



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:21 PM UTC

PDB ID : 4Q0L / pdb_00004q0l
Title : Crystal structure of catalytic domain of human carbonic anhydrase isozyme XII with inhibitor
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2014-04-02
Resolution : 2.00 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

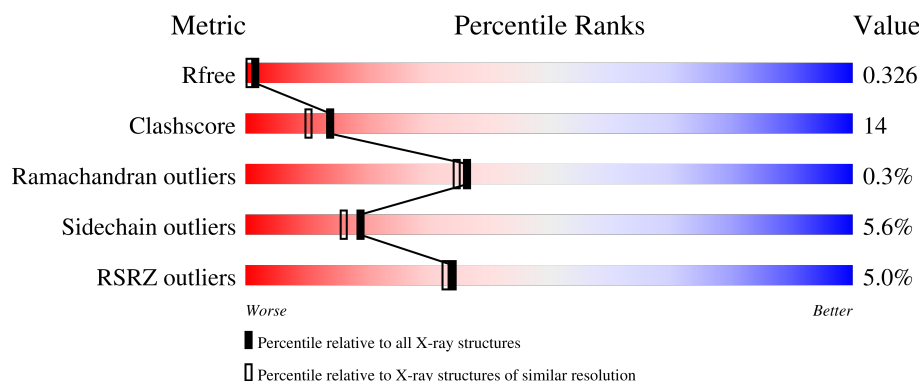
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

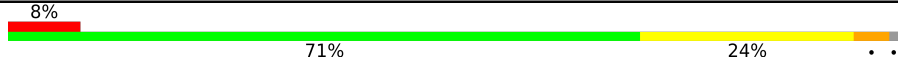
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	263	
1	B	263	
1	C	263	
1	D	263	

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
3	V14	D	302[B]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8894 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2098	1333	357	401	7			
1	B	260	Total	C	N	O	S	0	4	0
			2117	1346	360	404	7			
1	C	261	Total	C	N	O	S	0	2	0
			2115	1343	359	405	8			
1	D	260	Total	C	N	O	S	0	2	0
			2100	1334	357	402	7			

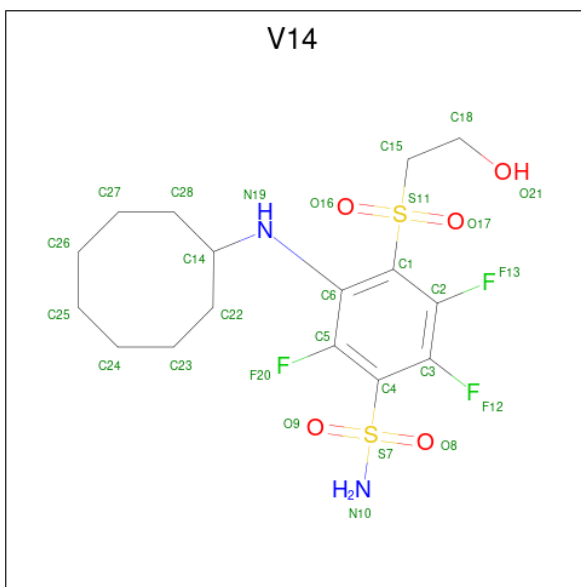
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP O43570
B	1	MET	-	expression tag	UNP O43570
C	1	MET	-	expression tag	UNP O43570
D	1	MET	-	expression tag	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 3-(cyclooctylamino)-2,5,6-trifluoro-4-[(2-hydroxyethyl)sulfonyl]benzenesulfonamide (CCD ID: V14) (formula: C₁₆H₂₃F₃N₂O₅S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 28	C 16	F 3	N 2	O 5	S 2	0	0
3	B	1	Total 28	C 16	F 3	N 2	O 5	S 2	0	0
3	C	1	Total 28	C 16	F 3	N 2	O 5	S 2	0	0
3	D	1	Total 56	C 32	F 6	N 4	O 10	S 4	0	1

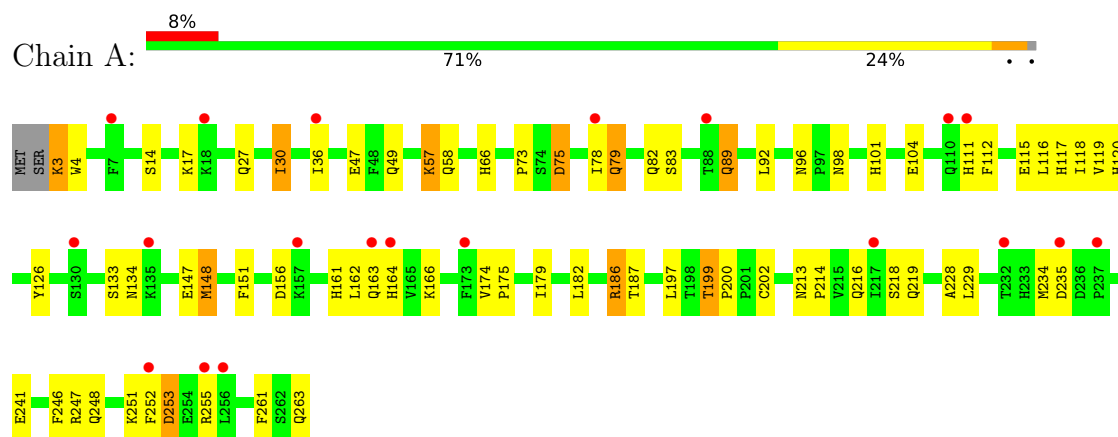
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	77	Total	O	0	0
			77	77		
4	C	89	Total	O	0	0
			89	89		
4	D	86	Total	O	0	0
			86	86		

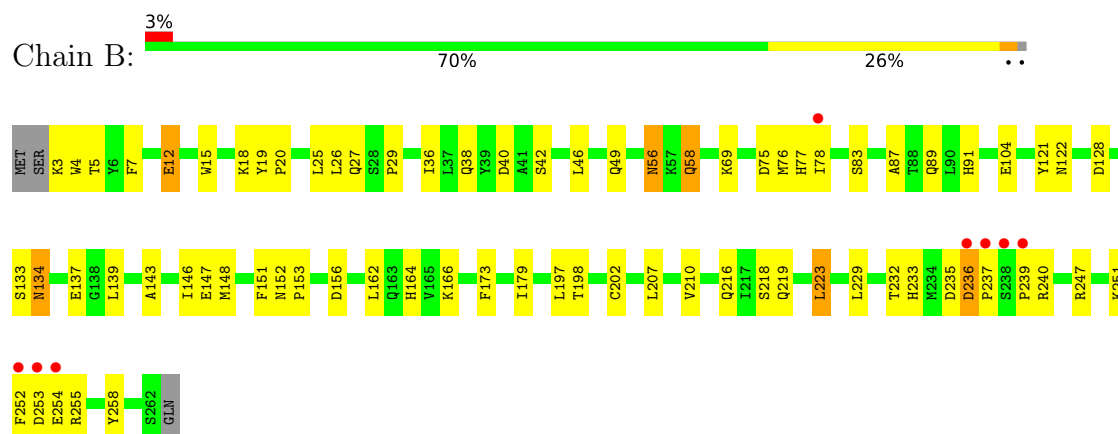
3 Residue-property plots [i](#)

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

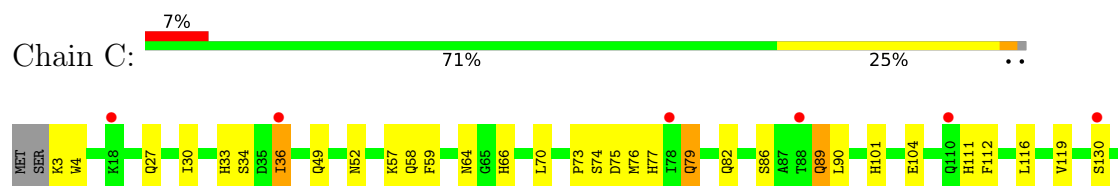
• Molecule 1: Carbonic anhydrase 12

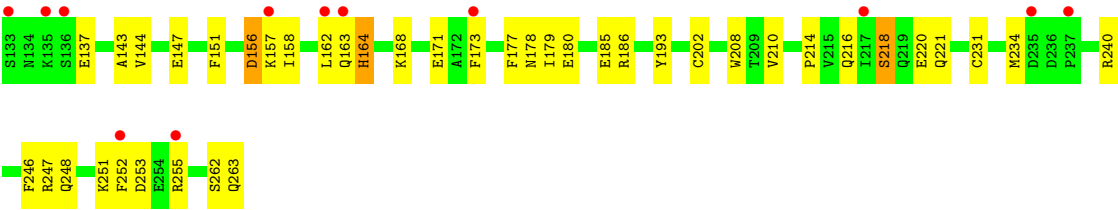


• Molecule 1: Carbonic anhydrase 12

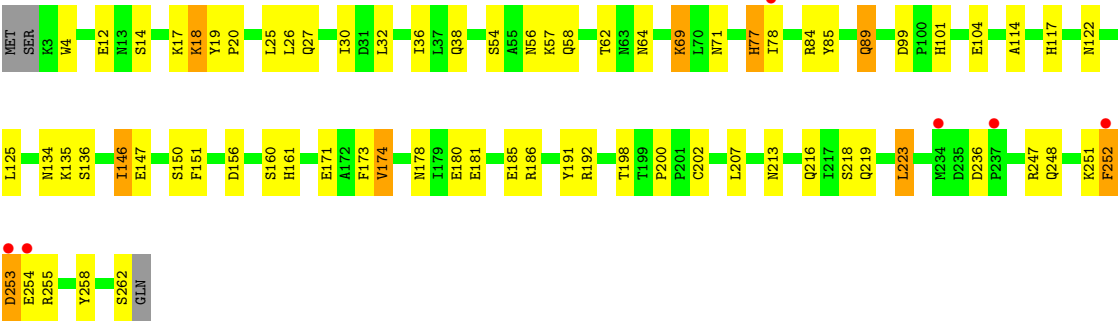


• Molecule 1: Carbonic anhydrase 12





● Molecule 1: Carbonic anhydrase 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.52Å 75.21Å 77.89Å 109.42° 101.60° 107.95°	Depositor
Resolution (Å)	22.09 – 2.00 22.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	74.5 (22.09-2.00) 74.5 (22.09-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.264 , 0.328 0.263 , 0.326	Depositor DCC
R_{free} test set	4525 reflections (7.52%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8894	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 71.21 % 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 2.7325e-06. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: V14, ZN

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	1.07	1/2161 (0.0%)	1.12	6/2942 (0.2%)
1	B	1.08	0/2180	1.11	4/2968 (0.1%)
1	C	1.06	1/2178 (0.0%)	1.14	5/2964 (0.2%)
1	D	1.08	0/2163	1.14	8/2946 (0.3%)
All	All	1.07	2/8682 (0.0%)	1.13	23/11820 (0.2%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	ILE	C-O	6.02	1.30	1.23
1	C	208	TRP	CA-C	-5.23	1.46	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	GLU	N-CA-C	-7.69	105.86	114.62
1	C	164	HIS	N-CA-C	7.41	122.16	113.20
1	B	12	GLU	N-CA-C	7.06	119.83	111.71
1	B	166	LYS	N-CA-C	6.47	119.16	111.33
1	C	34	SER	N-CA-C	6.27	118.91	111.33
1	A	213	ASN	CA-C-N	-6.21	114.14	120.85
1	A	213	ASN	C-N-CA	-6.21	114.14	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ILE	N-CA-C	6.15	116.72	107.80
1	D	12	GLU	N-CA-C	5.96	119.38	111.75
1	A	199	THR	CA-C-N	-5.86	114.35	120.38
1	A	199	THR	C-N-CA	-5.86	114.35	120.38
1	D	146	ILE	N-CA-C	5.62	115.96	107.80
1	D	174	VAL	CA-C-N	-5.40	114.21	119.78
1	D	174	VAL	C-N-CA	-5.40	114.21	119.78
1	D	77	HIS	N-CA-C	5.35	116.98	108.79
1	C	119	VAL	N-CA-C	5.35	116.42	108.23
1	A	126	TYR	CA-C-N	5.33	124.84	119.19
1	A	126	TYR	C-N-CA	5.33	124.84	119.19
1	C	234	MET	N-CA-C	5.33	117.09	111.28
1	D	78	ILE	CB-CA-C	-5.33	104.31	110.91
1	D	85	TYR	N-CA-C	5.26	122.00	110.80
1	D	252	PHE	N-CA-C	-5.21	96.68	107.67
1	C	218	SER	N-CA-C	5.01	117.31	110.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	253	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2098	0	1987	51	0
1	B	2117	0	2008	60	0
1	C	2115	0	2000	61	0
1	D	2100	0	1987	67	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	22	6	0
3	B	28	0	23	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	22	7	0
3	D	56	0	45	10	0
4	A	68	0	0	2	0
4	B	77	0	0	3	0
4	C	89	0	0	2	0
4	D	86	0	0	4	0
All	All	8894	0	8094	240	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 14.

All (240) 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:C:263:GLN:HA	4:C:461:HOH:O	1.61	1.01
1:A:148:MET:SD	1:A:219:GLN:OE1	2.25	0.94
1:D:252:PHE:CE1	1:D:255:ARG:HB3	2.03	0.94
1:B:252:PHE:O	1:B:252:PHE:CD2	2.22	0.92
1:C:58:GLN:HB3	1:C:173:PHE:CD2	2.05	0.92
1:A:186:ARG:HH21	1:A:186:ARG:HG3	1.33	0.91
1:C:248:GLN:HE21	1:D:251:LYS:NZ	1.70	0.89
1:C:248:GLN:HE21	1:D:251:LYS:HZ3	1.22	0.83
1:D:99:ASP:OD1	1:D:101:HIS:HD2	1.61	0.82
1:C:89:GLN:HE21	3:C:302:V14:H6	1.45	0.82
1:C:58:GLN:HB3	1:C:173:PHE:HD2	1.45	0.81
1:D:64:ASN:ND2	3:D:302[B]:V14:H4	1.95	0.80
1:C:220[B]:GLU:N	1:C:220[B]:GLU:OE1	2.15	0.78
1:B:252:PHE:CE1	1:B:255:ARG:HB3	2.19	0.77
1:D:27:GLN:HE22	1:D:202:CYS:HB3	1.49	0.77
1:B:27:GLN:HE21	1:B:247:ARG:HH22	1.32	0.76
1:B:252:PHE:CE1	1:B:255:ARG:CB	2.69	0.75
1:D:64:ASN:HD21	3:D:302[B]:V14:H4	1.52	0.74
1:C:156:ASP:OD2	1:C:221:GLN:NE2	2.21	0.74
1:C:164:HIS:HB3	4:C:480:HOH:O	1.87	0.74
1:D:54:SER:HB3	1:D:57:LYS:HG2	1.70	0.73
1:A:186:ARG:HH21	1:A:186:ARG:CG	2.02	0.72
1:D:36:ILE:HD13	1:D:252:PHE:CE2	2.24	0.72
1:D:27:GLN:HE21	1:D:247:ARG:HH22	1.36	0.72
1:C:27:GLN:NE2	1:C:247:ARG:HH12	1.86	0.71
1:D:252:PHE:CE1	1:D:255:ARG:CB	2.73	0.71
3:A:302:V14:H18	3:A:302:V14:H5	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLN:HE22	1:B:202:CYS:HB3	1.55	0.70
1:C:89:GLN:HE21	3:C:302:V14:C18	2.04	0.70
1:B:151:PHE:HB2	1:D:18:LYS:HE3	1.74	0.68
1:D:219:GLN:NE2	4:D:464:HOH:O	2.27	0.68
1:C:89:GLN:NE2	3:C:302:V14:H6	2.09	0.68
1:A:186:ARG:HG3	1:A:186:ARG:NH2	2.09	0.67
1:B:58:GLN:HB2	1:B:173:PHE:CD2	2.29	0.67
1:B:40:ASP:OD1	1:B:42:SER:HB3	1.95	0.67
1:D:36:ILE:HB	1:D:252:PHE:HE2	1.59	0.66
1:C:76:MET:HE1	1:C:179:ILE:HG13	1.75	0.66
1:A:27:GLN:NE2	1:A:247:ARG:HH12	1.93	0.66
1:D:178:ASN:HB3	1:D:181:GLU:OE2	1.96	0.66
1:D:30:ILE:HG21	1:D:255:ARG:HH11	1.62	0.64
3:A:302:V14:H6	3:A:302:V14:H8	1.62	0.64
1:D:223:LEU:CD2	4:D:462:HOH:O	2.45	0.64
1:A:27:GLN:HE22	1:A:202:CYS:HB3	1.63	0.63
1:D:26:LEU:HD22	1:D:255:ARG:HD2	1.80	0.63
1:B:252:PHE:CE1	1:B:255:ARG:HB2	2.33	0.63
1:B:252:PHE:O	1:B:252:PHE:HD2	1.81	0.63
1:B:207:LEU:HD23	4:B:430:HOH:O	1.99	0.62
1:B:164:HIS:CD2	4:B:433:HOH:O	2.52	0.62
1:D:252:PHE:HE1	1:D:255:ARG:HB3	1.58	0.62
1:A:147:GLU:OE2	1:A:216:GLN:NE2	2.33	0.62
1:A:166:LYS:HE3	1:A:228:ALA:O	2.00	0.61
1:C:27:GLN:HE21	1:C:247:ARG:HH12	1.47	0.61
1:C:253:ASP:O	1:C:255:ARG:HG3	2.01	0.60
1:B:49:GLN:OE1	1:B:77:HIS:NE2	2.33	0.60
1:A:248:GLN:HE21	1:B:251:LYS:NZ	1.99	0.60
3:A:302:V14:H8	3:A:302:V14:C18	2.15	0.60
3:C:302:V14:F20	3:C:302:V14:H9	1.91	0.60
1:D:69:LYS:NZ	1:D:71:ASN:OD1	2.32	0.59
1:B:26:LEU:HD22	1:B:255:ARG:HD3	1.83	0.59
1:C:30:ILE:HG21	1:C:252:PHE:CD1	2.37	0.59
1:A:118:ILE:HG22	1:A:120:HIS:CE1	2.38	0.59
1:A:166:LYS:HA	1:A:229:LEU:HD22	1.85	0.59
1:B:58:GLN:HB2	1:B:173:PHE:HD2	1.68	0.58
1:D:69:LYS:HD3	3:D:302[B]:V14:C18	2.32	0.58
1:D:26:LEU:HA	1:D:255:ARG:NH2	2.19	0.58
1:A:248:GLN:HE21	1:B:251:LYS:HZ3	1.50	0.58
1:A:4:TRP:O	1:A:66:HIS:HE1	1.87	0.58
1:D:64:ASN:HD21	3:D:302[B]:V14:C15	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:HB3	1:A:17:LYS:HD2	1.86	0.57
1:B:4:TRP:HZ2	3:B:302:V14:H5	1.68	0.57
1:C:157:LYS:HB2	1:C:177:PHE:CE2	2.39	0.57
1:B:133:SER:HB3	3:B:302:V14:H17	1.86	0.57
1:A:27:GLN:HE21	1:A:247:ARG:HH22	1.52	0.57
1:C:27:GLN:HE22	1:C:202:CYS:HB3	1.70	0.57
1:A:73:PRO:HB2	1:A:75:ASP:OD1	2.05	0.57
1:A:47:GLU:HG3	1:A:79:GLN:HB3	1.86	0.57
1:D:30:ILE:HG21	1:D:255:ARG:NH1	2.19	0.57
1:C:251:LYS:HZ2	1:D:248:GLN:HE21	1.53	0.56
1:D:186:ARG:CZ	1:D:213:ASN:HD21	2.19	0.56
1:A:151:PHE:HA	1:A:218:SER:HB3	1.88	0.56
3:C:302:V14:C18	3:C:302:V14:H8	2.19	0.56
1:A:253:ASP:N	1:A:253:ASP:OD1	2.39	0.56
1:C:73:PRO:HB2	1:C:75:ASP:OD1	2.05	0.56
1:D:151:PHE:HA	1:D:218:SER:HB3	1.88	0.55
1:D:99:ASP:OD1	1:D:101:HIS:CD2	2.51	0.55
1:D:64:ASN:ND2	3:D:302[B]:V14:C15	2.69	0.55
1:C:58:GLN:HB3	1:C:173:PHE:CE2	2.42	0.55
1:C:251:LYS:NZ	1:D:248:GLN:HE21	2.04	0.55
1:A:104:GLU:HG2	1:A:246:PHE:HB2	1.89	0.54
1:A:163:GLN:NE2	4:A:462:HOH:O	2.38	0.54
1:B:5:THR:OG1	1:B:7:PHE:O	2.24	0.54
1:B:83:SER:CB	1:B:122:ASN:HD21	2.20	0.54
1:A:251:LYS:HB3	1:A:253:ASP:OD1	2.08	0.54
1:B:252:PHE:HE1	1:B:255:ARG:HB3	1.72	0.54
1:A:101:HIS:HB3	1:A:111:HIS:HB3	1.90	0.54
1:B:252:PHE:CD1	1:B:255:ARG:HB2	2.44	0.53
1:D:36:ILE:CB	1:D:252:PHE:HE2	2.22	0.53
1:D:178:ASN:ND2	1:D:180:GLU:OE1	2.41	0.53
1:A:252:PHE:CZ	1:A:255:ARG:HB3	2.44	0.53
1:A:179:ILE:HG23	1:A:182:LEU:HD12	1.90	0.52
1:D:36:ILE:HB	1:D:252:PHE:CE2	2.44	0.52
1:C:27:GLN:HE21	1:C:247:ARG:HH22	1.57	0.52
1:A:92:LEU:HG	1:A:116:LEU:HD12	1.91	0.52
1:C:147:GLU:OE2	1:C:216:GLN:NE2	2.43	0.52
1:B:237:PRO:C	1:B:239:PRO:HD3	2.35	0.51
1:A:133:SER:OG	3:A:302:V14:H21	2.09	0.51
1:B:121:TYR:CE1	1:B:128:ASP:HA	2.45	0.51
1:B:133:SER:CB	3:B:302:V14:H17	2.41	0.51
1:C:248:GLN:NE2	1:D:251:LYS:HZ3	2.01	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ARG:HD2	1:D:207:LEU:HD11	1.91	0.51
1:C:30:ILE:HD13	1:C:252:PHE:CE1	2.46	0.51
1:C:151:PHE:CZ	1:C:156:ASP:OD1	2.64	0.51
1:C:74:SER:O	1:C:86:SER:HB3	2.11	0.50
1:B:162:LEU:HD22	1:B:229:LEU:HD21	1.94	0.50
1:A:96:ASN:OD1	1:A:98:ASN:HB2	2.11	0.50
1:C:253:ASP:C	1:C:255:ARG:HG3	2.36	0.50
1:C:185:GLU:OE1	1:C:186:ARG:NH2	2.41	0.50
1:D:26:LEU:HD22	1:D:255:ARG:CD	2.41	0.50
1:C:248:GLN:HE21	1:D:251:LYS:HZ2	1.57	0.49
1:B:46:LEU:HD22	1:B:78:ILE:CG2	2.43	0.49
1:C:168:LYS:HD2	1:C:231:CYS:O	2.12	0.49
1:D:69:LYS:HD3	3:D:302[B]:V14:H6	1.94	0.49
1:A:248:GLN:HA	4:A:429:HOH:O	2.12	0.49
1:A:89:GLN:HE21	3:A:302:V14:H6	1.76	0.49
1:D:252:PHE:HD1	1:D:255:ARG:NE	2.10	0.49
1:B:83:SER:HB2	1:B:122:ASN:HD21	1.78	0.49
1:A:261:PHE:HE1	1:A:263:GLN:HE21	1.60	0.48
1:B:76:MET:HB3	1:B:87:ALA:HB3	1.95	0.48
1:B:233:HIS:O	1:B:236:ASP:HB2	2.13	0.48
1:D:26:LEU:HA	1:D:255:ARG:HH21	1.76	0.48
1:B:27:GLN:HE21	1:B:247:ARG:NH2	2.06	0.48
1:B:29:PRO:HG3	1:B:104:GLU:HB3	1.96	0.48
1:C:4:TRP:O	1:C:66:HIS:HE1	1.96	0.48
1:C:151:PHE:HA	1:C:218:SER:HB3	1.96	0.48
1:A:115:GLU:OE1	1:A:117:HIS:NE2	2.42	0.48
1:A:252:PHE:CE1	1:A:255:ARG:HD2	2.48	0.48
1:C:64:ASN:O	1:C:168:LYS:HE3	2.14	0.48
1:D:223:LEU:HD22	4:D:462:HOH:O	2.11	0.48
3:B:302:V14:F20	3:B:302:V14:H9	2.04	0.48
1:D:122:ASN:OD1	1:D:125:LEU:HG	2.13	0.47
1:D:104:GLU:OE1	1:D:117:HIS:HE1	1.97	0.47
1:B:27:GLN:NE2	1:B:247:ARG:HH12	2.12	0.47
1:C:77:HIS:CD2	1:C:79:GLN:HE22	2.33	0.47
1:D:252:PHE:HD1	1:D:255:ARG:HE	1.63	0.47
1:A:82:GLN:OE1	1:A:83:SER:N	2.47	0.47
1:A:162:LEU:C	1:A:164:HIS:H	2.21	0.47
1:C:162:LEU:O	1:C:163:GLN:C	2.58	0.47
1:D:58:GLN:HB2	1:D:173:PHE:HB3	1.95	0.47
1:A:27:GLN:HE21	1:A:247:ARG:HH12	1.58	0.47
1:B:252:PHE:CZ	1:B:255:ARG:C	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:GLN:NE2	1:D:247:ARG:HH12	2.13	0.47
1:C:101:HIS:HB3	1:C:111:HIS:HB3	1.97	0.47
1:C:156:ASP:C	1:C:158:ILE:N	2.72	0.46
1:D:69:LYS:HZ2	1:D:89:GLN:HB3	1.79	0.46
1:B:252:PHE:O	1:B:252:PHE:CG	2.65	0.46
1:B:76:MET:HE1	1:B:179:ILE:HG21	1.98	0.46
1:C:137:GLU:OE2	1:C:137:GLU:HA	2.16	0.46
1:C:253:ASP:N	1:C:253:ASP:OD1	2.49	0.46
1:A:82:GLN:OE1	1:A:82:GLN:C	2.59	0.46
1:C:151:PHE:HZ	1:C:156:ASP:OD1	1.99	0.46
1:C:178:ASN:OD1	1:C:180:GLU:HB2	2.16	0.46
1:C:240:ARG:HE	1:C:240:ARG:HB2	1.51	0.46
1:D:69:LYS:HD3	3:D:302[B]:V14:O21	2.15	0.46
1:A:161:HIS:CD2	1:A:174:VAL:HG22	2.51	0.46
1:B:148:MET:SD	1:B:219:GLN:HB3	2.56	0.46
1:C:112:PHE:HE2	1:C:214:PRO:HG3	1.81	0.46
1:B:151:PHE:HA	1:B:218:SER:HB3	1.98	0.46
1:D:27:GLN:HE21	1:D:247:ARG:NH2	2.10	0.46
1:C:57:LYS:HD3	1:C:59:PHE:CZ	2.51	0.46
3:D:302[B]:V14:F20	3:D:302[B]:V14:H9	2.06	0.46
1:B:36:ILE:HB	1:B:252:PHE:HE2	1.80	0.45
1:D:26:LEU:CD2	1:D:255:ARG:HD3	2.46	0.45
1:D:64:ASN:OD1	1:D:64:ASN:C	2.59	0.45
1:D:32:LEU:HD13	1:D:191:TYR:CD1	2.51	0.45
1:C:143:ALA:HB3	1:C:210:VAL:HG22	1.98	0.45
1:C:52:ASN:OD1	1:C:178:ASN:HB2	2.17	0.45
3:D:302[A]:V14:H12	3:D:302[A]:V14:H23	1.71	0.45
1:A:4:TRP:O	1:A:66:HIS:CE1	2.70	0.45
1:B:83:SER:HB2	1:B:122:ASN:ND2	2.32	0.45
1:B:19:TYR:HA	1:B:20:PRO:HD2	1.85	0.44
1:D:14:SER:HB3	1:D:17:LYS:HE2	2.00	0.44
1:D:223:LEU:HD21	4:D:462:HOH:O	2.13	0.44
1:A:30:ILE:HG21	1:A:252:PHE:CD1	2.52	0.44
1:D:252:PHE:CD1	1:D:255:ARG:HB2	2.53	0.44
1:A:57:LYS:HG2	1:A:58:GLN:H	1.83	0.44
1:D:252:PHE:CZ	1:D:255:ARG:O	2.70	0.44
1:B:27:GLN:NE2	1:B:247:ARG:HH22	2.09	0.44
1:A:199:THR:O	1:A:200:PRO:C	2.59	0.44
1:B:198:THR:OG1	3:B:302:V14:N10	2.50	0.43
1:B:235:ASP:O	1:B:237:PRO:HD3	2.17	0.43
1:C:33:HIS:O	1:C:36:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ALA:C	1:A:229:LEU:HD23	2.43	0.43
1:D:62:THR:HG23	1:D:171:GLU:HG2	1.99	0.43
1:C:27:GLN:HE21	1:C:247:ARG:NH1	2.15	0.43
1:C:156:ASP:O	1:C:158:ILE:N	2.52	0.43
3:C:302:V14:H8	3:C:302:V14:H5	1.84	0.43
1:C:162:LEU:C	1:C:164:HIS:N	2.75	0.43
1:A:134:ASN:O	1:A:134:ASN:ND2	2.52	0.43
1:B:134:ASN:HD22	1:B:134:ASN:H	1.67	0.43
1:D:26:LEU:CD2	1:D:255:ARG:CD	2.97	0.43
1:C:30:ILE:HG12	1:C:193:TYR:CZ	2.53	0.43
1:D:4:TRP:CD2	1:D:200:PRO:HG2	2.54	0.43
1:D:147:GLU:HG3	1:D:216:GLN:HG2	2.00	0.43
1:A:3:LYS:HD3	1:A:3:LYS:N	2.34	0.42
1:B:223:LEU:HD22	4:B:472:HOH:O	2.19	0.42
1:B:12:GLU:HA	1:B:15:TRP:CD1	2.54	0.42
1:C:164:HIS:N	1:C:164:HIS:CD2	2.85	0.42
1:D:114:ALA:HB3	1:D:146:ILE:HB	2.01	0.42
1:B:143:ALA:HB3	1:B:210:VAL:HG22	2.01	0.42
1:D:19:TYR:HA	1:D:20:PRO:HD2	1.85	0.42
1:B:56:ASN:N	1:B:56:ASN:OD1	2.52	0.42
1:D:38:GLN:O	1:D:258:TYR:HA	2.20	0.42
1:B:83:SER:CB	1:B:122:ASN:ND2	2.83	0.42
1:D:77:HIS:HD2	1:D:84:ARG:HG2	1.85	0.42
1:D:198:THR:OG1	3:D:302[B]:V14:N10	2.53	0.42
1:B:3[B]:LYS:HD2	1:B:3[B]:LYS:HA	1.47	0.42
1:B:232:THR:CG2	1:B:240:ARG:H	2.33	0.42
1:B:252:PHE:CZ	1:B:255:ARG:O	2.73	0.42
1:B:147:GLU:O	1:B:216:GLN:HA	2.20	0.41
1:C:156:ASP:C	1:C:158:ILE:H	2.27	0.41
3:C:302:V14:H6	3:C:302:V14:H8	1.85	0.41
1:B:152:ASN:HA	1:B:153:PRO:HD2	1.84	0.41
1:A:119:VAL:HG11	3:A:302:V14:H23	2.03	0.41
1:A:197:LEU:O	1:A:202:CYS:HA	2.21	0.41
1:A:58:GLN:HG2	1:A:175:PRO:HA	2.01	0.41
1:D:253:ASP:C	1:D:255:ARG:H	2.28	0.41
1:A:58:GLN:HA	1:A:174:VAL:O	2.21	0.41
1:A:186:ARG:CG	1:A:186:ARG:NH2	2.72	0.41
1:B:91:HIS:CE1	3:B:302:V14:C4	3.04	0.41
1:C:70:LEU:HB3	1:C:90:LEU:HG	2.03	0.41
1:C:104:GLU:HG2	1:C:246:PHE:HB2	2.03	0.41
1:C:157:LYS:CB	1:C:177:PHE:CE2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLN:HE21	1:C:58:GLN:HA	1.86	0.40
1:B:46:LEU:HD22	1:B:78:ILE:HG21	2.03	0.40
1:A:112:PHE:HE2	1:A:214:PRO:HG3	1.86	0.40
1:B:38:GLN:O	1:B:258:TYR:HA	2.22	0.40
1:C:116:LEU:HB3	1:C:144:VAL:HB	2.02	0.40
1:D:161:HIS:CD2	1:D:174:VAL:HG22	2.56	0.40
1:B:139:LEU:HD13	1:B:197:LEU:HD21	2.03	0.40
1:C:151:PHE:CZ	1:C:156:ASP:CG	2.99	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	259/263 (98%)	245 (95%)	13 (5%)	1 (0%)	30	27
1	B	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
1	C	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
1	D	260/263 (99%)	251 (96%)	7 (3%)	2 (1%)	16	11
All	All	1041/1052 (99%)	997 (96%)	41 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	THR
1	D	160	SER
1	D	254	GLU

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	233/235 (99%)	218 (94%)	15 (6%)	16	12
1	B	236/235 (100%)	223 (94%)	13 (6%)	19	17
1	C	235/235 (100%)	225 (96%)	10 (4%)	26	25
1	D	234/235 (100%)	218 (93%)	16 (7%)	14	11
All	All	938/940 (100%)	884 (94%)	54 (6%)	19	15

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	36	ILE
1	A	49	GLN
1	A	57	LYS
1	A	75	ASP
1	A	78	ILE
1	A	79	GLN
1	A	89	GLN
1	A	148	MET
1	A	156	ASP
1	A	186	ARG
1	A	234	MET
1	A	235	ASP
1	A	241	GLU
1	A	253	ASP
1	B	18	LYS
1	B	25[A]	LEU
1	B	25[B]	LEU
1	B	56	ASN
1	B	58	GLN
1	B	69	LYS
1	B	75	ASP
1	B	89	GLN
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	137	GLU
1	B	156	ASP
1	B	223	LEU
1	B	236	ASP
1	C	3	LYS
1	C	36	ILE
1	C	49	GLN
1	C	79	GLN
1	C	82	GLN
1	C	89	GLN
1	C	130	SER
1	C	156	ASP
1	C	171	GLU
1	C	262	SER
1	D	18	LYS
1	D	25	LEU
1	D	56	ASN
1	D	69	LYS
1	D	89	GLN
1	D	134	ASN
1	D	135	LYS
1	D	136	SER
1	D	150[A]	SER
1	D	150[B]	SER
1	D	156	ASP
1	D	185	GLU
1	D	223	LEU
1	D	236	ASP
1	D	253	ASP
1	D	262	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	27	GLN
1	A	66	HIS
1	A	79	GLN
1	A	98	ASN
1	A	111	HIS
1	A	134	ASN
1	A	161	HIS

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Mol	Chain	Res	Type
1	A	163	GLN
1	A	164	HIS
1	A	219	GLN
1	A	248	GLN
1	A	263	GLN
1	B	27	GLN
1	B	33	HIS
1	B	38	GLN
1	B	66	HIS
1	B	101	HIS
1	B	111	HIS
1	B	134	ASN
1	B	164	HIS
1	B	248	GLN
1	B	250	GLN
1	C	13	ASN
1	C	27	GLN
1	C	58	GLN
1	C	66	HIS
1	C	79	GLN
1	C	134	ASN
1	C	152	ASN
1	C	213	ASN
1	C	216	GLN
1	C	233	HIS
1	C	248	GLN
1	C	250	GLN
1	D	13	ASN
1	D	27	GLN
1	D	33	HIS
1	D	38	GLN
1	D	82	GLN
1	D	101	HIS
1	D	161	HIS
1	D	213	ASN
1	D	219	GLN
1	D	233	HIS
1	D	248	GLN
1	D	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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$
3	V14	D	302[A]	2	29,29,29	2.93	7 (24%)	37,43,43	3.80	12 (32%)
3	V14	D	302[B]	2	29,29,29	2.92	5 (17%)	37,43,43	4.18	12 (32%)
3	V14	A	302	2	29,29,29	3.32	11 (37%)	37,43,43	4.44	14 (37%)
3	V14	B	302	2	29,29,29	2.86	6 (20%)	37,43,43	3.28	13 (35%)
3	V14	C	302	2	29,29,29	3.23	8 (27%)	37,43,43	4.30	14 (37%)

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
3	V14	D	302[A]	2	-	15/20/30/30	0/2/2/2
3	V14	D	302[B]	2	-	7/20/30/30	0/2/2/2
3	V14	A	302	2	-	11/20/30/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	V14	B	302	2	-	10/20/30/30	0/2/2/2
3	V14	C	302	2	-	10/20/30/30	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	V14	S7-N10	9.12	1.78	1.60
3	A	302	V14	O17-S11	8.99	1.56	1.44
3	C	302	V14	S7-N10	8.87	1.77	1.60
3	C	302	V14	O17-S11	7.89	1.54	1.44
3	D	302[A]	V14	S7-N10	7.59	1.75	1.60
3	B	302	V14	O17-S11	7.56	1.54	1.44
3	D	302[B]	V14	O16-S11	7.54	1.54	1.44
3	D	302[A]	V14	O17-S11	7.36	1.54	1.44
3	D	302[B]	V14	S7-N10	7.27	1.74	1.60
3	B	302	V14	S7-N10	7.24	1.74	1.60
3	D	302[B]	V14	O17-S11	7.15	1.53	1.44
3	B	302	V14	O16-S11	7.12	1.53	1.44
3	C	302	V14	O16-S11	7.00	1.53	1.44
3	D	302[A]	V14	O16-S11	6.85	1.53	1.44
3	C	302	V14	O9-S7	6.30	1.54	1.43
3	D	302[B]	V14	O9-S7	6.25	1.54	1.43
3	D	302[A]	V14	O9-S7	6.15	1.54	1.43
3	A	302	V14	O8-S7	6.06	1.54	1.43
3	A	302	V14	O16-S11	6.03	1.52	1.44
3	C	302	V14	O8-S7	5.96	1.54	1.43
3	B	302	V14	O9-S7	5.93	1.54	1.43
3	A	302	V14	O9-S7	5.66	1.53	1.43
3	D	302[B]	V14	O8-S7	5.54	1.53	1.43
3	D	302[A]	V14	O8-S7	5.28	1.53	1.43
3	B	302	V14	O8-S7	5.00	1.52	1.43
3	A	302	V14	C15-S11	3.32	1.84	1.77
3	C	302	V14	C15-S11	3.12	1.83	1.77
3	C	302	V14	C22-C14	3.10	1.56	1.52
3	A	302	V14	C2-C1	2.67	1.44	1.39
3	A	302	V14	C22-C14	2.60	1.55	1.52
3	D	302[A]	V14	C15-S11	2.54	1.82	1.77
3	A	302	V14	C28-C14	2.49	1.55	1.52
3	A	302	V14	C6-C5	2.48	1.43	1.39
3	A	302	V14	C4-S7	-2.38	1.75	1.78
3	D	302[A]	V14	C6-C5	2.21	1.42	1.39
3	B	302	V14	C6-C5	2.14	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	V14	C28-C14	2.10	1.55	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302[B]	V14	O17-S11-O16	-19.42	97.64	118.45
3	A	302	V14	O17-S11-O16	-18.50	98.62	118.45
3	C	302	V14	O17-S11-O16	-18.13	99.02	118.45
3	D	302[A]	V14	O17-S11-O16	-17.06	100.16	118.45
3	B	302	V14	O17-S11-O16	-11.02	106.64	118.45
3	C	302	V14	O8-S7-O9	-10.27	102.99	118.80
3	B	302	V14	O8-S7-O9	-10.02	103.38	118.80
3	D	302[B]	V14	O8-S7-O9	-9.91	103.55	118.80
3	A	302	V14	C3-C4-C5	9.86	123.41	116.65
3	D	302[A]	V14	O8-S7-O9	-8.84	105.19	118.80
3	A	302	V14	O8-S7-O9	-8.32	106.00	118.80
3	A	302	V14	C4-S7-N10	7.91	122.50	108.26
3	C	302	V14	O8-S7-C4	7.64	118.50	107.28
3	D	302[B]	V14	C3-C4-C5	7.48	121.78	116.65
3	D	302[A]	V14	C3-C4-C5	6.97	121.43	116.65
3	A	302	V14	O9-S7-N10	-6.39	98.14	107.35
3	C	302	V14	C4-S7-N10	6.24	119.49	108.26
3	A	302	V14	C15-S11-C1	6.00	133.03	108.15
3	C	302	V14	O9-S7-N10	-5.54	99.36	107.35
3	B	302	V14	C3-C4-C5	5.48	120.41	116.65
3	C	302	V14	C3-C4-C5	5.33	120.30	116.65
3	C	302	V14	C15-S11-C1	4.93	128.60	108.15
3	B	302	V14	C2-C1-S11	-4.87	108.93	120.87
3	B	302	V14	O9-S7-C4	4.72	114.22	107.28
3	B	302	V14	C15-S11-C1	4.64	127.41	108.15
3	D	302[B]	V14	O9-S7-C4	4.44	113.80	107.28
3	D	302[A]	V14	C2-C1-S11	-4.30	110.32	120.87
3	D	302[A]	V14	C15-S11-C1	4.19	125.51	108.15
3	B	302	V14	O8-S7-N10	4.07	113.21	107.35
3	D	302[A]	V14	O9-S7-C4	3.98	113.12	107.28
3	A	302	V14	C2-C3-C4	-3.59	117.44	121.78
3	D	302[B]	V14	C2-C1-S11	-3.58	112.08	120.87
3	D	302[A]	V14	O8-S7-C4	3.49	112.40	107.28
3	C	302	V14	O21-C18-C15	3.21	117.55	109.82
3	A	302	V14	F13-C2-C3	-3.06	113.19	119.27
3	D	302[B]	V14	C2-C3-C4	-2.99	118.16	121.78
3	D	302[B]	V14	O17-S11-C15	2.93	112.99	108.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	V14	O8-S7-C4	2.82	111.42	107.28
3	C	302	V14	O16-S11-C1	-2.80	99.50	106.59
3	A	302	V14	F20-C5-C4	-2.79	115.73	120.76
3	C	302	V14	F13-C2-C3	-2.73	113.84	119.27
3	D	302[B]	V14	O8-S7-C4	2.72	111.27	107.28
3	B	302	V14	C18-C15-S11	-2.72	106.72	114.27
3	A	302	V14	F20-C5-C6	2.68	123.51	119.54
3	D	302[A]	V14	F20-C5-C6	2.58	123.36	119.54
3	D	302[B]	V14	C4-S7-N10	2.55	112.85	108.26
3	B	302	V14	F12-C3-C4	2.53	125.31	120.76
3	C	302	V14	C26-C27-C28	-2.43	107.06	117.37
3	D	302[A]	V14	O9-S7-N10	-2.43	103.85	107.35
3	D	302[B]	V14	C15-S11-C1	2.43	118.22	108.15
3	D	302[B]	V14	C18-C15-S11	-2.42	107.54	114.27
3	A	302	V14	F13-C2-C1	2.42	125.11	120.76
3	B	302	V14	O9-S7-N10	-2.36	103.94	107.35
3	A	302	V14	O16-S11-C1	-2.24	100.90	106.59
3	C	302	V14	C2-C3-C4	-2.21	119.10	121.78
3	A	302	V14	O21-C18-C15	2.20	115.12	109.82
3	D	302[A]	V14	O8-S7-N10	2.20	110.52	107.35
3	B	302	V14	C2-C3-C4	-2.11	119.23	121.78
3	C	302	V14	O17-S11-C15	2.09	111.60	108.18
3	D	302[A]	V14	C2-C3-C4	-2.07	119.27	121.78
3	B	302	V14	O17-S11-C15	-2.07	104.79	108.18
3	B	302	V14	C4-S7-N10	2.06	111.97	108.26
3	D	302[A]	V14	F20-C5-C4	-2.06	117.06	120.76
3	C	302	V14	O8-S7-N10	-2.02	104.44	107.35
3	D	302[B]	V14	F12-C3-C4	2.02	124.40	120.76

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	V14	C3-C4-S7-N10
3	A	302	V14	C2-C1-S11-C15
3	A	302	V14	C6-C1-S11-O17
3	A	302	V14	C6-C1-S11-C15
3	A	302	V14	C18-C15-S11-C1
3	A	302	V14	C18-C15-S11-O16
3	A	302	V14	C18-C15-S11-O17
3	A	302	V14	S11-C15-C18-O21
3	B	302	V14	C3-C4-S7-N10

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Mol	Chain	Res	Type	Atoms
3	B	302	V14	C2-C1-S11-O17
3	B	302	V14	C6-C1-S11-O16
3	B	302	V14	C6-C1-S11-O17
3	B	302	V14	C6-C1-S11-C15
3	B	302	V14	C18-C15-S11-O16
3	B	302	V14	S11-C15-C18-O21
3	C	302	V14	C5-C4-S7-O8
3	C	302	V14	C3-C4-S7-N10
3	C	302	V14	C2-C1-S11-C15
3	C	302	V14	C6-C1-S11-O16
3	C	302	V14	C6-C1-S11-O17
3	C	302	V14	C6-C1-S11-C15
3	C	302	V14	C18-C15-S11-C1
3	C	302	V14	S11-C15-C18-O21
3	D	302[A]	V14	C5-C4-S7-O8
3	D	302[A]	V14	C3-C4-S7-N10
3	D	302[A]	V14	C3-C4-S7-O8
3	D	302[A]	V14	C1-C6-N19-C14
3	D	302[A]	V14	C2-C1-S11-O17
3	D	302[A]	V14	C6-C1-S11-O16
3	D	302[A]	V14	C6-C1-S11-O17
3	D	302[A]	V14	C6-C1-S11-C15
3	D	302[A]	V14	C18-C15-S11-C1
3	D	302[A]	V14	C18-C15-S11-O16
3	D	302[A]	V14	C18-C15-S11-O17
3	D	302[B]	V14	C3-C4-S7-N10
3	D	302[B]	V14	C6-C1-S11-O16
3	D	302[B]	V14	C18-C15-S11-O16
3	D	302[B]	V14	S11-C15-C18-O21
3	B	302	V14	C18-C15-S11-C1
3	D	302[B]	V14	C18-C15-S11-C1
3	D	302[A]	V14	C28-C14-N19-C6
3	D	302[B]	V14	C28-C14-N19-C6
3	A	302	V14	C2-C1-S11-O17
3	D	302[B]	V14	C2-C1-S11-O16
3	A	302	V14	C5-C4-S7-O8
3	D	302[A]	V14	S11-C15-C18-O21
3	A	302	V14	C5-C4-S7-N10
3	C	302	V14	C5-C4-S7-N10
3	D	302[A]	V14	C5-C4-S7-N10
3	C	302	V14	C3-C4-S7-O8
3	B	302	V14	C2-C1-S11-C15

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Mol	Chain	Res	Type	Atoms
3	D	302[A]	V14	C2-C1-S11-C15
3	B	302	V14	C5-C6-N19-C14

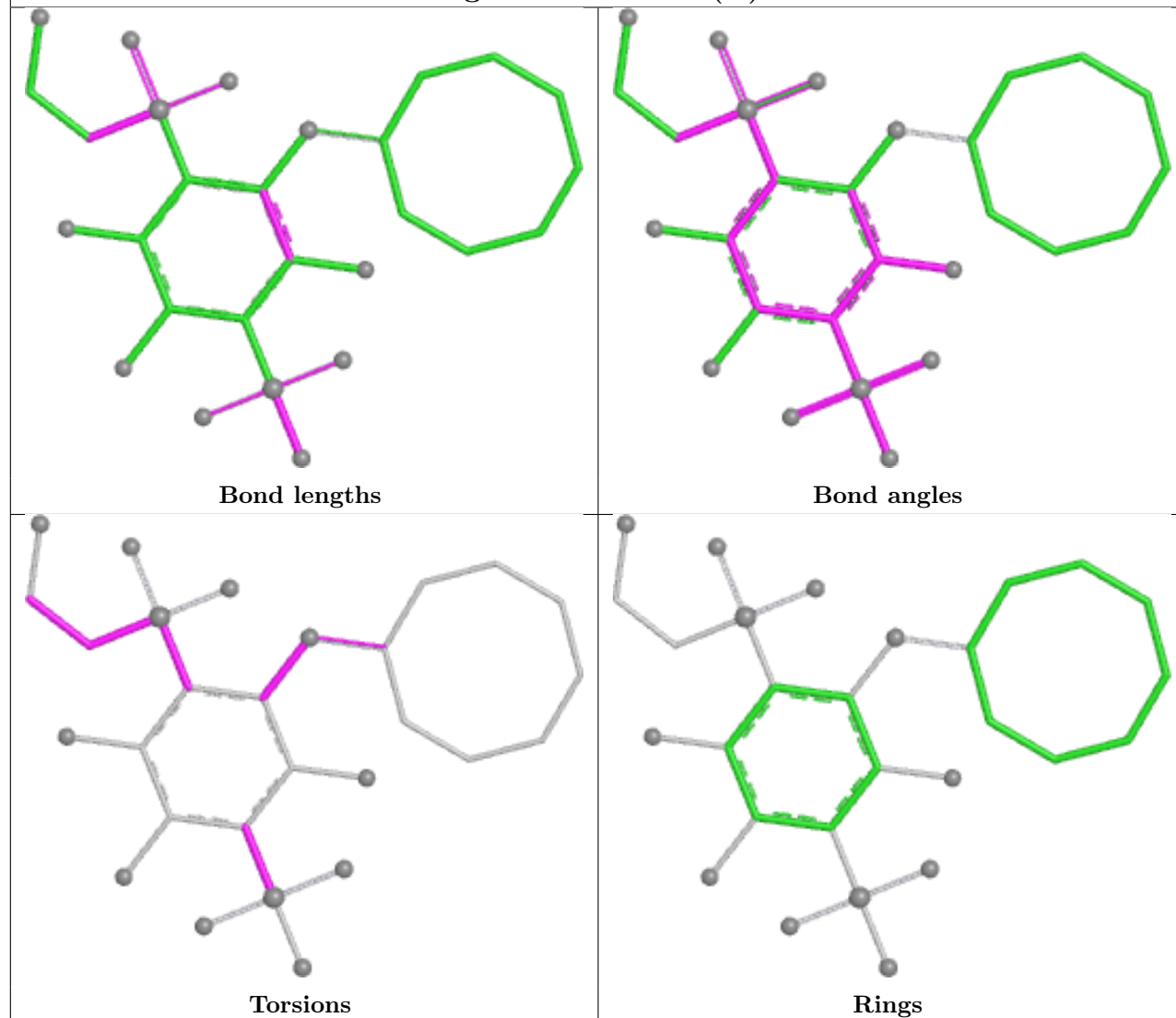
There are no ring outliers.

5 monomers are involved in 29 short contacts:

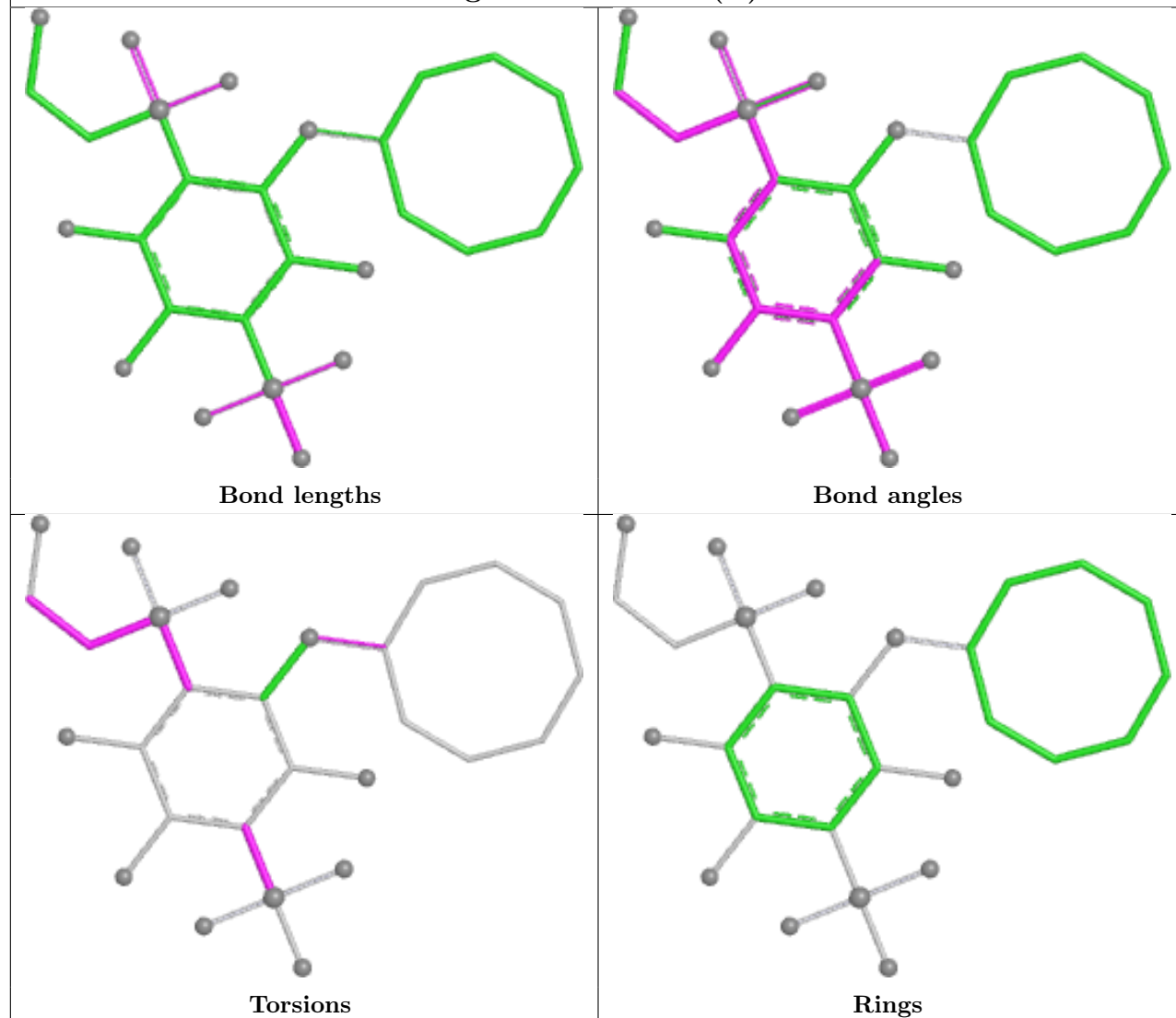
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302[A]	V14	1	0
3	D	302[B]	V14	9	0
3	A	302	V14	6	0
3	B	302	V14	6	0
3	C	302	V14	7	0

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

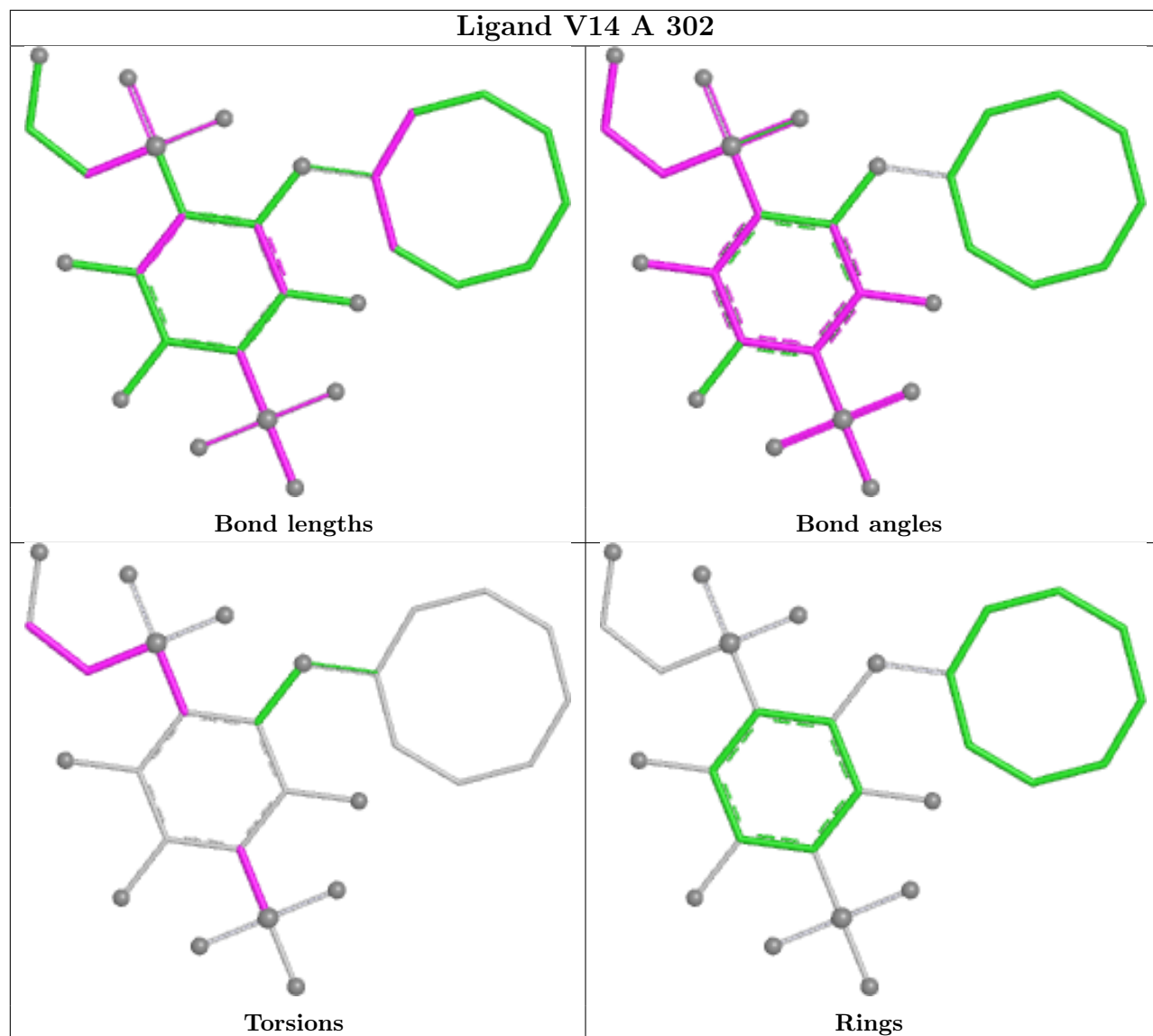
Ligand V14 D 302 (A)



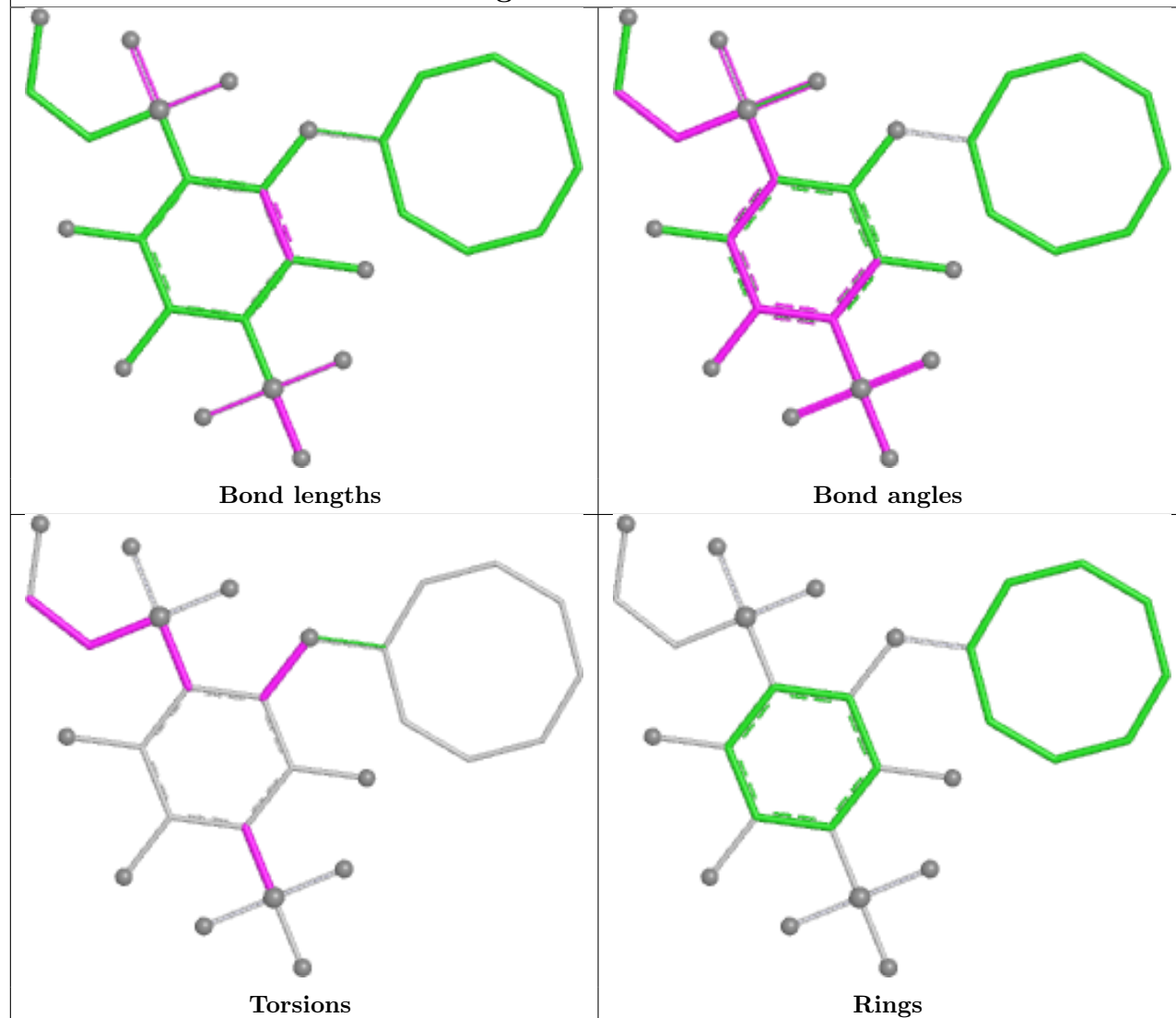
Ligand V14 D 302 (B)

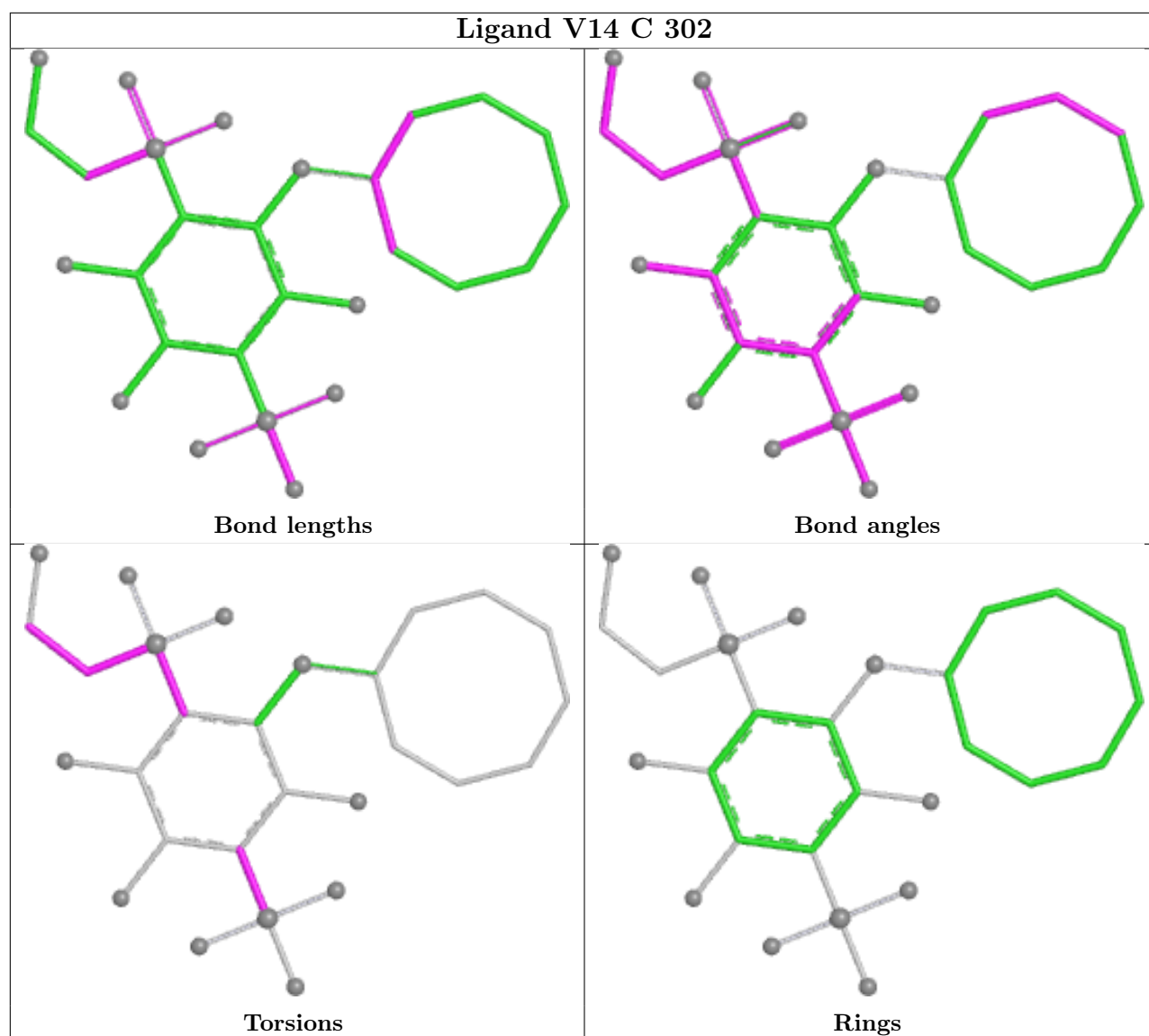


Ligand V14 A 302



Ligand V14 B 302





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	261/263 (99%)	0.41	20 (7%)	19 18	5, 19, 37, 48	17 (6%)
1	B	260/263 (98%)	0.14	8 (3%)	51 50	7, 18, 29, 59	8 (3%)
1	C	261/263 (99%)	0.39	18 (6%)	23 21	5, 19, 35, 49	19 (7%)
1	D	260/263 (98%)	0.10	6 (2%)	61 60	7, 18, 30, 59	6 (2%)
All	All	1042/1052 (99%)	0.26	52 (4%)	34 33	5, 18, 34, 59	50 (4%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	PHE	5.9
1	A	130	SER	5.5
1	D	253	ASP	5.4
1	A	78	ILE	5.2
1	A	235	ASP	4.8
1	D	78	ILE	4.7
1	C	130	SER	4.4
1	C	235	ASP	4.0
1	A	237	PRO	3.9
1	C	135	LYS	3.9
1	D	254	GLU	3.9
1	A	217	ILE	3.9
1	B	237	PRO	3.7
1	C	78	ILE	3.6
1	A	255	ARG	3.5
1	C	217	ILE	3.5
1	B	78	ILE	3.3
1	C	36	ILE	3.3
1	B	253	ASP	3.3
1	D	234	MET	3.2
1	A	88	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	173	PHE	3.1
1	A	173	PHE	3.1
1	A	36	ILE	3.1
1	C	88	THR	3.0
1	A	157	LYS	3.0
1	C	255	ARG	3.0
1	A	135	LYS	2.9
1	C	237	PRO	2.8
1	A	111	HIS	2.8
1	A	110	GLN	2.6
1	C	110	GLN	2.6
1	C	163	GLN	2.6
1	C	252	PHE	2.6
1	B	238	SER	2.6
1	A	256	LEU	2.6
1	B	252	PHE	2.5
1	B	236	ASP	2.5
1	A	7	PHE	2.4
1	A	18	LYS	2.4
1	C	162	LEU	2.3
1	C	133	SER	2.2
1	B	254	GLU	2.2
1	A	163	GLN	2.1
1	A	252	PHE	2.1
1	C	136	SER	2.1
1	D	237	PRO	2.1
1	C	157	LYS	2.1
1	A	164	HIS	2.0
1	A	232	THR	2.0
1	B	239	PRO	2.0
1	C	18	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

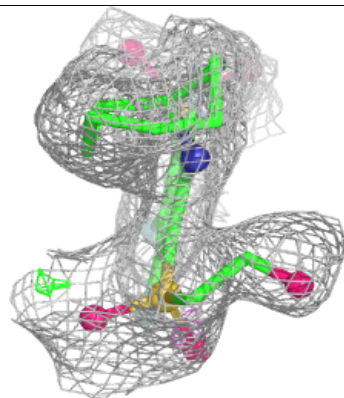
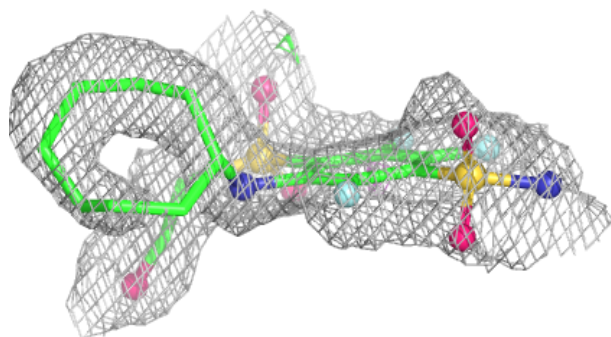
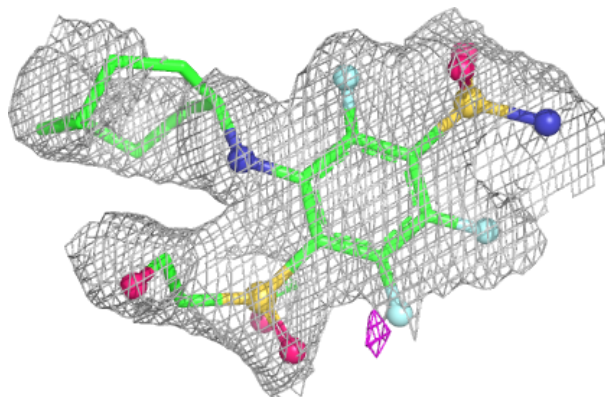
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	V14	A	302	28/28	0.91	0.11	21,27,31,33	0
3	V14	B	302	28/28	0.94	0.08	13,19,24,29	0
3	V14	C	302	28/28	0.95	0.08	20,27,30,31	0
3	V14	D	302[A]	28/28	0.95	0.08	12,15,17,17	28
3	V14	D	302[B]	28/28	0.95	0.08	15,20,22,23	28
2	ZN	C	301	1/1	0.98	0.03	14,14,14,14	0
2	ZN	A	301	1/1	0.98	0.02	12,12,12,12	0
2	ZN	D	301	1/1	0.99	0.02	11,11,11,11	0
2	ZN	B	301	1/1	0.99	0.02	14,14,14,14	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.

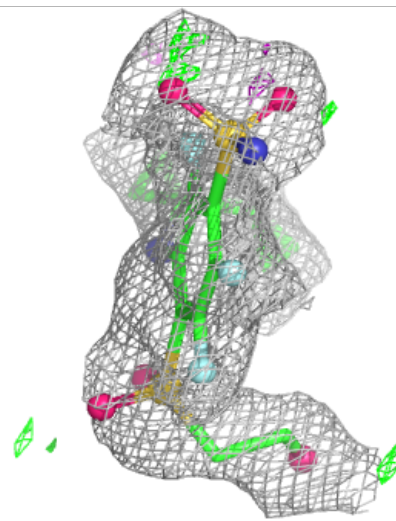
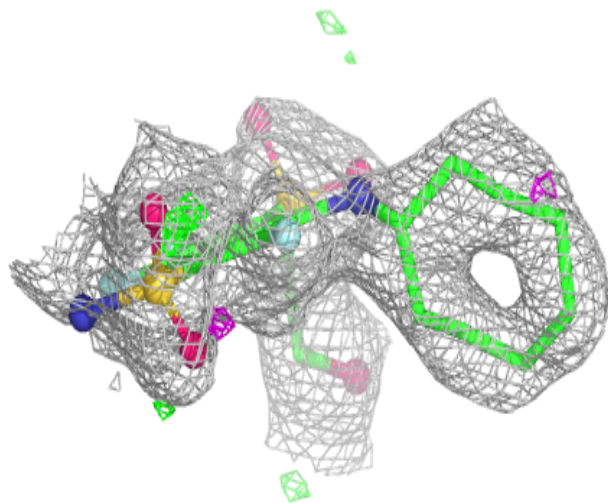
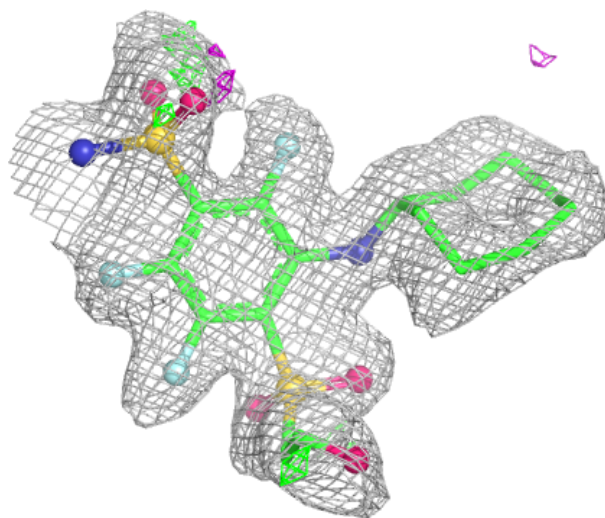
Electron density around V14 A 302:

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



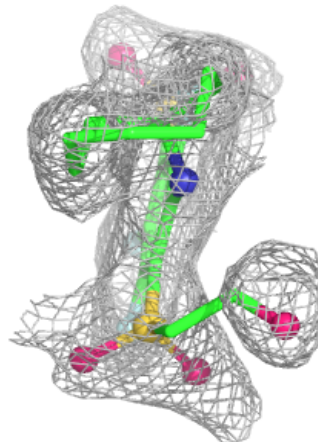
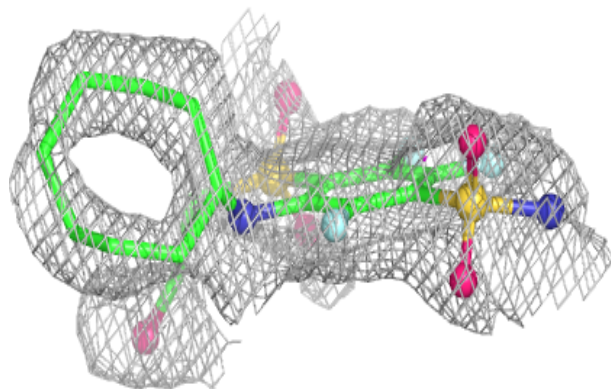
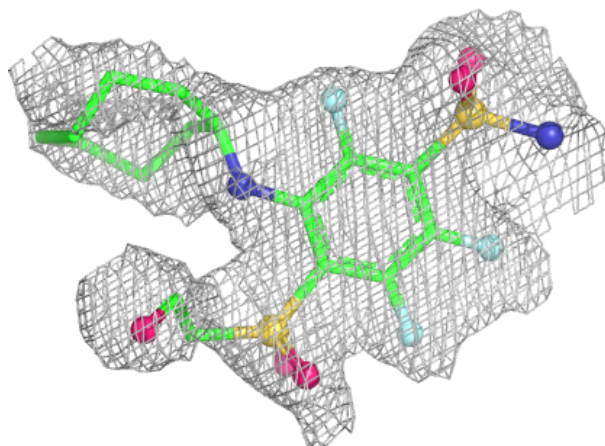
Electron density around V14 B 302:

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



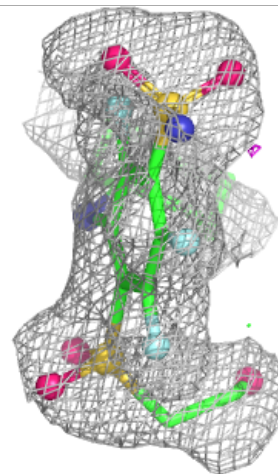
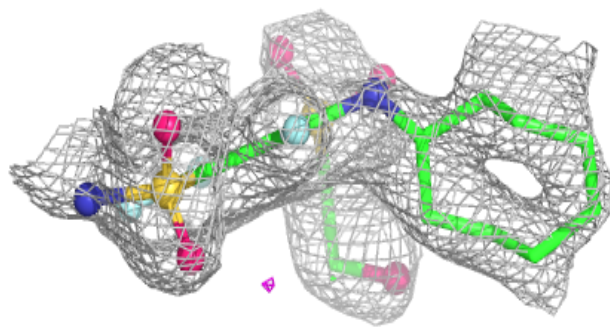
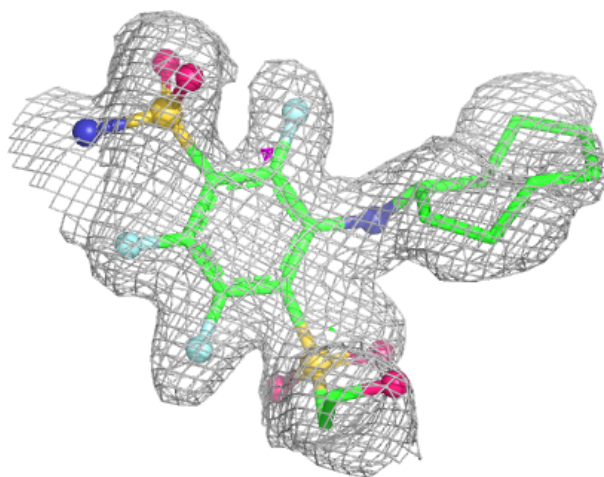
Electron density around V14 C 302:

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



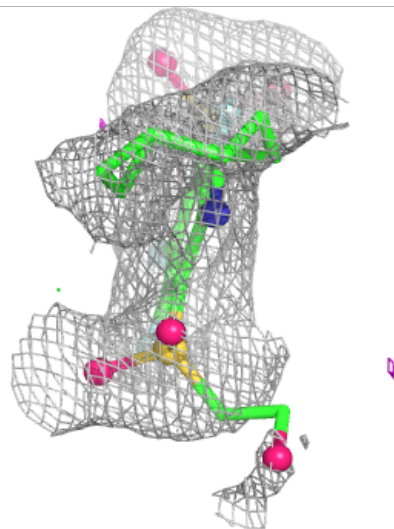
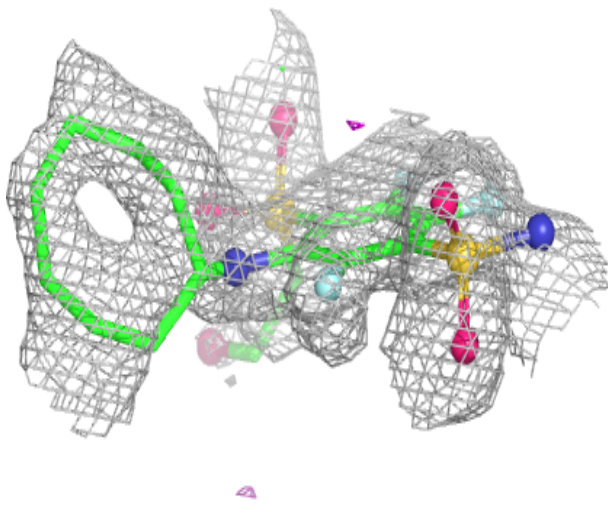
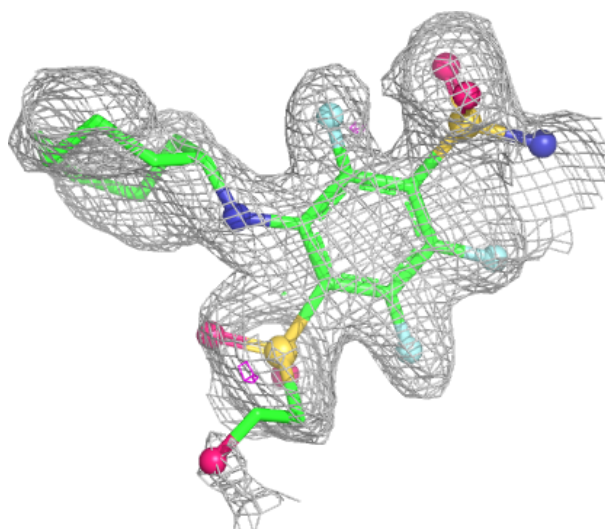
Electron density around V14 D 302 (A):

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



Electron density around V14 D 302 (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.