



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:51 PM UTC

PDB ID : 9FDD / pdb_00009fdd
Title : The crystal structure of full length tetramer CysB from *Klebsiella aerogenes* in complex with N-acetylserine
Authors : Verschueren, K.H.G.; Dodson, E.J.; Wilkinson, A.J.
Deposited on : 2024-05-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

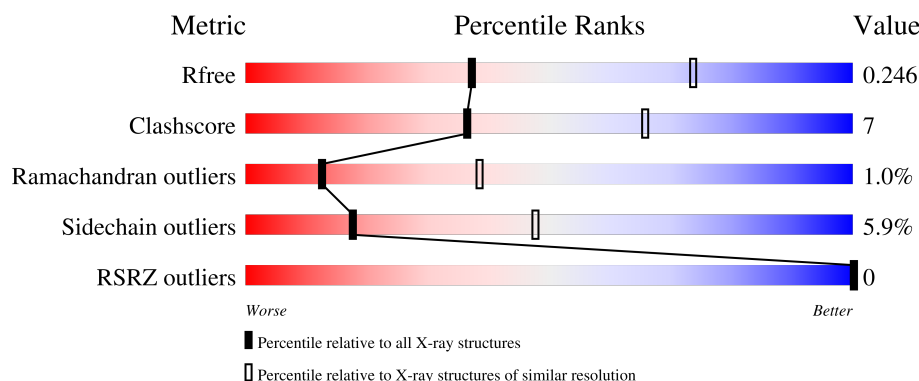
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	324	 81% 16% .
1	B	324	 74% 22% .
1	C	324	 82% 17% .
1	D	324	 76% 21% .
1	E	324	 78% 19% .

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Mol	Chain	Length	Quality of chain
1	F	324	 77% 21% •
1	G	324	 81% 17% •
1	H	324	 73% 23% •

2 Entry composition

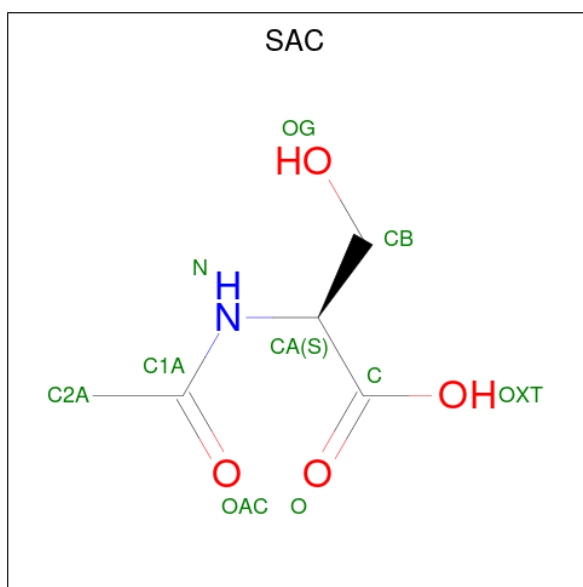
There are 3 unique types of molecules in this entry. The entry contains 41037 atoms, of which 20612 are hydrogens and 0 are deuteriums.

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 HTH-type transcriptional regulator CysB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	H	N	O	S	82	2	0
			5118	1619	2573	442	476	8			
1	B	324	Total	C	H	N	O	S	82	0	0
			5100	1614	2564	440	474	8			
1	C	324	Total	C	H	N	O	S	82	2	0
			5118	1619	2573	442	476	8			
1	D	324	Total	C	H	N	O	S	82	0	0
			5100	1614	2564	440	474	8			
1	E	324	Total	C	H	N	O	S	82	2	0
			5118	1619	2573	442	476	8			
1	F	324	Total	C	H	N	O	S	82	0	0
			5100	1614	2564	440	474	8			
1	G	324	Total	C	H	N	O	S	82	2	0
			5118	1619	2573	442	476	8			
1	H	324	Total	C	H	N	O	S	82	0	0
			5100	1614	2564	440	474	8			

- Molecule 2 is N-ACETYL-SERINE (CCD ID: SAC) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	4	0
			18	5	8	1	4		
2	B	1	Total	C	H	N	O	4	0
			18	5	8	1	4		
2	C	1	Total	C	H	N	O	4	0
			18	5	8	1	4		
2	D	1	Total	C	H	N	O	4	0
			18	5	8	1	4		
2	E	1	Total	C	H	N	O	4	0
			18	5	8	1	4		
2	F	1	Total	C	H	N	O	4	0
			18	5	8	1	4		
2	G	1	Total	C	H	N	O	4	0
			18	5	8	1	4		
2	H	1	Total	C	H	N	O	4	0
			18	5	8	1	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	2	Total	O	0	0
			2	2		
3	C	4	Total	O	0	0
			4	4		
3	D	1	Total	O	0	0
			1	1		

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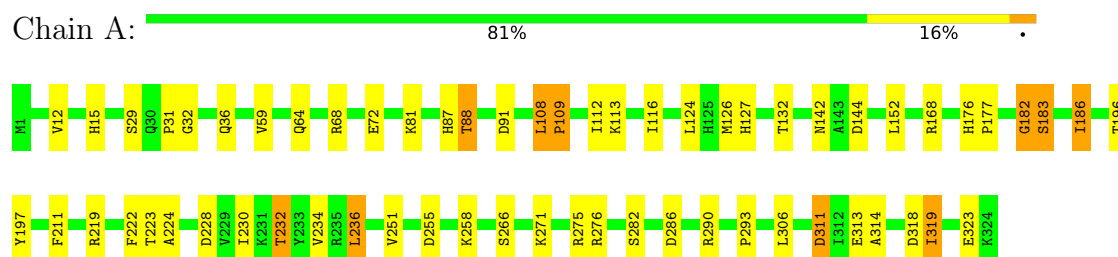
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total 3	O 3	0	0
3	F	2	Total 2	O 2	0	0
3	G	3	Total 3	O 3	0	0
3	H	1	Total 1	O 1	0	0

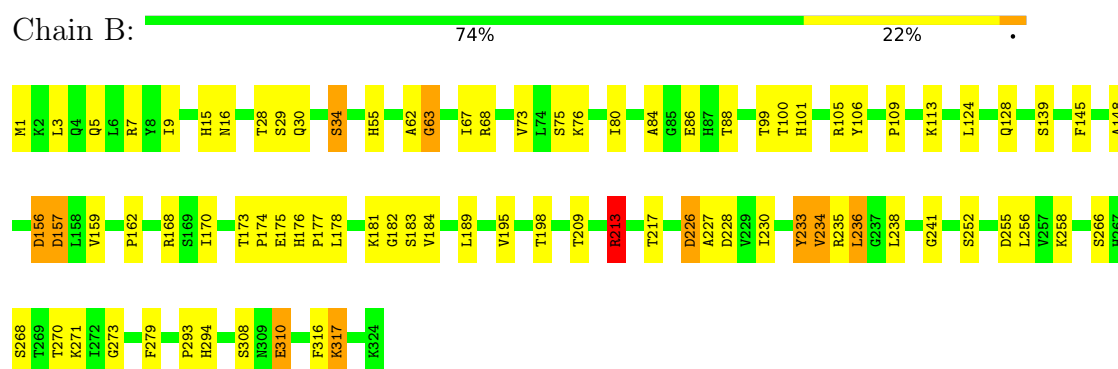
3 Residue-property plots

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

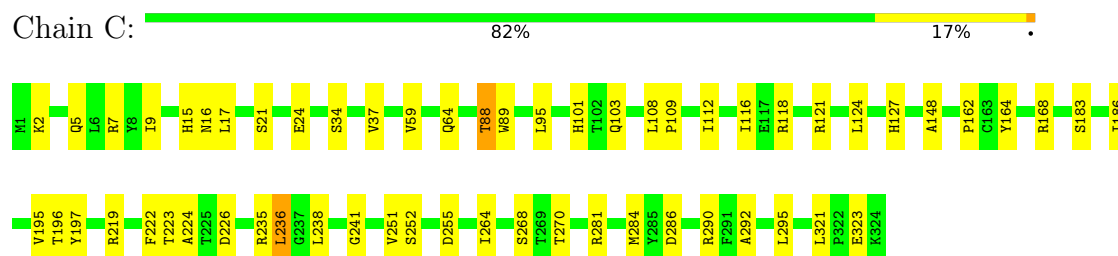
- Molecule 1: HTH-type transcriptional regulator CysB



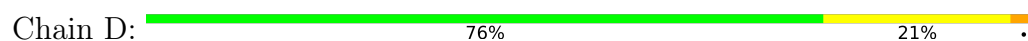
- Molecule 1: HTH-type transcriptional regulator CysB

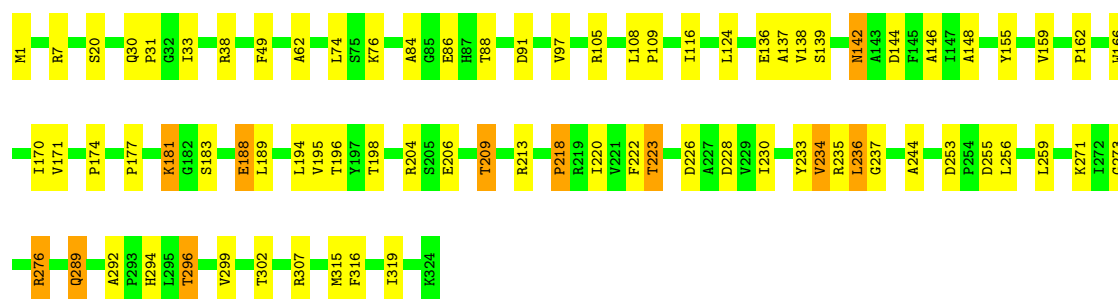


- Molecule 1: HTH-type transcriptional regulator CysB



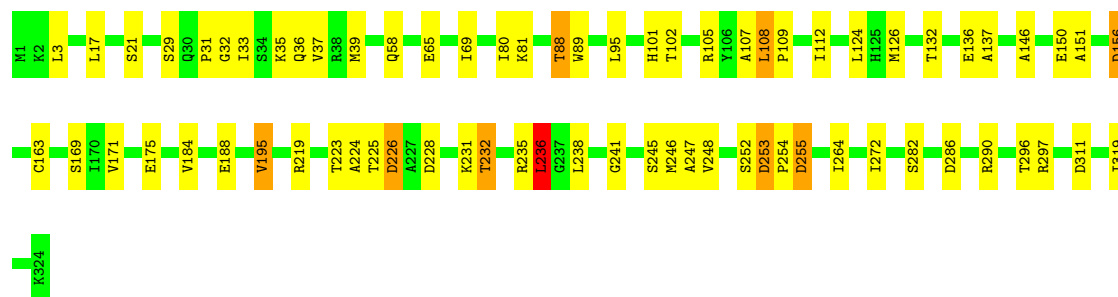
- Molecule 1: HTH-type transcriptional regulator CysB





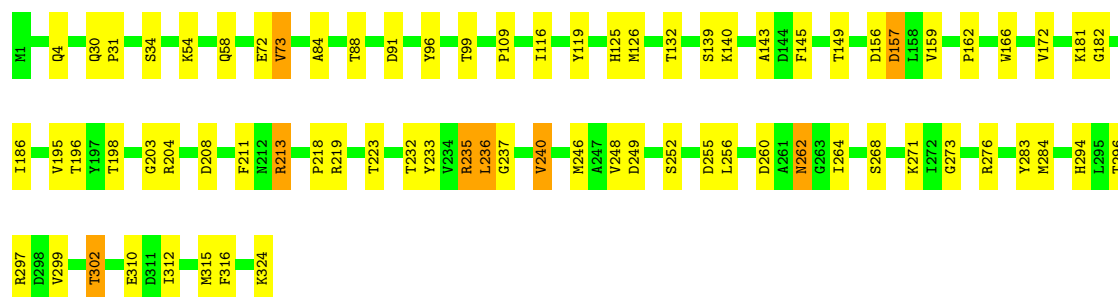
- Molecule 1: HTH-type transcriptional regulator CysB

Chain E: 78% 19%



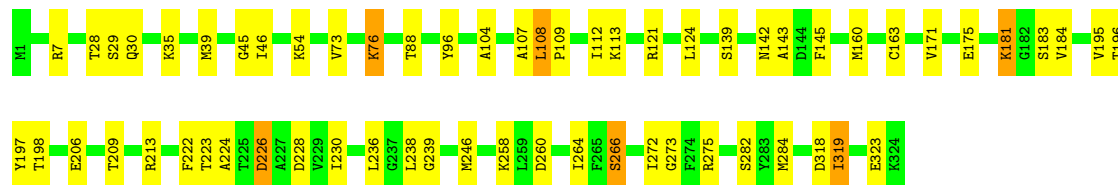
- Molecule 1: HTH-type transcriptional regulator CysB

Chain F: 77% 21%



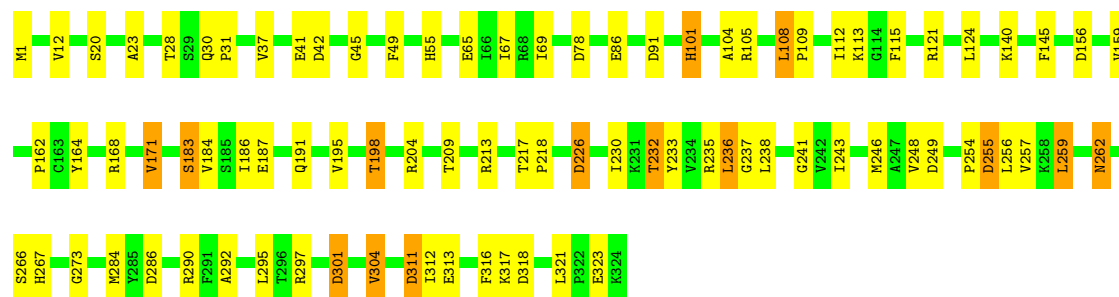
- Molecule 1: HTH-type transcriptional regulator CysB

Chain G: 81% 17%



- Molecule 1: HTH-type transcriptional regulator CysB

Chain H: 73% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	187.44Å 187.44Å 224.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.46 – 2.80 41.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.46-2.80) 99.9 (41.46-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0425, REFMAC 5.8.0425	Depositor
R, R_{free}	0.180 , 0.246 0.180 , 0.246	Depositor DCC
R_{free} test set	3626 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 14.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.030 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.019 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.023 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.019 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.020 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.033 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.164 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	41037	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1784e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SAC

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	0.63	0/2612	1.20	9/3548 (0.3%)
1	B	0.60	0/2590	1.31	16/3517 (0.5%)
1	C	0.62	0/2612	1.20	3/3548 (0.1%)
1	D	0.60	0/2590	1.26	12/3517 (0.3%)
1	E	0.62	0/2612	1.21	7/3548 (0.2%)
1	F	0.61	0/2590	1.24	7/3517 (0.2%)
1	G	0.63	0/2612	1.23	7/3548 (0.2%)
1	H	0.62	0/2590	1.30	14/3517 (0.4%)
All	All	0.62	0/20808	1.25	75/28260 (0.3%)

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	A	0	2
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	2
1	H	0	1
All	All	0	9

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	198	THR	CA-CB-OG1	-9.40	95.50	109.60
1	H	232	THR	CA-CB-OG1	-7.57	98.24	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	ARG	N-CA-CB	7.48	121.28	110.06
1	B	217	THR	CA-CB-OG1	-7.47	98.40	109.60
1	H	65	GLU	CB-CA-C	7.38	122.56	110.90
1	B	7	ARG	CB-CA-C	-7.12	98.58	110.68
1	E	226	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	15	HIS	CA-CB-CG	7.00	120.80	113.80
1	F	73	VAL	N-CA-CB	6.98	118.72	110.55
1	C	226	ASP	CA-CB-CG	6.94	119.54	112.60
1	G	258	LYS	CB-CA-C	6.76	120.83	109.48
1	H	213	ARG	N-CA-CB	6.68	120.05	110.16
1	G	226	ASP	CA-CB-CG	6.59	119.19	112.60
1	G	88	THR	CA-CB-OG1	-6.48	99.88	109.60
1	F	91	ASP	CA-CB-CG	6.40	119.00	112.60
1	G	258	LYS	N-CA-CB	-6.34	100.05	110.52
1	D	209	THR	CA-CB-OG1	-6.33	100.11	109.60
1	B	55	HIS	CA-CB-CG	6.28	120.08	113.80
1	H	49	PHE	CA-CB-CG	6.25	120.05	113.80
1	D	296	THR	CA-CB-OG1	-6.21	100.28	109.60
1	D	206	GLU	CB-CG-CD	6.11	122.98	112.60
1	D	276	ARG	N-CA-CB	-6.10	101.17	110.01
1	E	296	THR	CA-CB-OG1	-6.08	100.48	109.60
1	G	7	ARG	N-CA-CB	6.07	119.04	110.12
1	B	157	ASP	CA-CB-CG	6.03	118.63	112.60
1	E	195	VAL	N-CA-CB	-5.89	103.81	111.82
1	D	259	LEU	N-CA-CB	-5.84	101.28	110.69
1	B	145	PHE	CB-CA-C	-5.84	97.17	109.38
1	B	258	LYS	N-CA-CB	-5.82	100.39	110.17
1	H	235	ARG	N-CA-CB	-5.82	100.77	110.42
1	F	195	VAL	N-CA-CB	-5.78	104.39	111.67
1	A	144	ASP	CA-CB-CG	5.75	118.35	112.60
1	F	99	THR	CA-CB-OG1	-5.68	101.08	109.60
1	C	88	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	132	THR	CA-CB-OG1	-5.65	101.13	109.60
1	D	144	ASP	CA-CB-CG	5.63	118.23	112.60
1	D	91	ASP	CA-CB-CG	5.63	118.23	112.60
1	E	311	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	310	GLU	CB-CG-CD	5.51	121.97	112.60
1	B	233	TYR	N-CA-CB	5.49	118.79	110.28
1	H	191	GLN	CB-CA-C	-5.49	100.66	110.70
1	A	91	ASP	CA-CB-CG	5.48	118.08	112.60
1	E	156	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	293	PRO	N-CA-C	5.45	121.72	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	THR	CA-CB-OG1	-5.43	101.45	109.60
1	G	260	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	253	ASP	CA-CB-CG	5.37	117.97	112.60
1	G	209	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	73	VAL	N-CA-C	-5.32	105.31	110.42
1	H	226	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	218	PRO	N-CA-CB	-5.23	98.22	103.19
1	A	311	ASP	CA-CB-CG	5.22	117.82	112.60
1	H	255	ASP	CA-CB-CG	5.22	117.82	112.60
1	H	55	HIS	CA-CB-CG	5.20	119.00	113.80
1	D	276	ARG	CB-CA-C	5.19	119.03	110.88
1	H	318	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	258	LYS	N-CA-CB	-5.16	102.18	110.69
1	C	15	HIS	CA-CB-CG	5.12	118.92	113.80
1	H	156	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	253	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	49	PHE	CA-CB-CG	5.08	118.88	113.80
1	F	204	ARG	CB-CA-C	-5.08	100.32	110.42
1	F	219	ARG	CB-CA-C	5.07	118.40	110.19
1	E	132	THR	OG1-CB-CG2	-5.06	99.19	109.30
1	H	78	ASP	CA-CB-CG	5.05	117.65	112.60
1	H	235	ARG	CB-CA-C	5.05	119.78	111.50
1	F	310	GLU	CB-CA-C	-5.04	102.93	110.90
1	A	109	PRO	CA-C-N	5.03	126.43	120.14
1	A	109	PRO	C-N-CA	5.03	126.43	120.14
1	A	142	ASN	CB-CA-C	-5.03	101.43	110.37
1	B	106	TYR	CB-CA-C	5.03	120.42	110.42
1	B	226	ASP	CA-CB-CG	5.01	117.61	112.60
1	D	223	THR	CA-CB-OG1	-5.01	102.08	109.60
1	B	173	THR	CA-CB-OG1	-5.00	102.09	109.60
1	B	213	ARG	N-CA-CB	5.00	118.04	110.28

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	ARG	Sidechain
1	A	275	ARG	Sidechain
1	D	38	ARG	Sidechain
1	E	225	THR	Peptide
1	F	235	ARG	Sidechain
1	F	276	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	121	ARG	Sidechain
1	G	275	ARG	Sidechain
1	H	204	ARG	Sidechain

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	2545	2573	2552	31	0
1	B	2536	2564	2553	50	0
1	C	2545	2573	2552	36	0
1	D	2536	2564	2553	55	0
1	E	2545	2573	2552	46	0
1	F	2536	2564	2553	40	0
1	G	2545	2573	2552	27	0
1	H	2536	2564	2553	38	0
2	A	10	8	8	0	0
2	B	10	8	8	0	0
2	C	10	8	8	0	0
2	D	10	8	8	2	0
2	E	10	8	8	0	0
2	F	10	8	8	3	0
2	G	10	8	8	0	0
2	H	10	8	8	0	0
3	A	5	0	0	1	0
3	B	2	0	0	0	0
3	C	4	0	0	1	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
All	All	20425	20612	20484	296	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 7.

All (296) 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:E:231:LYS:HE3	1:E:253:ASP:OD2	1.82	0.80
1:E:101:HIS:HB3	1:E:105:ARG:HH12	1.49	0.78
1:B:234:VAL:O	1:B:235:ARG:HG3	1.85	0.77
1:C:112:ILE:HD12	1:C:124:LEU:HD21	1.69	0.75
1:H:297:ARG:O	1:H:301:ASP:HB2	1.91	0.71
1:C:127:HIS:NE2	1:D:198:THR:HG21	2.08	0.69
1:D:138:VAL:HG21	1:D:146:ALA:HB2	1.75	0.69
1:B:101:HIS:CG	1:B:226:ASP:HB3	2.29	0.68
1:B:84:ALA:HB1	1:B:88:THR:HG21	1.77	0.67
1:A:255:ASP:HB2	3:A:502:HOH:O	1.94	0.67
1:E:107:ALA:HB2	1:E:246:MET:HE1	1.77	0.66
1:B:178:LEU:HA	1:B:181:LYS:HD3	1.78	0.65
1:A:228:ASP:OD2	1:B:105:ARG:HD3	1.96	0.65
1:D:276:ARG:HH11	1:D:276:ARG:HG3	1.61	0.64
1:B:195:VAL:HG12	1:B:230:ILE:HG23	1.79	0.63
1:C:121:ARG:HG2	1:C:121:ARG:HH11	1.64	0.63
1:F:296:THR:OG1	1:F:299:VAL:HG23	2.00	0.61
1:E:228:ASP:O	1:E:232:THR:HG23	2.00	0.61
1:C:235:ARG:O	1:C:236:LEU:HB3	1.98	0.61
1:D:181:LYS:HE2	1:D:188:GLU:OE1	2.00	0.61
1:F:246:MET:HE3	2:F:401:SAC:H2A2	1.81	0.61
1:B:234:VAL:C	1:B:235:ARG:HG3	2.23	0.61
1:E:184:VAL:O	1:E:264:ILE:HD11	2.01	0.60
1:E:223:THR:OG1	1:F:125:HIS:HD2	1.84	0.60
1:A:32:GLY:O	1:A:36:GLN:HG2	2.03	0.59
1:H:168:ARG:HG3	1:H:168:ARG:HH11	1.68	0.59
3:C:501:HOH:O	1:D:116:ILE:HD11	2.02	0.58
1:E:184:VAL:HA	1:E:188:GLU:OE1	2.02	0.58
1:E:235:ARG:O	1:E:236:LEU:HD23	2.02	0.58
1:D:296:THR:OG1	1:D:299:VAL:HG23	2.02	0.58
1:A:152:LEU:HD13	1:A:271:LYS:HE3	1.85	0.58
1:E:286:ASP:O	1:E:290:ARG:HG3	2.03	0.58
1:C:124:LEU:O	1:D:222:PHE:HA	2.03	0.58
1:H:236:LEU:HG	1:H:237:GLY:N	2.18	0.58
1:A:222:PHE:HA	1:B:124:LEU:O	2.04	0.57
1:A:59:VAL:HG12	1:A:64:GLN:HG3	1.85	0.57
1:E:319:ILE:HD12	1:E:319:ILE:N	2.20	0.57
1:F:162:PRO:O	1:F:294:HIS:HE1	1.87	0.57
1:F:233:TYR:CZ	1:F:236:LEU:HD13	2.40	0.57
1:H:145:PHE:HZ	1:H:284:MET:HB3	1.68	0.57
1:A:87:HIS:CD2	1:D:62:ALA:HB2	2.41	0.56
1:F:196:THR:O	1:F:223:THR:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASP:O	1:A:319:ILE:HG13	2.05	0.56
1:H:262:ASN:HD22	1:H:262:ASN:N	2.03	0.56
1:F:156:ASP:O	1:F:157:ASP:HB2	2.05	0.56
1:G:107:ALA:HB2	1:G:246:MET:HE1	1.87	0.56
1:A:228:ASP:O	1:A:232:THR:HG23	2.06	0.55
1:A:112:ILE:HD12	1:A:124:LEU:HD21	1.86	0.55
1:D:174:PRO:HD3	1:D:255:ASP:O	2.07	0.55
1:G:28:THR:OG1	1:G:29:SER:N	2.39	0.55
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.72	0.55
1:H:286:ASP:OD2	1:H:290:ARG:NH1	2.33	0.55
1:E:156:ASP:O	1:G:213:ARG:HG3	2.07	0.54
1:C:112:ILE:HG23	1:C:124:LEU:HD22	1.89	0.54
1:D:233:TYR:C	1:D:235:ARG:H	2.15	0.54
1:C:103:GLN:NE2	1:C:164:TYR:OH	2.40	0.54
1:F:156:ASP:O	1:F:157:ASP:CB	2.56	0.54
1:D:316:PHE:HA	1:D:319:ILE:HD12	1.90	0.54
1:A:127:HIS:NE2	1:B:198:THR:HG21	2.23	0.53
1:A:230:ILE:O	1:A:234:VAL:HG23	2.09	0.53
1:B:170:ILE:HD11	1:B:189:LEU:HD22	1.89	0.53
1:E:102:THR:HG22	1:E:246:MET:HE2	1.90	0.53
1:F:84:ALA:HB1	1:F:88:THR:HG21	1.90	0.53
1:B:105:ARG:O	1:B:109:PRO:CD	2.57	0.53
1:D:7:ARG:HA	1:D:74:LEU:HD11	1.89	0.53
1:B:308:SER:OG	1:B:310:GLU:HG2	2.08	0.53
1:A:112:ILE:O	1:A:116:ILE:HG12	2.09	0.52
1:D:138:VAL:CG2	1:D:146:ALA:HB2	2.38	0.52
1:C:112:ILE:O	1:C:116:ILE:HG12	2.09	0.52
1:E:171:VAL:HG11	1:E:248:VAL:HG21	1.90	0.52
1:D:30:GLN:N	1:D:31:PRO:HD2	2.24	0.52
1:D:307:ARG:HG3	1:D:307:ARG:HH11	1.74	0.52
1:F:312:ILE:O	1:F:316:PHE:HD2	1.93	0.52
1:B:156:ASP:O	1:B:157:ASP:HB2	2.10	0.52
1:F:159:VAL:O	1:F:273:GLY:HA2	2.10	0.52
1:G:160:MET:SD	1:G:273:GLY:HA3	2.50	0.52
1:C:2:LYS:O	1:C:5:GLN:HB2	2.10	0.52
1:C:118:ARG:NH1	1:C:118:ARG:HG3	2.25	0.52
1:E:252:SER:O	1:E:254:PRO:HD3	2.10	0.51
1:C:127:HIS:CD2	1:D:198:THR:HG21	2.46	0.51
1:H:30:GLN:HB3	1:H:31:PRO:HD3	1.93	0.51
1:B:28:THR:OG1	1:B:29:SER:N	2.43	0.51
1:C:112:ILE:HD12	1:C:124:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE1	1:D:76:LYS:HD2	2.10	0.51
1:B:233:TYR:CD1	1:B:233:TYR:C	2.89	0.51
1:D:236:LEU:CG	1:D:237:GLY:N	2.73	0.51
1:E:286:ASP:OD2	1:E:290:ARG:NE	2.42	0.51
1:G:112:ILE:HD12	1:G:124:LEU:HD21	1.92	0.51
1:B:230:ILE:O	1:B:234:VAL:HG23	2.11	0.51
1:H:195:VAL:O	1:H:241:GLY:HA2	2.09	0.51
1:B:101:HIS:HB3	1:B:105:ARG:HH22	1.76	0.51
1:B:148:ALA:O	1:B:270:THR:HA	2.11	0.50
1:D:196:THR:O	1:D:223:THR:HA	2.11	0.50
1:H:292:ALA:HB3	1:H:295:LEU:HD12	1.93	0.50
1:E:17:LEU:HD11	1:E:58:GLN:HA	1.94	0.50
1:H:195:VAL:HG12	1:H:230:ILE:HG23	1.93	0.50
1:D:276:ARG:HG3	1:D:276:ARG:NH1	2.25	0.50
1:B:105:ARG:O	1:B:109:PRO:HG2	2.12	0.50
1:F:262:ASN:N	1:F:262:ASN:HD22	2.10	0.50
1:C:121:ARG:HG2	1:C:121:ARG:NH1	2.27	0.49
1:C:112:ILE:HG23	1:C:124:LEU:CD2	2.42	0.49
1:F:235:ARG:N	1:F:235:ARG:HD2	2.27	0.49
1:H:262:ASN:N	1:H:262:ASN:ND2	2.56	0.49
1:C:88:THR:HG22	1:C:89:TRP:CE3	2.47	0.49
1:B:159:VAL:O	1:B:273:GLY:HA2	2.12	0.49
1:E:29:SER:OG	1:E:31:PRO:HD2	2.13	0.49
1:E:146:ALA:O	1:E:272:ILE:HA	2.13	0.49
1:H:257:VAL:HG12	1:H:259:LEU:HD13	1.95	0.49
1:E:235:ARG:O	1:E:236:LEU:CB	2.60	0.49
1:H:91:ASP:OD1	1:H:121:ARG:NH2	2.42	0.49
1:H:168:ARG:HG3	1:H:168:ARG:NH1	2.28	0.49
1:D:234:VAL:HG12	1:D:234:VAL:O	2.13	0.49
1:E:255:ASP:OD1	1:E:255:ASP:N	2.45	0.48
1:F:186:ILE:HB	1:F:264:ILE:HG23	1.93	0.48
1:D:302:THR:HB	1:D:315:MET:HE1	1.93	0.48
1:A:113:LYS:HA	1:B:236:LEU:HD11	1.96	0.48
1:B:101:HIS:CD2	1:B:226:ASP:HB3	2.47	0.48
1:G:222:PHE:HA	1:H:124:LEU:O	2.12	0.48
1:B:1:MET:HA	1:B:5:GLN:OE1	2.14	0.48
1:C:108:LEU:O	1:C:112:ILE:HG12	2.13	0.48
1:A:59:VAL:CG1	1:A:64:GLN:HG3	2.43	0.48
1:B:233:TYR:CD1	1:B:233:TYR:O	2.67	0.48
1:F:72:GLU:OE1	1:G:76:LYS:HD2	2.13	0.48
1:C:286:ASP:OD2	1:C:290:ARG:NE	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LEU:HD23	1:D:237:GLY:N	2.29	0.48
1:E:112:ILE:HD12	1:E:124:LEU:CD2	2.44	0.48
1:C:168:ARG:NH2	1:C:268:SER:OG	2.29	0.47
1:E:112:ILE:HD12	1:E:124:LEU:HD21	1.95	0.47
1:A:108:LEU:O	1:A:112:ILE:HG12	2.14	0.47
1:F:233:TYR:CD1	1:F:233:TYR:C	2.91	0.47
1:D:162:PRO:HA	1:D:271:LYS:HG2	1.96	0.47
1:D:307:ARG:HG3	1:D:307:ARG:NH1	2.29	0.47
1:D:108:LEU:N	1:D:109:PRO:CD	2.77	0.47
1:D:213:ARG:HG3	1:D:213:ARG:HH11	1.79	0.47
1:E:195:VAL:O	1:E:241:GLY:HA2	2.14	0.47
1:D:236:LEU:HG	1:D:237:GLY:N	2.29	0.47
1:E:231:LYS:CE	1:E:253:ASP:OD2	2.60	0.47
1:B:105:ARG:O	1:B:109:PRO:CG	2.62	0.47
1:B:156:ASP:O	1:B:157:ASP:CB	2.61	0.47
1:C:59:VAL:HG12	1:C:64:GLN:HG3	1.97	0.47
1:C:222:PHE:HA	1:D:124:LEU:O	2.14	0.47
1:G:96:TYR:HB3	1:G:143:ALA:HA	1.96	0.47
1:G:181:LYS:C	1:G:183:SER:H	2.22	0.47
1:B:316:PHE:O	1:B:317:LYS:C	2.58	0.47
1:H:233:TYR:CD1	1:H:233:TYR:C	2.92	0.47
1:E:81:LYS:HE3	1:H:1:MET:HE3	1.96	0.47
1:H:312:ILE:O	1:H:316:PHE:HD2	1.97	0.47
1:H:316:PHE:O	1:H:317:LYS:C	2.58	0.47
1:B:235:ARG:O	1:B:236:LEU:HB2	2.15	0.46
1:F:73:VAL:HG13	1:G:73:VAL:HG13	1.95	0.46
1:D:162:PRO:O	1:D:294:HIS:HE1	1.99	0.46
1:B:178:LEU:HD23	1:B:181:LYS:HD3	1.98	0.46
1:E:163:CYS:SG	1:E:272:ILE:HG22	2.55	0.46
1:F:162:PRO:HA	1:F:271:LYS:HG2	1.96	0.46
1:H:112:ILE:O	1:H:113:LYS:C	2.58	0.46
1:B:176:HIS:CE1	1:B:178:LEU:HD12	2.50	0.46
1:E:35:LYS:O	1:E:39:MET:HG3	2.16	0.46
1:H:101:HIS:CD2	1:H:226:ASP:HB3	2.51	0.46
1:D:166:TRP:CE3	2:D:401:SAC:H2A1	2.51	0.46
1:G:35:LYS:O	1:G:39:MET:HG3	2.16	0.46
1:A:176:HIS:CG	1:A:177:PRO:HD2	2.51	0.46
1:C:196:THR:O	1:C:223:THR:HA	2.16	0.46
1:D:233:TYR:O	1:D:235:ARG:N	2.48	0.46
1:G:108:LEU:H	1:G:109:PRO:CD	2.28	0.46
1:B:101:HIS:CD2	1:B:128:GLN:HG2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:ASP:C	1:G:319:ILE:HD12	2.41	0.46
1:A:87:HIS:CG	1:D:62:ALA:HB2	2.51	0.46
1:E:150:GLU:O	1:E:151:ALA:C	2.59	0.46
1:B:76:LYS:O	1:B:80:ILE:HG13	2.16	0.46
1:C:108:LEU:O	1:C:109:PRO:C	2.57	0.46
1:B:213:ARG:NH1	1:B:213:ARG:HG3	2.31	0.45
1:D:289:GLN:HG3	1:D:296:THR:HA	1.98	0.45
1:D:233:TYR:C	1:D:233:TYR:CD1	2.94	0.45
1:G:108:LEU:N	1:G:109:PRO:CD	2.78	0.45
1:A:196:THR:O	1:A:223:THR:HA	2.16	0.45
1:D:159:VAL:O	1:D:273:GLY:HA2	2.16	0.45
1:D:166:TRP:CZ3	1:D:244:ALA:HB2	2.52	0.45
1:E:95:LEU:HB3	1:E:124:LEU:HD12	1.97	0.45
1:H:104:ALA:HA	1:H:108:LEU:HD12	1.98	0.45
1:C:195:VAL:O	1:C:241:GLY:HA2	2.17	0.45
1:H:164:TYR:CE1	1:H:246:MET:HE1	2.52	0.45
1:A:108:LEU:O	1:A:109:PRO:C	2.59	0.45
1:B:63:GLY:O	1:B:67:ILE:HG12	2.17	0.45
1:D:148:ALA:HB2	1:D:155:TYR:CE2	2.52	0.45
1:E:65:GLU:O	1:E:69:ILE:HG13	2.17	0.45
1:H:23:ALA:HB1	1:H:28:THR:O	2.16	0.45
1:C:162:PRO:HB2	1:C:321:LEU:HD11	1.98	0.45
1:F:96:TYR:HB3	1:F:143:ALA:HA	1.99	0.45
1:C:186:ILE:HB	1:C:264:ILE:HG23	1.98	0.45
1:A:81:LYS:HE2	1:D:1:MET:HE3	1.99	0.44
1:A:182:GLY:O	1:A:183:SER:CB	2.65	0.44
1:E:112:ILE:CD1	1:E:124:LEU:HD21	2.47	0.44
1:G:228:ASP:OD2	1:H:105:ARG:HD3	2.17	0.44
1:A:108:LEU:H	1:A:109:PRO:CD	2.29	0.44
1:B:9:ILE:HD12	1:B:67:ILE:HD13	1.99	0.44
1:B:195:VAL:O	1:B:241:GLY:HA2	2.18	0.44
1:B:294:HIS:CD2	1:B:294:HIS:H	2.35	0.44
1:E:36:GLN:OE1	1:E:39:MET:HE3	2.17	0.44
1:G:45:GLY:C	1:G:46:ILE:HG13	2.42	0.44
1:G:145:PHE:HZ	1:G:284:MET:HB3	1.83	0.44
1:C:292:ALA:HB3	1:C:295:LEU:HD12	1.99	0.44
1:F:172:VAL:HG12	1:F:240:VAL:HG22	1.98	0.44
1:H:301:ASP:O	1:H:304:VAL:HG22	2.18	0.44
1:H:311:ASP:OD1	1:H:311:ASP:N	2.49	0.44
1:H:42:ASP:O	1:H:45:GLY:N	2.50	0.44
1:G:104:ALA:O	1:G:109:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:NH2	1:B:268:SER:OG	2.45	0.44
1:D:194:LEU:HD12	1:D:218:PRO:HB2	2.00	0.44
1:E:235:ARG:O	1:E:236:LEU:HB3	2.18	0.44
1:B:101:HIS:CG	1:B:226:ASP:CB	3.00	0.43
1:F:211:PHE:CE2	1:F:218:PRO:HB3	2.53	0.43
1:C:9:ILE:HG22	1:C:37:VAL:HG22	2.00	0.43
1:D:84:ALA:HB1	1:D:88:THR:HG21	1.99	0.43
1:B:175:GLU:OE1	1:B:175:GLU:N	2.52	0.43
1:B:279:PHE:CE1	1:E:39:MET:HG2	2.53	0.43
1:C:197:TYR:HA	1:C:224:ALA:O	2.18	0.43
1:H:104:ALA:O	1:H:109:PRO:HD3	2.18	0.43
1:B:162:PRO:HA	1:B:271:LYS:HG2	2.00	0.43
1:D:136:GLU:O	1:D:137:ALA:C	2.62	0.43
1:E:101:HIS:CD2	1:E:226:ASP:OD2	2.71	0.43
1:A:286:ASP:OD2	1:A:290:ARG:NE	2.49	0.43
1:B:227:ALA:O	1:B:228:ASP:C	2.61	0.43
1:D:1:MET:HE2	1:D:1:MET:HB3	1.90	0.43
1:G:196:THR:O	1:G:223:THR:HA	2.18	0.43
1:E:223:THR:OG1	1:F:125:HIS:CD2	2.69	0.43
1:A:311:ASP:O	1:A:314:ALA:HB3	2.18	0.43
1:D:195:VAL:HG12	1:D:230:ILE:HG23	2.01	0.43
1:C:16:ASN:O	1:C:17:LEU:HB2	2.18	0.43
1:E:80:ILE:HG13	1:H:69:ILE:HG21	2.01	0.43
1:F:302:THR:HB	1:F:315:MET:HE1	2.01	0.43
1:E:136:GLU:O	1:E:137:ALA:C	2.61	0.43
1:G:195:VAL:HG12	1:G:230:ILE:HG23	2.01	0.43
1:D:233:TYR:OH	1:D:236:LEU:HD22	2.19	0.43
1:G:112:ILE:HD12	1:G:124:LEU:CD2	2.49	0.43
1:H:112:ILE:O	1:H:115:PHE:N	2.52	0.42
1:E:245:SER:C	1:E:247:ALA:H	2.27	0.42
1:F:119:TYR:CE2	1:F:283:TYR:HB3	2.54	0.42
1:G:238:LEU:HD12	1:G:239:GLY:H	1.83	0.42
1:F:296:THR:O	1:F:297:ARG:C	2.62	0.42
1:H:37:VAL:O	1:H:41:GLU:HG3	2.18	0.42
1:A:29:SER:OG	1:A:31:PRO:HD2	2.20	0.42
1:G:108:LEU:O	1:G:112:ILE:HG12	2.19	0.42
1:D:142:ASN:OD1	1:D:142:ASN:N	2.51	0.42
1:D:170:ILE:CD1	1:D:189:LEU:HD13	2.49	0.42
1:H:186:ILE:HG23	1:H:187:GLU:N	2.34	0.42
1:D:230:ILE:O	1:D:234:VAL:HG23	2.19	0.42
1:A:197:TYR:HA	1:A:224:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:MET:HE3	1:E:126:MET:HB3	1.85	0.42
1:F:149:THR:HG21	2:F:401:SAC:OAC	2.19	0.42
1:D:234:VAL:O	1:D:235:ARG:HG3	2.20	0.42
1:F:30:GLN:N	1:F:31:PRO:HD2	2.34	0.42
1:F:233:TYR:CD1	1:F:233:TYR:O	2.73	0.42
1:H:145:PHE:CZ	1:H:284:MET:HB3	2.53	0.42
1:B:30:GLN:O	1:B:34:SER:HB2	2.20	0.42
1:C:281:ARG:O	1:C:284:MET:HB2	2.19	0.42
1:D:233:TYR:C	1:D:235:ARG:N	2.78	0.42
1:E:33:ILE:O	1:E:37:VAL:HG23	2.20	0.42
1:G:197:TYR:HA	1:G:224:ALA:O	2.20	0.42
1:H:159:VAL:O	1:H:273:GLY:HA2	2.19	0.42
1:F:246:MET:HE3	2:F:401:SAC:C2A	2.48	0.41
1:B:3:LEU:HD23	1:B:3:LEU:HA	1.91	0.41
1:E:224:ALA:HA	1:F:126:MET:O	2.20	0.41
1:B:99:THR:OG1	1:B:100:THR:N	2.53	0.41
1:G:184:VAL:O	1:G:264:ILE:HD11	2.21	0.41
1:F:213:ARG:O	1:F:213:ARG:HG3	2.21	0.41
1:C:95:LEU:HB3	1:C:124:LEU:HD12	2.02	0.41
1:F:203:GLY:H	1:F:208:ASP:CG	2.28	0.41
1:G:109:PRO:O	1:G:113:LYS:HB2	2.20	0.41
1:G:163:CYS:SG	1:G:272:ILE:HG22	2.61	0.41
1:C:118:ARG:HG3	1:C:118:ARG:HH11	1.84	0.41
1:D:292:ALA:HB1	1:D:294:HIS:NE2	2.36	0.41
1:E:32:GLY:O	1:E:36:GLN:HG2	2.21	0.41
1:F:145:PHE:HZ	1:F:284:MET:HB3	1.85	0.41
1:E:88:THR:HG22	1:E:89:TRP:N	2.36	0.41
1:F:236:LEU:CG	1:F:237:GLY:N	2.82	0.41
1:H:101:HIS:CG	1:H:226:ASP:HB2	2.55	0.41
1:A:186:ILE:HD11	1:A:211:PHE:CD1	2.56	0.41
1:B:170:ILE:CD1	1:B:184:VAL:HG11	2.51	0.41
1:C:101:HIS:HD2	1:D:226:ASP:OD2	2.03	0.41
1:D:166:TRP:CD2	2:D:401:SAC:H2A1	2.56	0.41
1:E:108:LEU:O	1:E:109:PRO:C	2.64	0.41
1:F:235:ARG:N	1:F:235:ARG:CD	2.84	0.41
1:H:162:PRO:HB3	1:H:321:LEU:HD11	2.02	0.41
1:A:108:LEU:N	1:A:109:PRO:CD	2.84	0.41
1:A:126:MET:HE3	1:A:126:MET:HB3	1.85	0.41
1:B:174:PRO:HD3	1:B:255:ASP:O	2.21	0.41
1:C:219:ARG:HD3	1:D:88:THR:O	2.21	0.41
1:F:249:ASP:OD1	1:F:252:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ALA:O	1:C:270:THR:HA	2.22	0.40
1:H:171:VAL:HG11	1:H:243:ILE:HD11	2.02	0.40
1:F:166:TRP:CE2	1:F:268:SER:HB2	2.56	0.40
1:F:166:TRP:HA	1:F:324:LYS:OXT	2.21	0.40
1:B:62:ALA:O	1:B:63:GLY:C	2.64	0.40
1:C:124:LEU:HD23	1:D:222:PHE:HE2	1.87	0.40
1:E:219:ARG:NH1	1:F:88:THR:OG1	2.55	0.40
1:F:198:THR:HA	1:F:223:THR:HB	2.02	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	324/324 (100%)	302 (93%)	17 (5%)	5 (2%)	8	28
1	B	322/324 (99%)	300 (93%)	17 (5%)	5 (2%)	7	27
1	C	324/324 (100%)	304 (94%)	17 (5%)	3 (1%)	14	41
1	D	322/324 (99%)	298 (92%)	23 (7%)	1 (0%)	36	66
1	E	324/324 (100%)	302 (93%)	19 (6%)	3 (1%)	14	41
1	F	322/324 (99%)	302 (94%)	17 (5%)	3 (1%)	14	41
1	G	324/324 (100%)	304 (94%)	16 (5%)	4 (1%)	10	34
1	H	322/324 (99%)	296 (92%)	24 (8%)	2 (1%)	21	51
All	All	2584/2592 (100%)	2408 (93%)	150 (6%)	26 (1%)	12	38

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	SER
1	A	236	LEU

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Mol	Chain	Res	Type
1	B	236	LEU
1	C	236	LEU
1	E	236	LEU
1	G	236	LEU
1	A	182	GLY
1	B	63	GLY
1	D	234	VAL
1	E	88	THR
1	F	157	ASP
1	C	183	SER
1	G	181	LYS
1	H	108	LEU
1	A	306	LEU
1	B	317	LYS
1	F	109	PRO
1	G	266	SER
1	B	182	GLY
1	H	183	SER
1	A	108	LEU
1	F	182	GLY
1	C	251	VAL
1	B	234	VAL
1	E	108	LEU
1	G	108	LEU

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	278/276 (101%)	262 (94%)	16 (6%)	18	49
1	B	276/276 (100%)	261 (95%)	15 (5%)	20	51
1	C	278/276 (101%)	270 (97%)	8 (3%)	37	73
1	D	276/276 (100%)	257 (93%)	19 (7%)	14	41
1	E	278/276 (101%)	268 (96%)	10 (4%)	31	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	276/276 (100%)	257 (93%)	19 (7%)	14	41
1	G	278/276 (101%)	264 (95%)	14 (5%)	22	54
1	H	276/276 (100%)	246 (89%)	30 (11%)	6	21
All	All	2216/2208 (100%)	2085 (94%)	131 (6%)	18	48

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	15	HIS
1	A	68	ARG
1	A	88	THR
1	A	186	ILE
1	A	219	ARG
1	A	232	THR
1	A	236	LEU
1	A	251	VAL
1	A	266	SER
1	A	276	ARG
1	A	282	SER
1	A	293	PRO
1	A	313	GLU
1	A	319	ILE
1	A	323	GLU
1	B	16	ASN
1	B	34	SER
1	B	75	SER
1	B	86	GLU
1	B	113	LYS
1	B	139	SER
1	B	156	ASP
1	B	177	PRO
1	B	183	SER
1	B	209	THR
1	B	213	ARG
1	B	238	LEU
1	B	252	SER
1	B	256	LEU
1	B	266	SER
1	C	7	ARG
1	C	21	SER

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Mol	Chain	Res	Type
1	C	24	GLU
1	C	34	SER
1	C	238	LEU
1	C	252	SER
1	C	255	ASP
1	C	323	GLU
1	D	20	SER
1	D	33	ILE
1	D	86	GLU
1	D	97	VAL
1	D	105	ARG
1	D	139	SER
1	D	142	ASN
1	D	171	VAL
1	D	177	PRO
1	D	181	LYS
1	D	183	SER
1	D	188	GLU
1	D	204	ARG
1	D	209	THR
1	D	220	ILE
1	D	228	ASP
1	D	236	LEU
1	D	256	LEU
1	D	289	GLN
1	E	3	LEU
1	E	21	SER
1	E	169	SER
1	E	175	GLU
1	E	232	THR
1	E	236	LEU
1	E	238	LEU
1	E	255	ASP
1	E	282	SER
1	E	297	ARG
1	F	4	GLN
1	F	34	SER
1	F	54	LYS
1	F	58	GLN
1	F	116	ILE
1	F	132	THR
1	F	139	SER

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Mol	Chain	Res	Type
1	F	140	LYS
1	F	181	LYS
1	F	213	ARG
1	F	232	THR
1	F	236	LEU
1	F	240	VAL
1	F	248	VAL
1	F	255	ASP
1	F	256	LEU
1	F	260	ASP
1	F	262	ASN
1	F	302	THR
1	G	30	GLN
1	G	54	LYS
1	G	76	LYS
1	G	139	SER
1	G	142	ASN
1	G	171	VAL
1	G	175	GLU
1	G	198	THR
1	G	206	GLU
1	G	226	ASP
1	G	266	SER
1	G	282	SER
1	G	319	ILE
1	G	323	GLU
1	H	12	VAL
1	H	20	SER
1	H	67	ILE
1	H	86	GLU
1	H	101	HIS
1	H	140	LYS
1	H	171	VAL
1	H	183	SER
1	H	184	VAL
1	H	198	THR
1	H	209	THR
1	H	217	THR
1	H	218	PRO
1	H	232	THR
1	H	236	LEU
1	H	238	LEU

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Mol	Chain	Res	Type
1	H	248	VAL
1	H	249	ASP
1	H	254	PRO
1	H	255	ASP
1	H	256	LEU
1	H	259	LEU
1	H	262	ASN
1	H	266	SER
1	H	267	HIS
1	H	301	ASP
1	H	304	VAL
1	H	311	ASP
1	H	313	GLU
1	H	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	153	HIS
1	A	167	ASN
1	B	15	HIS
1	B	18	ASN
1	B	36	GLN
1	B	47	GLN
1	B	58	GLN
1	B	125	HIS
1	B	128	GLN
1	B	153	HIS
1	B	212	ASN
1	B	294	HIS
1	C	16	ASN
1	C	36	GLN
1	C	101	HIS
1	C	167	ASN
1	D	212	ASN
1	D	289	GLN
1	D	294	HIS
1	E	16	ASN
1	E	30	GLN
1	E	101	HIS
1	E	103	GLN

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Mol	Chain	Res	Type
1	E	153	HIS
1	E	167	ASN
1	F	18	ASN
1	F	36	GLN
1	F	125	HIS
1	F	212	ASN
1	F	262	ASN
1	F	294	HIS
1	G	30	GLN
1	G	36	GLN
1	G	58	GLN
1	G	153	HIS
1	H	15	HIS
1	H	125	HIS
1	H	212	ASN
1	H	262	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	SAC	C	401	-	9,9,9	1.04	1 (11%)	11,11,11	0.49	0
2	SAC	B	401	-	9,9,9	0.87	0	11,11,11	0.66	0
2	SAC	A	401	-	9,9,9	0.66	0	11,11,11	0.71	0
2	SAC	E	401	-	9,9,9	0.69	0	11,11,11	0.97	1 (9%)
2	SAC	D	401	-	9,9,9	0.80	1 (11%)	11,11,11	0.67	0
2	SAC	G	401	-	9,9,9	0.87	0	11,11,11	0.60	0
2	SAC	F	401	-	9,9,9	0.92	1 (11%)	11,11,11	0.67	0
2	SAC	H	401	-	9,9,9	0.72	0	11,11,11	0.72	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
2	SAC	C	401	-	-	2/10/10/10	-
2	SAC	B	401	-	-	1/10/10/10	-
2	SAC	A	401	-	-	0/10/10/10	-
2	SAC	E	401	-	-	1/10/10/10	-
2	SAC	D	401	-	-	0/10/10/10	-
2	SAC	G	401	-	-	0/10/10/10	-
2	SAC	F	401	-	-	1/10/10/10	-
2	SAC	H	401	-	-	0/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	SAC	OXT-C	-2.24	1.23	1.30
2	F	401	SAC	O-C	2.14	1.28	1.22
2	C	401	SAC	OXT-C	-2.14	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	SAC	O-C-CA	-2.21	115.13	122.26

There are no chirality outliers.

All (5) torsion outliers are listed below:

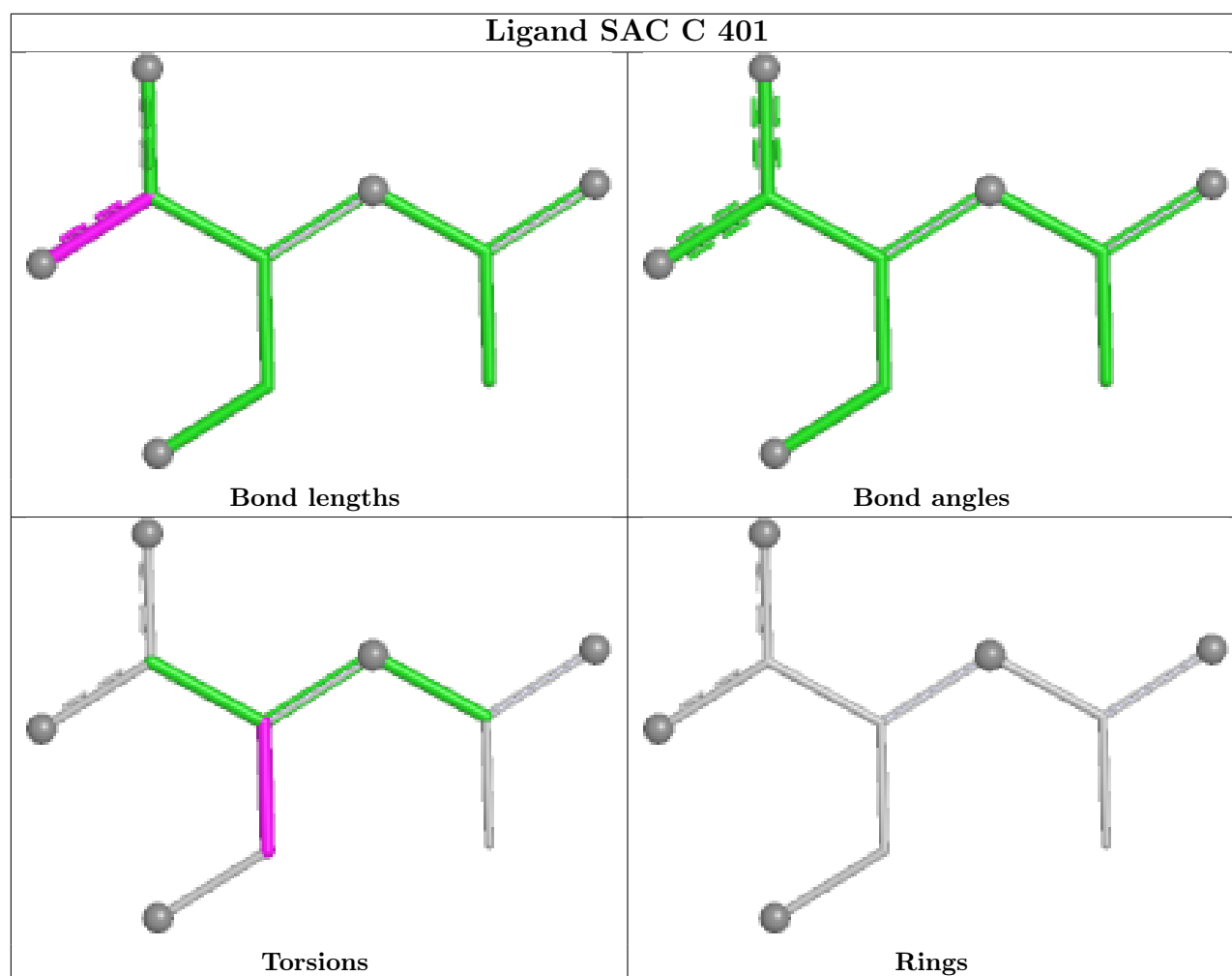
Mol	Chain	Res	Type	Atoms
2	C	401	SAC	C-CA-CB-OG
2	F	401	SAC	N-CA-CB-OG
2	E	401	SAC	C-CA-CB-OG
2	C	401	SAC	N-CA-CB-OG
2	B	401	SAC	C-CA-CB-OG

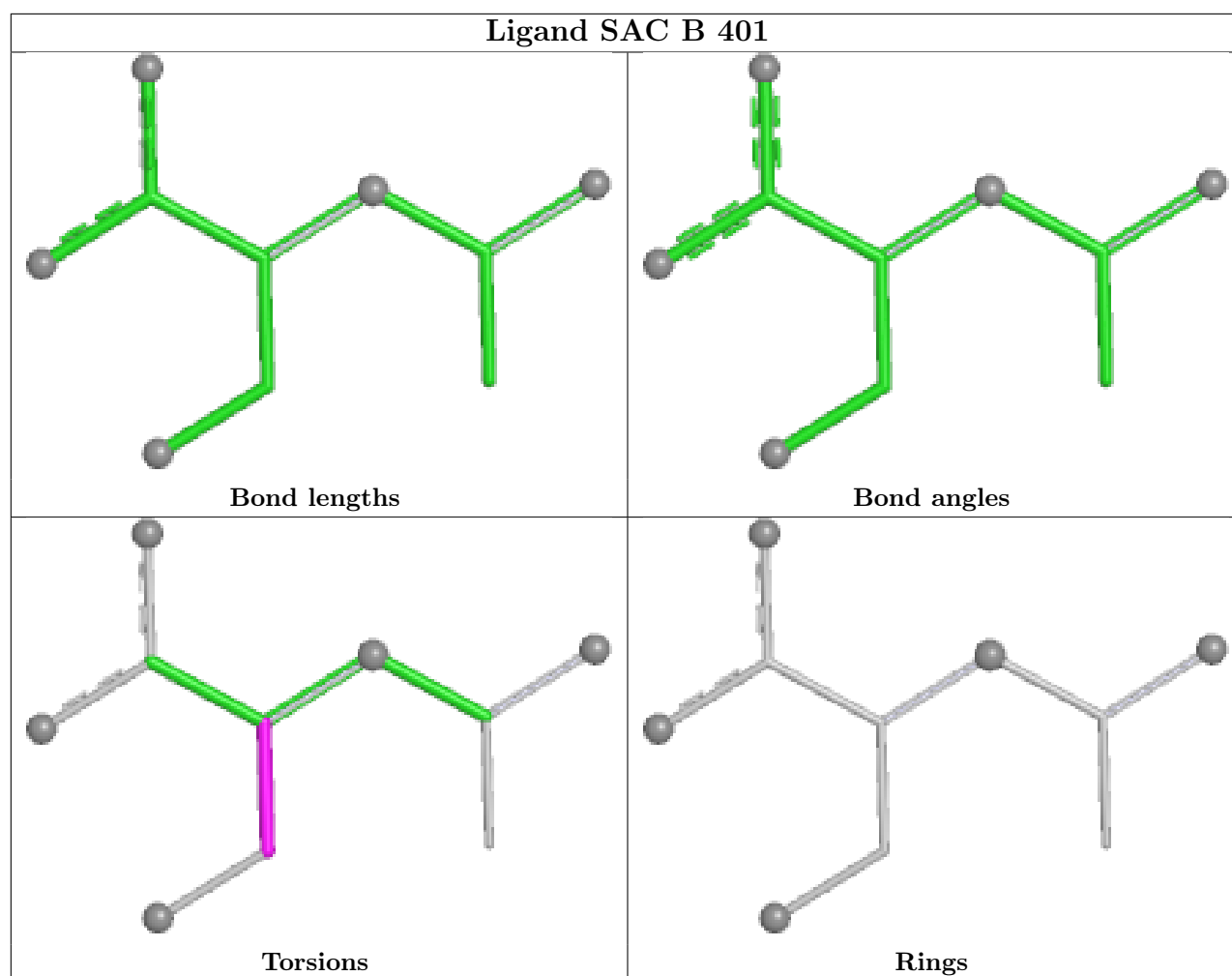
There are no ring outliers.

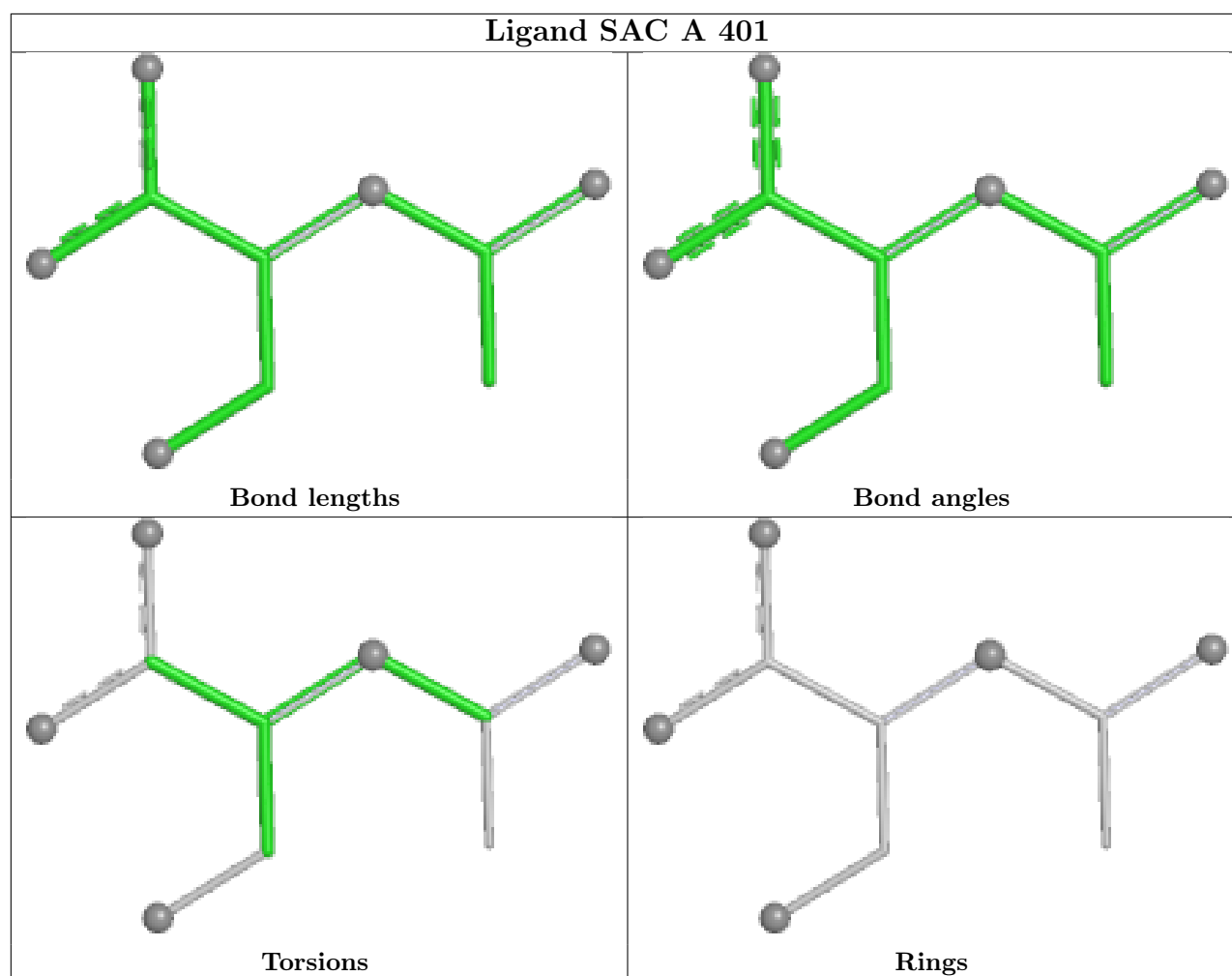
2 monomers are involved in 5 short contacts:

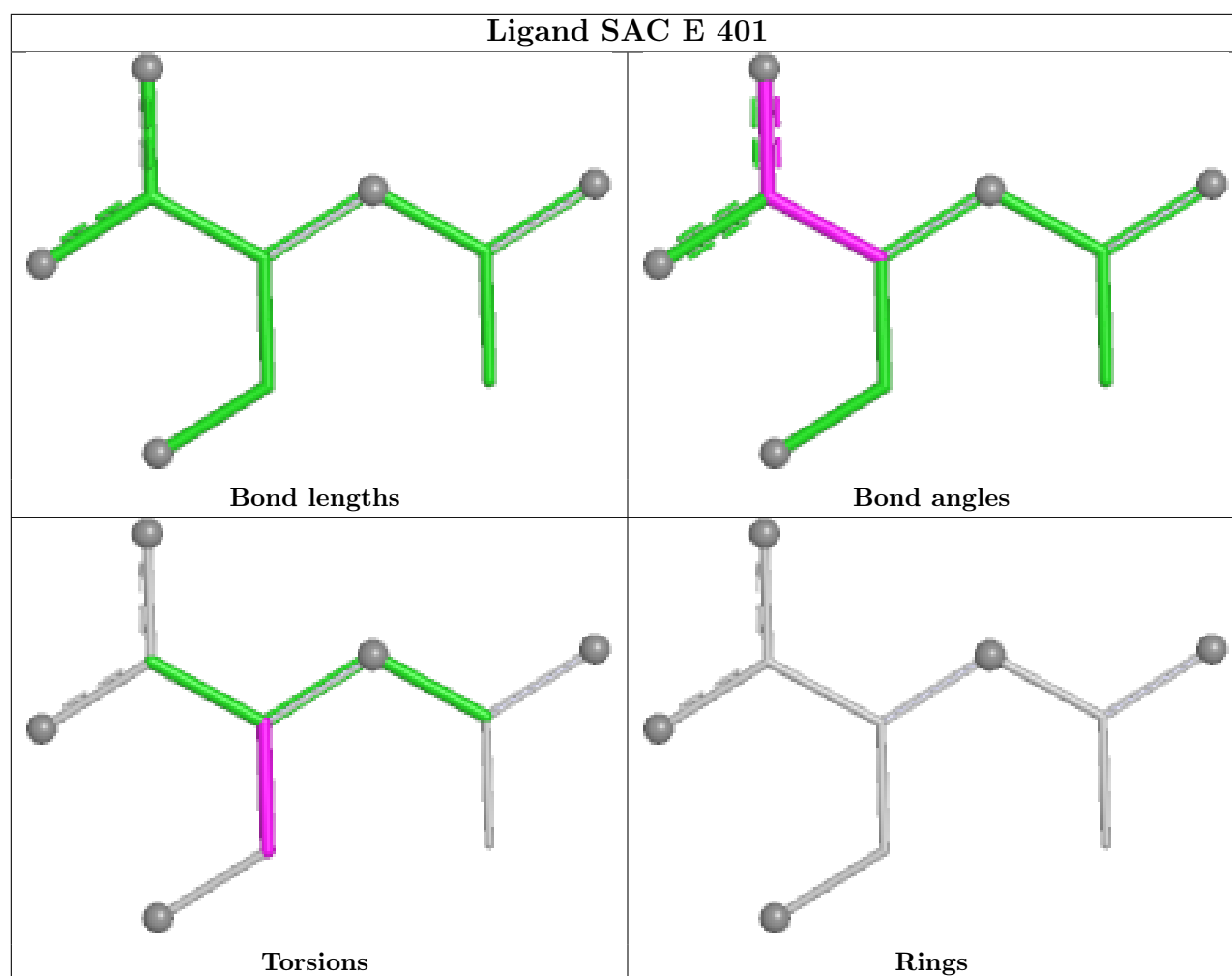
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	SAC	2	0
2	F	401	SAC	3	0

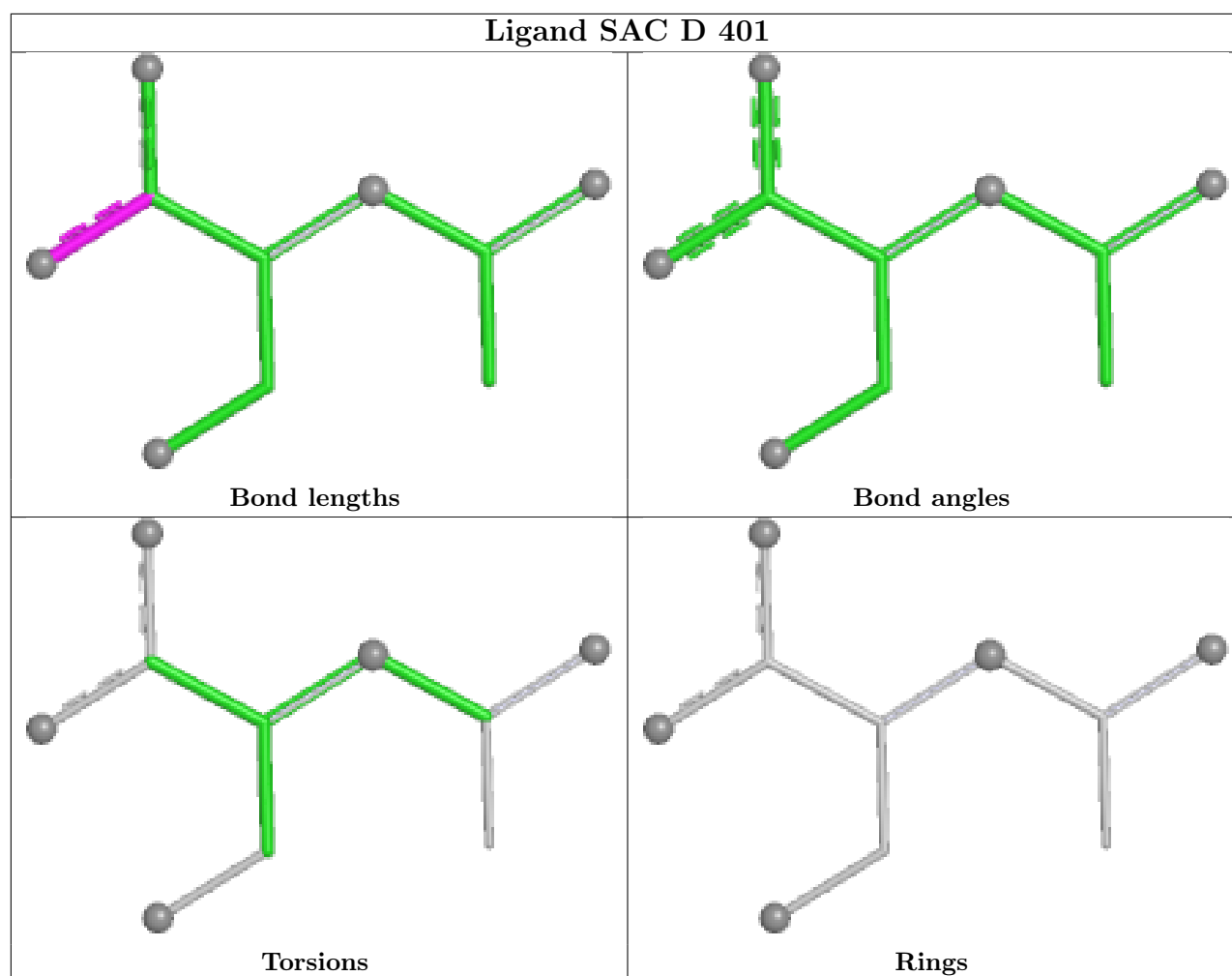
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

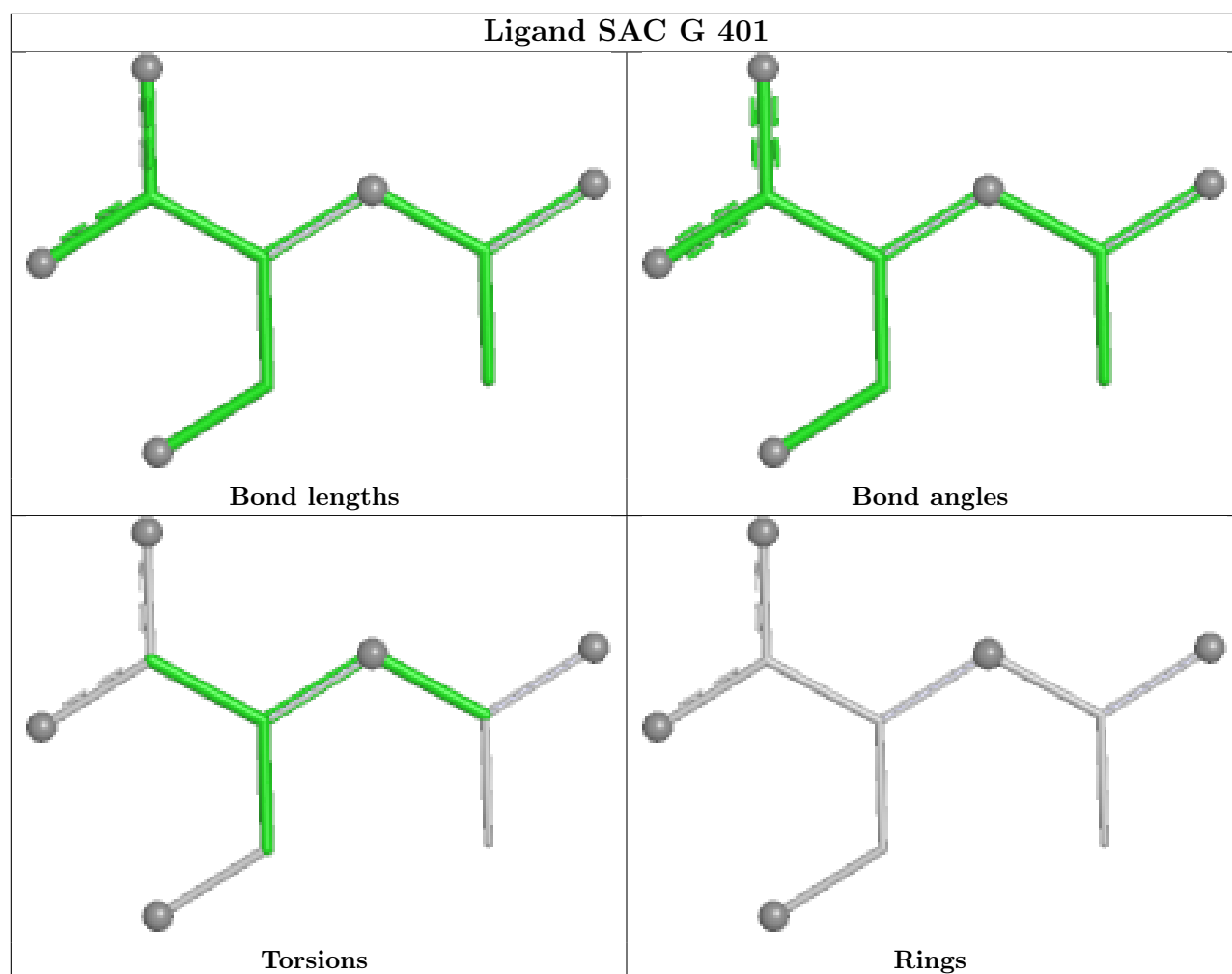


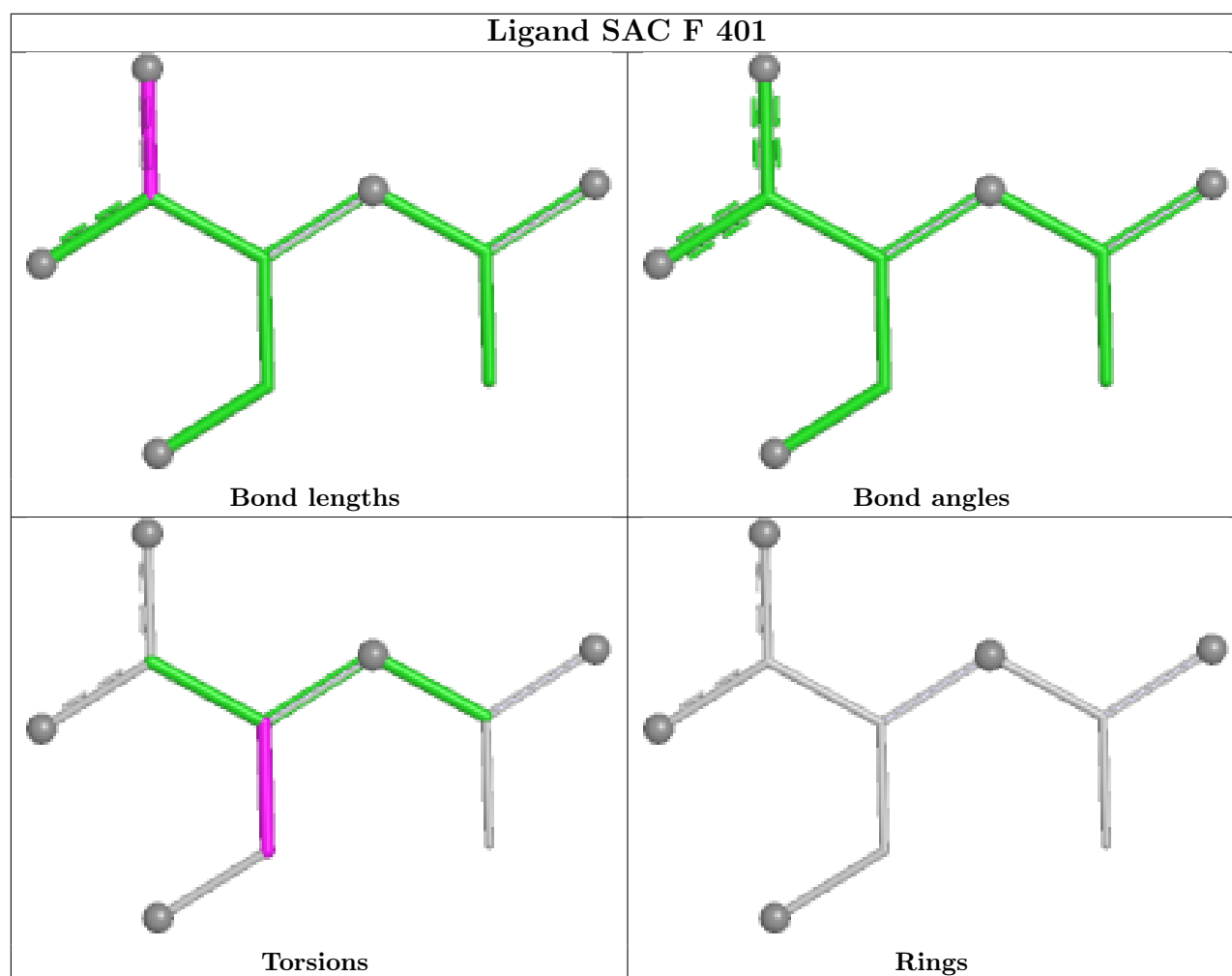


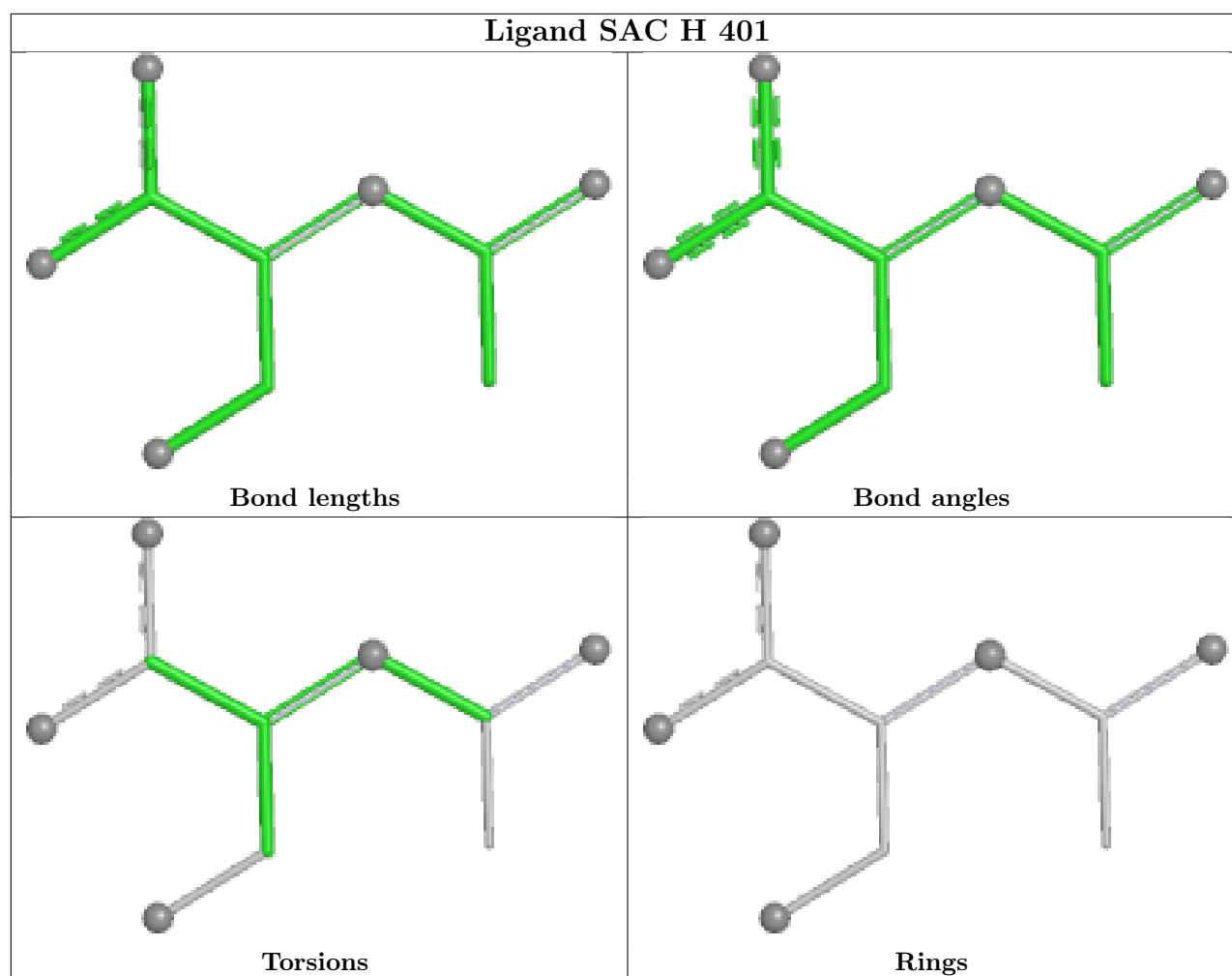












5.7 Other polymers [i](#)

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	324/324 (100%)	-1.57	0 100 100	18, 39, 76, 107	1 (0%)
1	B	324/324 (100%)	-1.51	0 100 100	25, 46, 83, 109	0
1	C	324/324 (100%)	-1.60	0 100 100	16, 36, 73, 100	1 (0%)
1	D	324/324 (100%)	-1.49	0 100 100	22, 50, 81, 115	0
1	E	324/324 (100%)	-1.58	0 100 100	20, 41, 75, 99	1 (0%)
1	F	324/324 (100%)	-1.57	0 100 100	20, 43, 74, 112	0
1	G	324/324 (100%)	-1.62	0 100 100	16, 35, 73, 97	1 (0%)
1	H	324/324 (100%)	-1.54	0 100 100	23, 45, 78, 106	0
All	All	2592/2592 (100%)	-1.56	0 100 100	16, 42, 77, 115	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

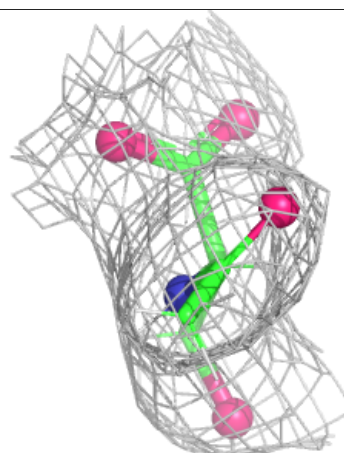
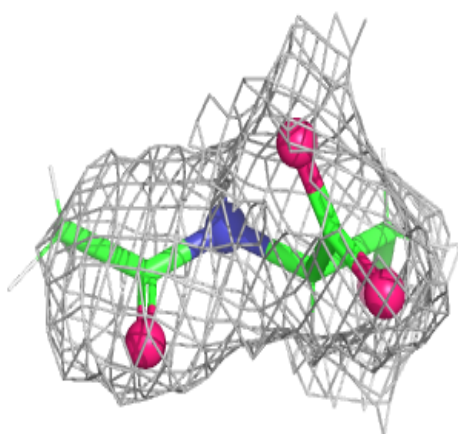
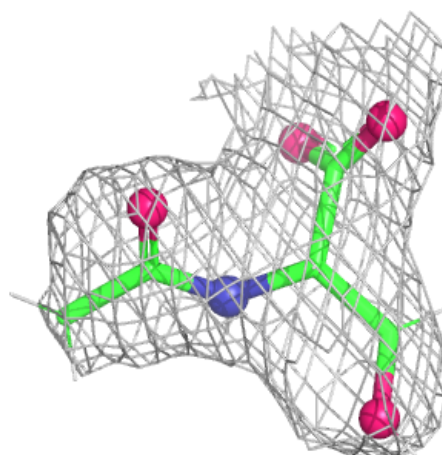
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAC	A	401	10/10	0.99	0.04	25,28,30,31	4
2	SAC	B	401	10/10	0.99	0.03	33,39,43,48	4
2	SAC	D	401	10/10	0.99	0.04	31,33,36,38	4
2	SAC	E	401	10/10	0.99	0.03	23,29,30,30	4
2	SAC	F	401	10/10	0.99	0.03	25,30,35,35	4
2	SAC	H	401	10/10	0.99	0.04	33,38,48,48	4
2	SAC	G	401	10/10	1.00	0.03	23,28,31,31	4
2	SAC	C	401	10/10	1.00	0.03	22,24,26,26	4

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.

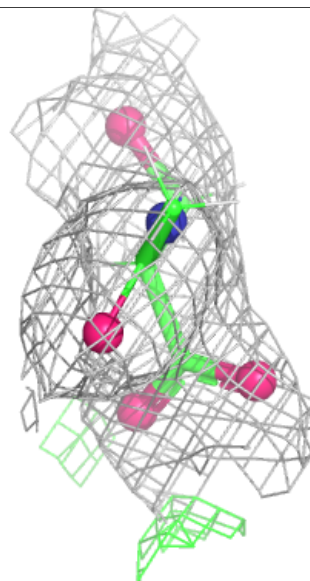
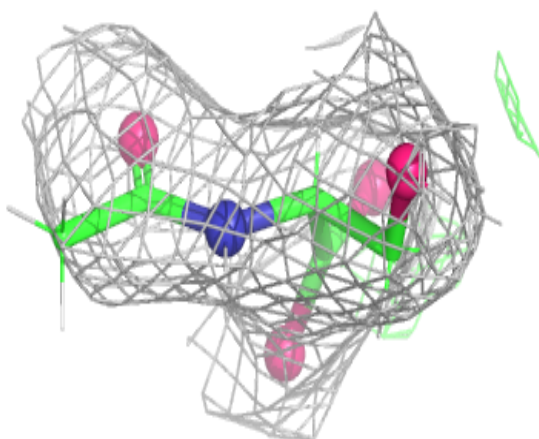
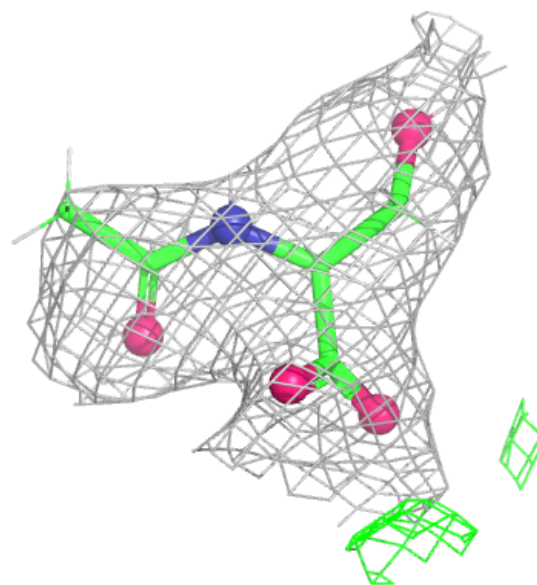
Electron density around SAC A 401:

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



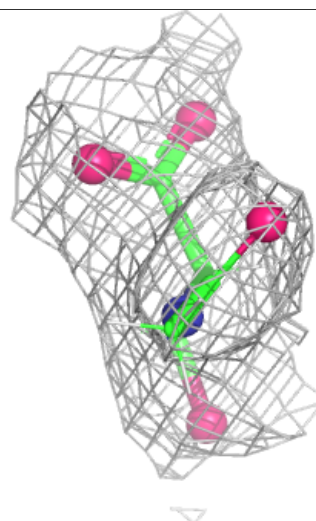
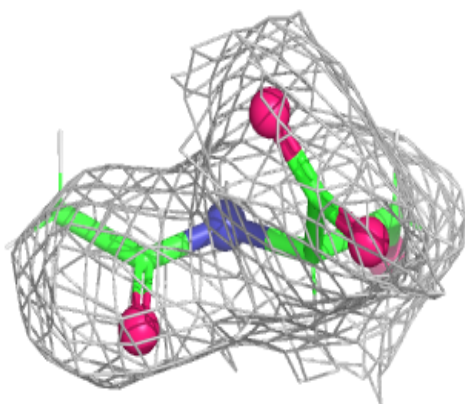
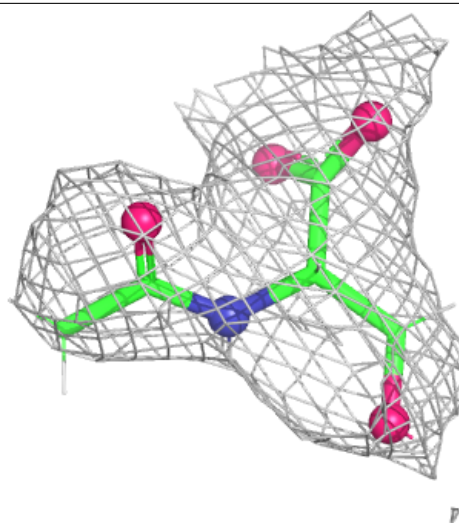
Electron density around SAC B 401:

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



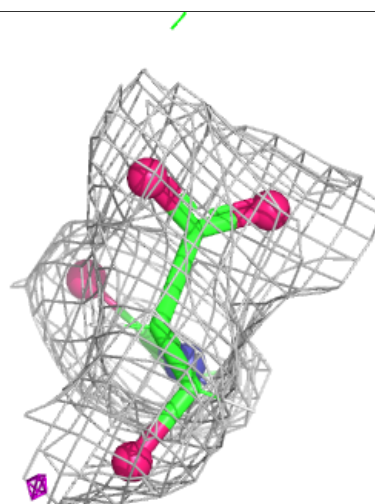
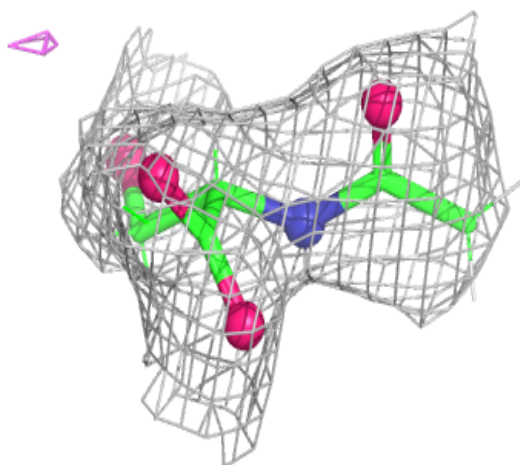
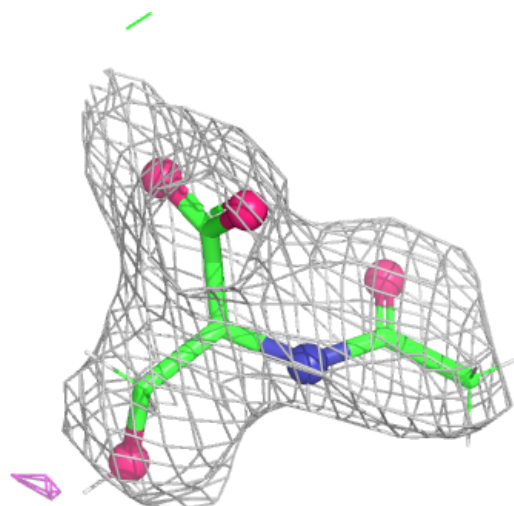
Electron density around SAC D 401:

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



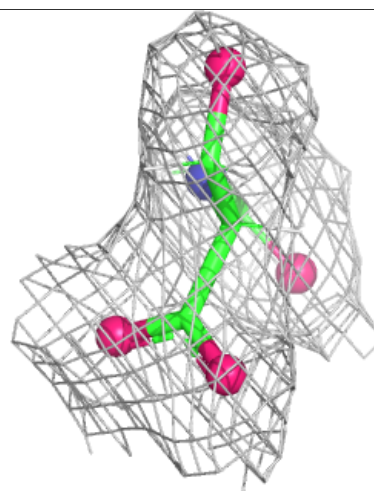
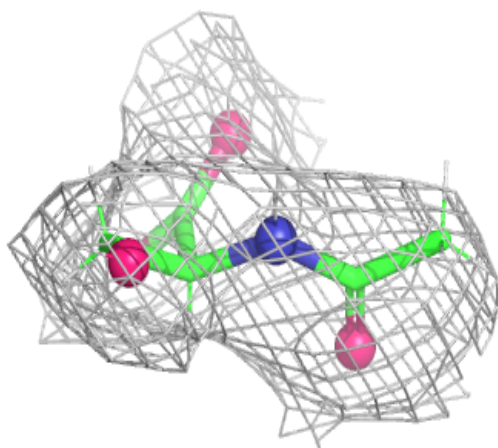
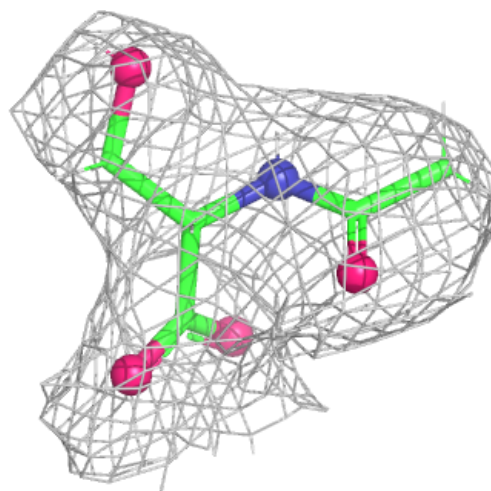
Electron density around SAC E 401:

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



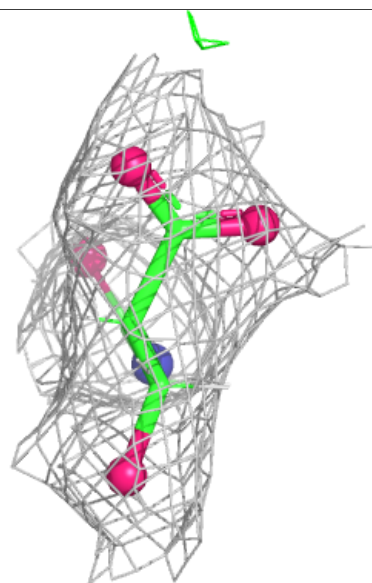
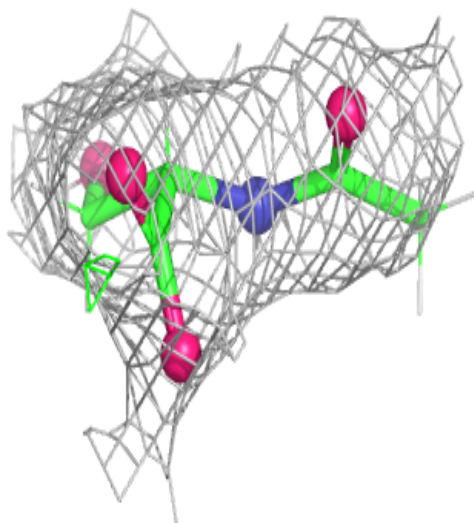
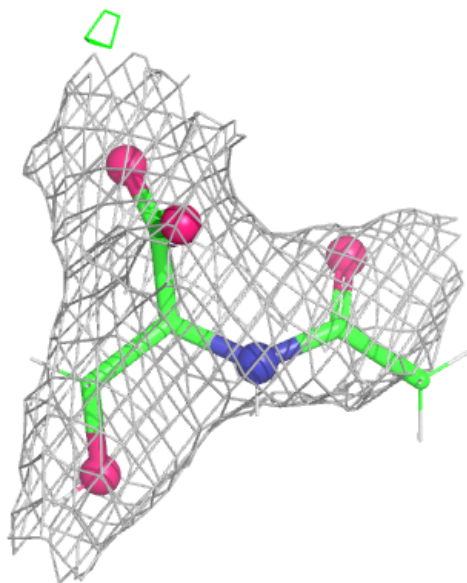
Electron density around SAC F 401:

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



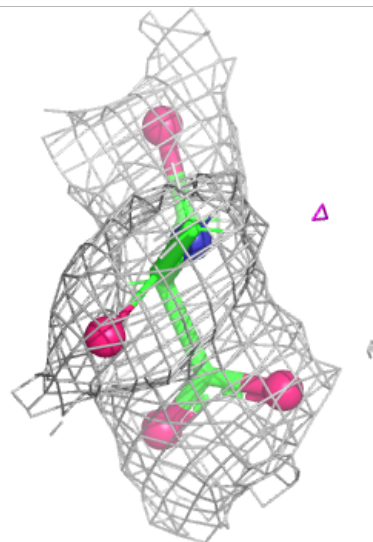
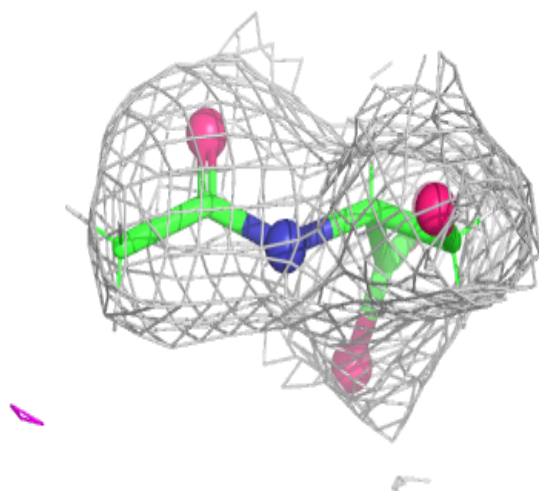
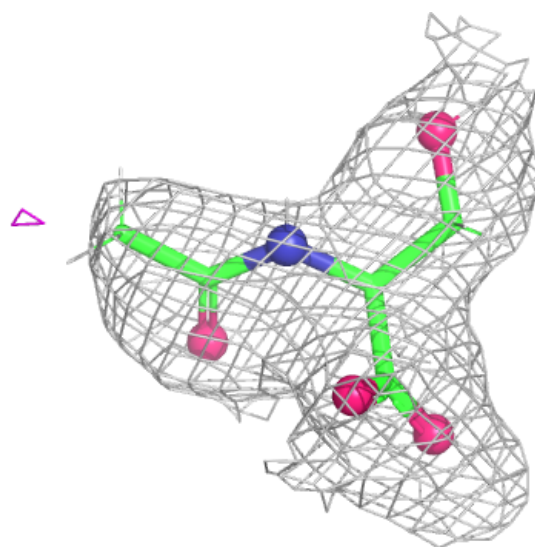
Electron density around SAC H 401:

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



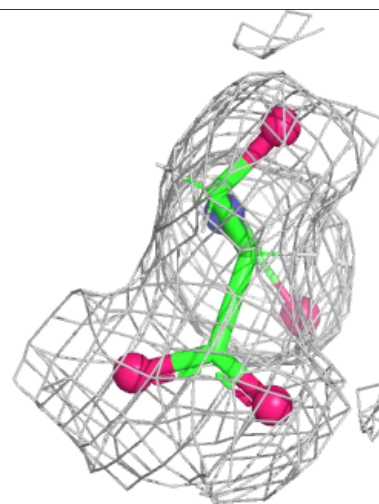
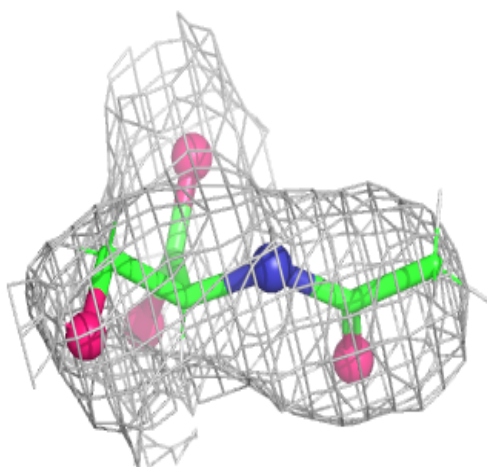
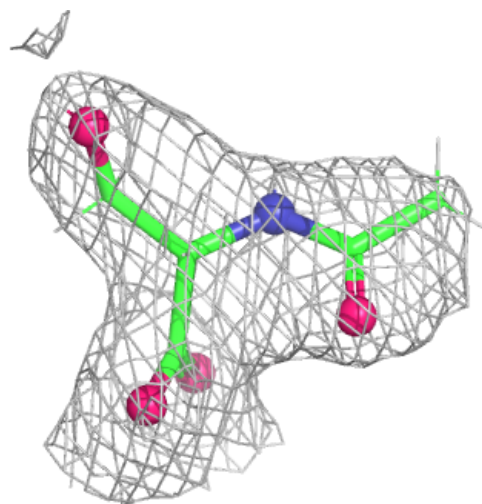
Electron density around SAC G 401:

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



Electron density around SAC C 401:

$2mF_o-DF_c$ (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.