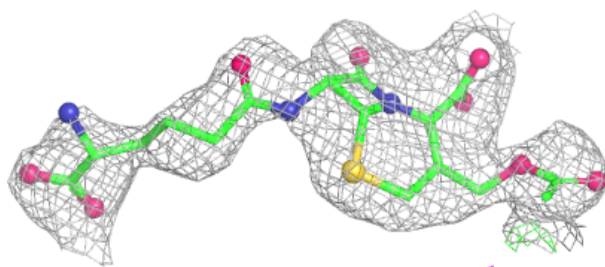
**Electron density around CSC B 1384 (B):**

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

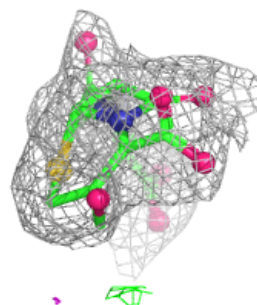
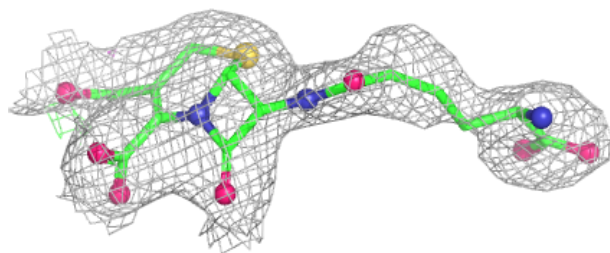
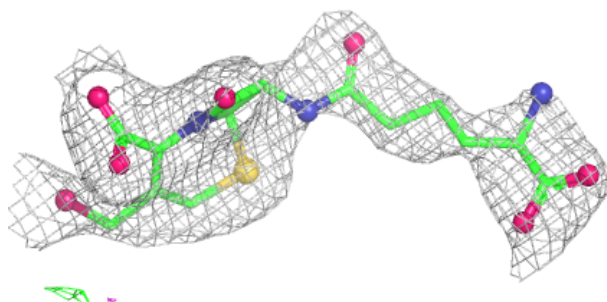


Electron density around CSC F 1383 (A):

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

**Electron density around CSC F 1383 (B):**

$2mF_o-DF_c$ (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.