



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:59 PM UTC

PDB ID : 8HPC / pdb_00008hpc
Title : Crystal structure of C171A Mutant of N-carbamyl-D-amino acid amidohydro-
lase complexed with N-carbamyl-D-Hydroxyphenylglycine
Authors : Zhang, L.D.; Song, W.
Deposited on : 2022-12-12
Resolution : 2.52 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

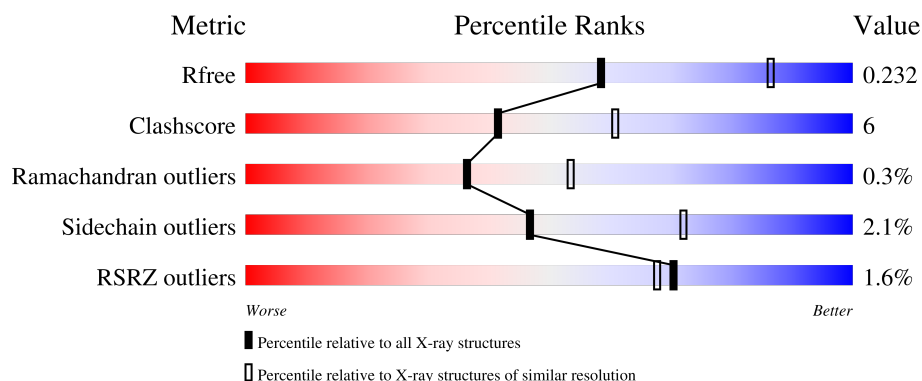
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	304	0% 85% 13% .
1	B	304	2% 81% 16% ..
1	C	304	0% 82% 17% .
1	D	304	0% 84% 15% .
1	E	304	2% 81% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	304	% 83% 15% ..
1	G	304	2% 80% 18% ..
1	H	304	3% 81% 17% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19517 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.

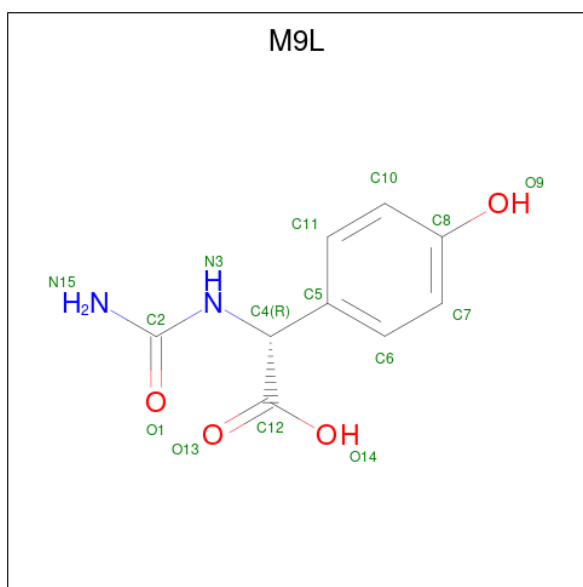
- Molecule 1 is a protein called N-carbamoyl-D-amino acid hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2390	1526	422	429	13			
1	B	300	Total	C	N	O	S	0	0	0
			2390	1526	422	429	13			
1	C	303	Total	C	N	O	S	0	0	0
			2405	1535	425	432	13			
1	D	303	Total	C	N	O	S	0	0	0
			2405	1535	425	432	13			
1	E	298	Total	C	N	O	S	0	0	0
			2374	1516	420	425	13			
1	F	299	Total	C	N	O	S	0	0	0
			2383	1522	421	427	13			
1	G	300	Total	C	N	O	S	0	0	0
			2390	1526	422	429	13			
1	H	300	Total	C	N	O	S	0	0	0
			2390	1526	422	429	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	CYS	engineered mutation	UNP P60327
B	192	ALA	CYS	engineered mutation	UNP P60327
C	192	ALA	CYS	engineered mutation	UNP P60327
D	192	ALA	CYS	engineered mutation	UNP P60327
E	192	ALA	CYS	engineered mutation	UNP P60327
F	192	ALA	CYS	engineered mutation	UNP P60327
G	192	ALA	CYS	engineered mutation	UNP P60327
H	192	ALA	CYS	engineered mutation	UNP P60327

- Molecule 2 is (2 {R})-2-(aminocarbonylamino)-2-(4-hydroxyphenyl)ethanoic acid (CCD ID: M9L) (formula: C₉H₁₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	9	2	4		
2	B	1	Total	C	N	O	0	0
			15	9	2	4		
2	C	1	Total	C	N	O	0	0
			15	9	2	4		
2	D	1	Total	C	N	O	0	0
			15	9	2	4		
2	E	1	Total	C	N	O	0	0
			15	9	2	4		
2	F	1	Total	C	N	O	0	0
			15	9	2	4		
2	G	1	Total	C	N	O	0	0
			15	9	2	4		
2	H	1	Total	C	N	O	0	0
			15	9	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	40	Total	O	0	0
			40	40		
3	C	38	Total	O	0	0
			38	38		
3	D	31	Total	O	0	0
			31	31		

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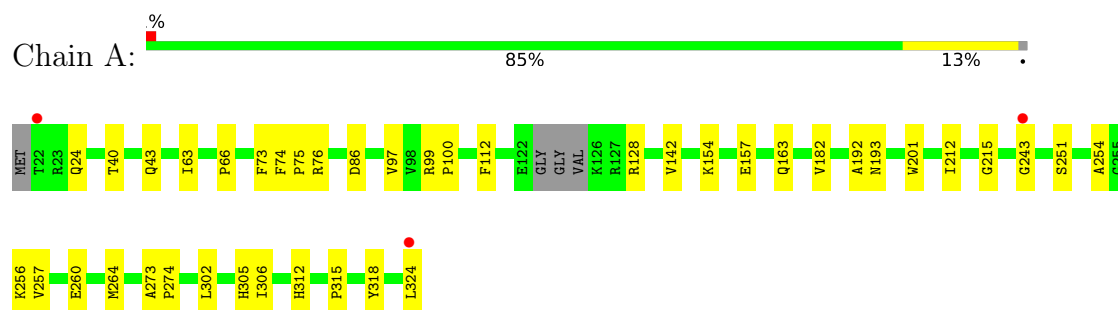
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	34	Total 34	O 34	0	0
3	F	31	Total 31	O 31	0	0
3	G	39	Total 39	O 39	0	0
3	H	20	Total 20	O 20	0	0

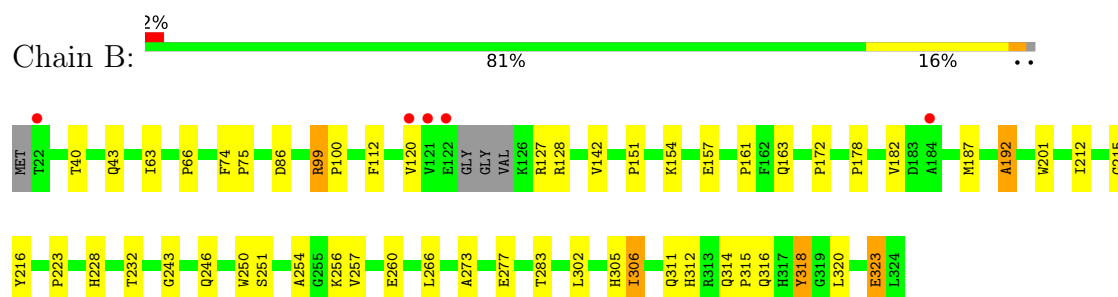
3 Residue-property plots [i](#)

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

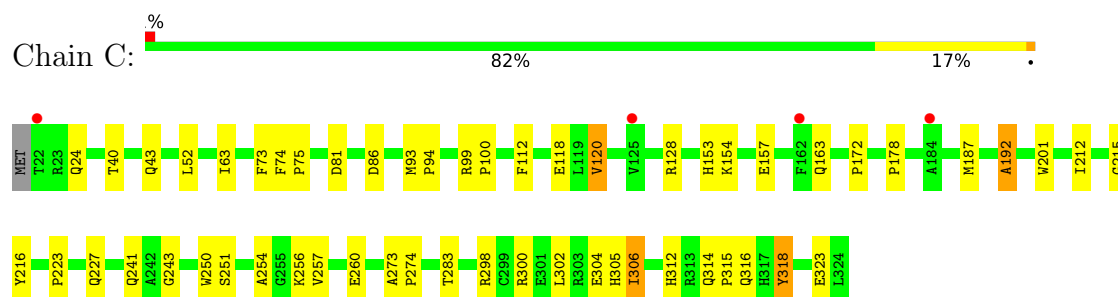
• Molecule 1: N-carbamoyl-D-amino acid hydrolase



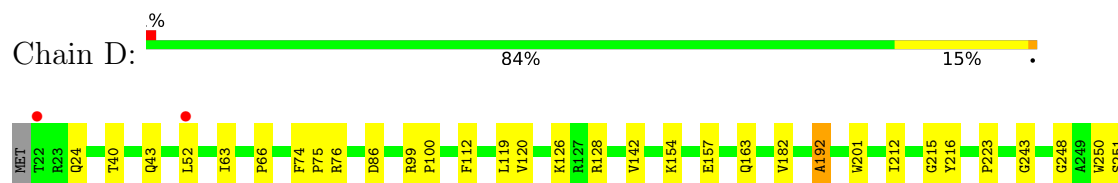
• Molecule 1: N-carbamoyl-D-amino acid hydrolase



• Molecule 1: N-carbamoyl-D-amino acid hydrolase

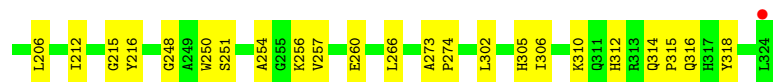
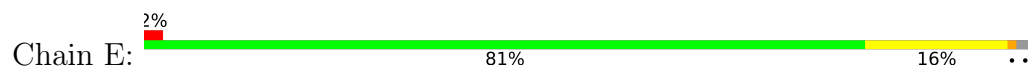


• Molecule 1: N-carbamoyl-D-amino acid hydrolase

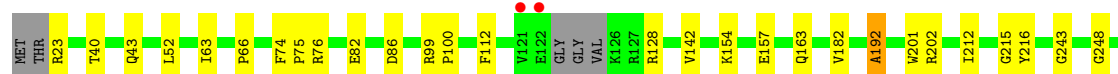
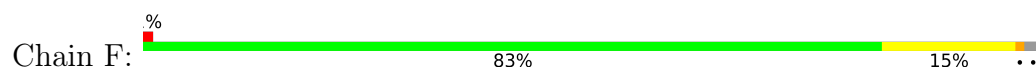




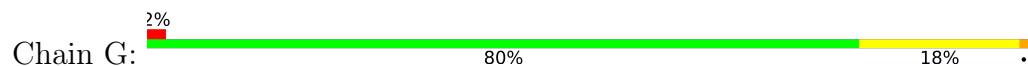
• Molecule 1: N-carbamoyl-D-amino acid hydrolase



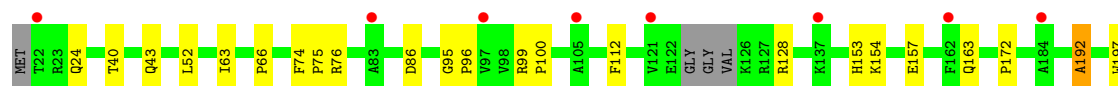
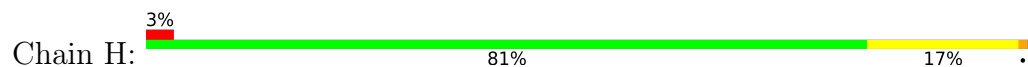
• Molecule 1: N-carbamoyl-D-amino acid hydrolase



• Molecule 1: N-carbamoyl-D-amino acid hydrolase



• Molecule 1: N-carbamoyl-D-amino acid hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.17Å 79.86Å 91.07Å 91.40° 98.48° 92.78°	Depositor
Resolution (Å)	46.59 – 2.52 46.59 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.59-2.52) 98.0 (46.59-2.52)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.218 , 0.253 0.202 , 0.232	Depositor DCC
R_{free} test set	3537 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19517	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.96% 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: M9L

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	1.03	0/2452	1.33	2/3321 (0.1%)
1	B	1.04	0/2452	1.34	8/3321 (0.2%)
1	C	1.04	1/2468 (0.0%)	1.37	11/3344 (0.3%)
1	D	1.04	0/2468	1.33	3/3344 (0.1%)
1	E	1.01	0/2436	1.32	3/3299 (0.1%)
1	F	1.02	0/2445	1.33	1/3311 (0.0%)
1	G	1.03	0/2452	1.34	2/3321 (0.1%)
1	H	1.01	2/2452 (0.1%)	1.32	4/3321 (0.1%)
All	All	1.03	3/19625 (0.0%)	1.33	34/26582 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	PRO	C-O	-5.93	1.16	1.23
1	H	228	HIS	CE1-NE2	5.87	1.38	1.32
1	H	153	HIS	CE1-NE2	5.46	1.38	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	324	LEU	CA-C-O	-6.91	109.05	120.80
1	B	323	GLU	CB-CG-CD	6.16	123.07	112.60
1	G	183	ASP	CA-C-O	-6.15	114.83	122.03
1	F	23	ARG	CA-C-O	-6.02	110.57	120.80
1	B	318	TYR	CA-C-N	5.94	126.69	120.03
1	B	318	TYR	C-N-CA	5.94	126.69	120.03
1	C	81	ASP	CA-C-N	5.74	128.43	120.29
1	C	81	ASP	C-N-CA	5.74	128.43	120.29
1	C	187	MET	CA-C-N	5.56	126.02	122.18
1	C	187	MET	C-N-CA	5.56	126.02	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	84	GLU	CB-CG-CD	5.33	121.67	112.60
1	H	318	TYR	CA-C-N	5.30	125.97	120.03
1	H	318	TYR	C-N-CA	5.30	125.97	120.03
1	C	172	PRO	CA-C-N	5.25	125.09	120.10
1	C	172	PRO	C-N-CA	5.25	125.09	120.10
1	B	187	MET	CA-C-N	5.24	125.79	122.18
1	B	187	MET	C-N-CA	5.24	125.79	122.18
1	A	73	PHE	CA-C-N	5.19	126.23	120.06
1	A	73	PHE	C-N-CA	5.19	126.23	120.06
1	C	223	PRO	N-CA-C	5.12	116.94	110.70
1	B	223	PRO	N-CA-C	5.11	116.93	110.70
1	E	187	MET	CA-C-N	5.08	125.69	122.18
1	E	187	MET	C-N-CA	5.08	125.69	122.18
1	D	318	TYR	CA-C-N	5.07	125.71	120.03
1	D	318	TYR	C-N-CA	5.07	125.71	120.03
1	D	223	PRO	N-CA-C	5.06	116.87	110.70
1	B	172	PRO	CA-C-N	5.03	124.88	120.10
1	B	172	PRO	C-N-CA	5.03	124.88	120.10
1	C	73	PHE	CA-C-N	5.03	126.04	120.06
1	C	73	PHE	C-N-CA	5.03	126.04	120.06
1	H	172	PRO	CA-C-N	5.02	124.87	120.10
1	H	172	PRO	C-N-CA	5.02	124.87	120.10
1	C	318	TYR	CA-C-N	5.01	125.64	120.03
1	C	318	TYR	C-N-CA	5.01	125.64	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2390	0	2345	26	0
1	B	2390	0	2345	36	0
1	C	2405	0	2361	34	0
1	D	2405	0	2361	24	0
1	E	2374	0	2330	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2383	0	2338	35	0
1	G	2390	0	2345	40	0
1	H	2390	0	2345	34	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
2	F	15	0	0	0	0
2	G	15	0	0	0	0
2	H	15	0	0	0	0
3	A	37	0	0	3	0
3	B	40	0	0	8	0
3	C	38	0	0	5	0
3	D	31	0	0	1	0
3	E	34	0	0	3	0
3	F	31	0	0	3	0
3	G	39	0	0	5	0
3	H	20	0	0	8	0
All	All	19517	0	18770	245	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 6.

All (245) 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:B:306:ILE:HB	3:B:536:HOH:O	1.27	1.32
1:A:306:ILE:HG23	3:H:519:HOH:O	1.39	1.18
1:A:306:ILE:CG2	3:H:519:HOH:O	2.02	1.01
1:B:311:GLN:O	3:B:501:HOH:O	1.83	0.96
1:E:256:LYS:NZ	3:E:502:HOH:O	2.08	0.82
3:B:526:HOH:O	1:G:306:ILE:HG23	1.83	0.77
1:B:178:PRO:HB3	1:E:310:LYS:HD2	1.67	0.75
1:A:97:VAL:O	3:A:501:HOH:O	2.05	0.75
1:H:95:GLY:HA3	3:H:514:HOH:O	1.85	0.74
1:C:241:GLN:OE1	3:C:501:HOH:O	2.06	0.72
1:C:153:HIS:HB2	3:C:521:HOH:O	1.90	0.72
1:H:300:ARG:N	1:H:300:ARG:HD2	2.03	0.71
1:E:266:LEU:O	3:E:501:HOH:O	2.06	0.71
1:H:306:ILE:O	3:H:501:HOH:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:PRO:HD2	3:H:518:HOH:O	1.93	0.69
1:B:161:PRO:HG2	3:B:534:HOH:O	1.93	0.68
1:H:246:GLN:NE2	3:H:502:HOH:O	2.27	0.68
1:H:95:GLY:CA	3:H:514:HOH:O	2.43	0.67
1:G:168:ARG:HD3	1:G:169:TYR:CE1	2.30	0.67
1:C:306:ILE:HD12	1:C:306:ILE:H	1.59	0.67
1:G:306:ILE:HD12	1:G:306:ILE:H	1.60	0.66
1:B:306:ILE:H	1:B:306:ILE:HD12	1.60	0.66
1:E:306:ILE:HD12	1:E:306:ILE:H	1.60	0.66
1:H:157:GLU:H	1:H:163:GLN:HE22	1.45	0.65
1:E:91:THR:HG22	1:E:119:LEU:HD23	1.79	0.65
1:D:157:GLU:H	1:D:163:GLN:HE22	1.45	0.65
1:A:306:ILE:HD12	1:A:306:ILE:H	1.61	0.64
1:B:157:GLU:H	1:B:163:GLN:HE22	1.46	0.64
1:A:157:GLU:H	1:A:163:GLN:HE22	1.46	0.64
1:C:300:ARG:NH1	1:C:304:GLU:OE2	2.31	0.63
1:F:157:GLU:H	1:F:163:GLN:HE22	1.46	0.62
1:C:256:LYS:NZ	3:C:502:HOH:O	2.27	0.62
1:G:162:PHE:HB2	3:G:536:HOH:O	2.00	0.62
1:D:306:ILE:H	1:D:306:ILE:HD12	1.63	0.62
1:C:157:GLU:H	1:C:163:GLN:HE22	1.46	0.61
1:G:157:GLU:H	1:G:163:GLN:HE22	1.47	0.61
1:H:324:LEU:HD12	1:H:324:LEU:H	1.66	0.60
1:F:256:LYS:NZ	3:F:501:HOH:O	2.27	0.60
1:B:246:GLN:NE2	3:B:503:HOH:O	2.35	0.59
1:B:320:LEU:HA	1:B:323:GLU:HG3	1.85	0.58
1:E:149:HIS:HE2	1:F:318:TYR:HH	1.51	0.58
1:G:183:ASP:O	1:G:184:ALA:HB3	2.03	0.57
1:H:300:ARG:HH11	1:H:300:ARG:HA	1.69	0.57
1:C:86:ASP:OD1	1:C:128:ARG:NH2	2.29	0.57
1:G:162:PHE:HD2	3:G:534:HOH:O	1.87	0.56
1:E:37:ARG:HD3	3:E:534:HOH:O	2.05	0.56
1:G:162:PHE:HB2	3:G:534:HOH:O	2.05	0.56
1:F:298:ARG:HH22	1:H:283:THR:CB	2.19	0.56
1:B:323:GLU:OE2	1:E:22:THR:HB	2.05	0.55
1:G:256:LYS:HE3	1:G:260:GLU:OE1	2.07	0.55
1:E:196:ARG:CD	1:F:306:ILE:HD11	2.37	0.55
1:A:99:ARG:HD2	3:A:532:HOH:O	2.07	0.55
1:F:266:LEU:HA	3:F:520:HOH:O	2.06	0.54
1:B:151:PRO:HG3	2:B:401:M9L:O1	2.08	0.54
1:B:127:ARG:NH1	1:F:320:LEU:HD13	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:ILE:HG22	3:F:528:HOH:O	2.08	0.54
1:H:256:LYS:HE3	1:H:260:GLU:OE1	2.07	0.53
1:E:186:LYS:HE2	1:G:316:GLN:HB3	1.88	0.53
1:A:193:ASN:HA	2:A:401:M9L:O13	2.09	0.53
1:A:256:LYS:HE3	1:A:260:GLU:OE1	2.08	0.53
1:C:256:LYS:HE3	1:C:260:GLU:OE1	2.09	0.53
1:B:86:ASP:OD1	1:B:128:ARG:NH2	2.34	0.52
1:D:256:LYS:HE3	1:D:260:GLU:OE1	2.08	0.52
1:F:256:LYS:HE3	1:F:260:GLU:OE1	2.10	0.52
1:G:152:GLY:HA2	3:G:532:HOH:O	2.08	0.52
1:E:256:LYS:HE3	1:E:260:GLU:OE1	2.09	0.52
1:B:302:LEU:N	1:B:302:LEU:HD22	2.25	0.52
1:E:120:VAL:HG22	1:E:127:ARG:H	1.75	0.52
1:B:256:LYS:HE3	1:B:260:GLU:OE1	2.10	0.51
1:D:314:GLN:HE21	1:D:316:GLN:HE22	1.59	0.51
1:E:314:GLN:HE21	1:E:316:GLN:HE22	1.58	0.51
1:C:302:LEU:N	1:C:302:LEU:HD22	2.24	0.51
1:E:86:ASP:OD1	1:E:128:ARG:NH2	2.34	0.51
1:B:315:PRO:HA	1:B:318:TYR:CD2	2.46	0.51
1:E:196:ARG:HD2	1:F:306:ILE:HD11	1.93	0.51
1:A:86:ASP:OD1	1:A:128:ARG:NH2	2.36	0.51
1:G:315:PRO:HA	1:G:318:TYR:CD2	2.46	0.51
1:C:316:GLN:HB3	1:D:324:LEU:HD21	1.92	0.51
1:A:302:LEU:HD22	1:A:302:LEU:N	2.25	0.50
1:A:315:PRO:HA	1:A:318:TYR:CD2	2.46	0.50
1:C:315:PRO:HA	1:C:318:TYR:CD2	2.46	0.50
1:D:315:PRO:HA	1:D:318:TYR:CD2	2.47	0.50
1:E:74:PHE:N	1:E:75:PRO:CD	2.74	0.50
1:H:314:GLN:HE21	1:H:316:GLN:HE22	1.59	0.50
1:F:86:ASP:OD1	1:F:128:ARG:NH2	2.35	0.50
1:H:315:PRO:HA	1:H:318:TYR:CD2	2.47	0.50
1:B:127:ARG:HH12	1:F:320:LEU:HD13	1.76	0.50
1:C:74:PHE:N	1:C:75:PRO:CD	2.75	0.50
1:E:315:PRO:HA	1:E:318:TYR:CD2	2.47	0.50
1:G:274:PRO:O	1:G:302:LEU:HD13	2.11	0.50
1:F:274:PRO:O	1:F:302:LEU:HD13	2.12	0.50
1:E:91:THR:HG22	1:E:119:LEU:CD2	2.41	0.50
1:H:74:PHE:N	1:H:75:PRO:CD	2.75	0.50
3:B:518:HOH:O	1:C:283:THR:HA	2.11	0.49
1:A:264:MET:CG	3:A:535:HOH:O	2.60	0.49
1:F:315:PRO:HA	1:F:318:TYR:CD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:GLU:CD	1:C:283:THR:HG22	2.37	0.49
1:D:74:PHE:N	1:D:75:PRO:CD	2.75	0.49
1:G:74:PHE:N	1:G:75:PRO:CD	2.76	0.49
1:B:120:VAL:HG11	1:F:323:GLU:HG2	1.93	0.49
1:F:314:GLN:HE21	1:F:316:GLN:HE22	1.60	0.49
1:C:314:GLN:HE21	1:C:316:GLN:HE22	1.59	0.49
1:E:40:THR:H	1:E:43:GLN:HE21	1.60	0.49
1:D:192:ALA:HB2	1:D:216:TYR:HA	1.95	0.49
1:E:274:PRO:O	1:E:302:LEU:HD13	2.13	0.49
1:B:74:PHE:N	1:B:75:PRO:CD	2.75	0.48
1:F:74:PHE:N	1:F:75:PRO:CD	2.76	0.48
1:G:56:ALA:HB2	1:G:110:ILE:HD11	1.95	0.48
1:D:86:ASP:OD1	1:D:128:ARG:NH2	2.34	0.48
1:A:74:PHE:N	1:A:75:PRO:CD	2.76	0.48
1:C:40:THR:H	1:C:43:GLN:HE21	1.60	0.48
1:E:248:GLY:HA2	1:E:302:LEU:HD13	1.96	0.48
1:H:40:THR:H	1:H:43:GLN:HE21	1.61	0.48
1:C:24:GLN:CG	3:C:535:HOH:O	2.61	0.48
1:G:192:ALA:HB2	1:G:216:TYR:HA	1.96	0.48
1:E:186:LYS:HE2	1:G:316:GLN:CB	2.44	0.48
1:F:40:THR:H	1:F:43:GLN:HE21	1.62	0.48
1:H:274:PRO:O	1:H:302:LEU:HD13	2.13	0.48
1:G:248:GLY:HA2	1:G:302:LEU:HD13	1.96	0.47
1:C:24:GLN:HG2	3:C:535:HOH:O	2.13	0.47
1:C:118:GLU:HG2	1:C:120:VAL:HG22	1.95	0.47
1:F:248:GLY:HA2	1:F:302:LEU:HD13	1.96	0.47
1:G:142:VAL:HG11	1:G:181:ASP:O	2.15	0.47
1:B:283:THR:CB	1:C:298:ARG:HH22	2.27	0.47
1:D:274:PRO:O	1:D:302:LEU:HD13	2.14	0.47
1:E:192:ALA:HB2	1:E:216:TYR:HA	1.97	0.47
1:A:212:ILE:O	1:A:251:SER:HA	2.15	0.47
1:G:314:GLN:HE21	1:G:316:GLN:HE22	1.63	0.47
1:B:314:GLN:HE21	1:B:316:GLN:HE22	1.61	0.46
1:B:212:ILE:O	1:B:251:SER:HA	2.16	0.46
1:H:212:ILE:O	1:H:251:SER:HA	2.15	0.46
1:C:192:ALA:HB2	1:C:216:TYR:HA	1.96	0.46
1:D:212:ILE:O	1:D:251:SER:HA	2.15	0.46
1:D:248:GLY:HA2	1:D:302:LEU:HD13	1.96	0.46
1:G:212:ILE:O	1:G:251:SER:HA	2.15	0.46
1:D:40:THR:H	1:D:43:GLN:HE21	1.62	0.46
1:H:248:GLY:HA2	1:H:302:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:H	1:A:43:GLN:HE21	1.64	0.46
1:C:215:GLY:HA2	1:C:254:ALA:O	2.16	0.46
1:B:192:ALA:HB2	1:B:216:TYR:HA	1.97	0.45
1:A:63:ILE:O	1:A:112:PHE:HA	2.17	0.45
1:D:215:GLY:HA2	1:D:254:ALA:O	2.16	0.45
1:H:209:ALA:O	1:H:303:ARG:NH2	2.48	0.45
1:C:212:ILE:O	1:C:251:SER:HA	2.15	0.45
1:F:212:ILE:O	1:F:251:SER:HA	2.15	0.45
1:H:192:ALA:HB2	1:H:216:TYR:HA	1.97	0.45
1:B:201:TRP:CD2	1:B:243:GLY:HA3	2.52	0.45
1:B:228:HIS:C	3:B:512:HOH:O	2.60	0.45
1:E:66:PRO:HA	1:E:215:GLY:HA3	1.99	0.45
1:E:212:ILE:O	1:E:251:SER:HA	2.16	0.45
1:F:192:ALA:HB2	1:F:216:TYR:HA	1.98	0.45
1:B:40:THR:H	1:B:43:GLN:HE21	1.64	0.45
1:G:122:GLU:OE2	1:G:127:ARG:NH1	2.50	0.45
1:D:283:THR:OG1	1:G:298:ARG:NH2	2.42	0.44
1:C:227:GLN:HA	1:G:285:LEU:HD11	2.00	0.44
1:A:215:GLY:HA2	1:A:254:ALA:O	2.18	0.44
1:B:302:LEU:HD13	1:B:306:ILE:HD13	1.99	0.44
1:C:201:TRP:CD2	1:C:243:GLY:HA3	2.53	0.44
1:H:95:GLY:HA3	3:H:518:HOH:O	2.17	0.44
1:A:201:TRP:CD2	1:A:243:GLY:HA3	2.53	0.44
1:G:230:HIS:HA	3:G:522:HOH:O	2.18	0.44
1:H:63:ILE:O	1:H:112:PHE:HA	2.18	0.44
1:H:215:GLY:HA2	1:H:254:ALA:O	2.18	0.44
1:B:127:ARG:NH1	1:F:323:GLU:OE2	2.51	0.43
3:B:526:HOH:O	1:G:306:ILE:CG2	2.54	0.43
1:A:142:VAL:HG21	1:A:182:VAL:HG22	1.99	0.43
1:G:215:GLY:HA2	1:G:254:ALA:O	2.19	0.43
1:H:86:ASP:OD1	1:H:128:ARG:NH2	2.35	0.43
1:F:215:GLY:HA2	1:F:254:ALA:O	2.19	0.43
1:D:201:TRP:CD2	1:D:243:GLY:HA3	2.54	0.43
1:A:273:ALA:HB1	1:A:274:PRO:HD2	2.01	0.43
1:E:206:LEU:HD13	1:F:320:LEU:HG	1.99	0.43
1:G:201:TRP:CD2	1:G:243:GLY:HA3	2.53	0.43
1:B:305:HIS:O	1:B:312:HIS:HE1	2.02	0.43
1:F:201:TRP:CD2	1:F:243:GLY:HA3	2.53	0.43
1:F:273:ALA:HB1	1:F:274:PRO:HD2	2.01	0.43
1:F:66:PRO:HA	1:F:215:GLY:HA3	2.01	0.42
1:C:306:ILE:CD1	3:D:514:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ILE:O	1:F:112:PHE:HA	2.19	0.42
1:F:142:VAL:HG21	1:F:182:VAL:HG22	2.01	0.42
1:H:66:PRO:HA	1:H:215:GLY:HA3	2.01	0.42
1:F:99:ARG:N	1:F:100:PRO:CD	2.82	0.42
1:A:99:ARG:N	1:A:100:PRO:CD	2.83	0.42
1:C:63:ILE:O	1:C:112:PHE:HA	2.20	0.42
1:C:99:ARG:N	1:C:100:PRO:CD	2.83	0.42
1:D:99:ARG:N	1:D:100:PRO:CD	2.83	0.42
1:G:56:ALA:HB2	1:G:110:ILE:CD1	2.49	0.42
1:A:66:PRO:HA	1:A:215:GLY:HA3	2.02	0.42
1:A:302:LEU:HD13	1:A:306:ILE:HD13	2.01	0.42
1:C:227:GLN:HA	1:G:285:LEU:CD1	2.50	0.42
1:E:273:ALA:HB1	1:E:274:PRO:HD2	2.02	0.42
1:G:273:ALA:HB1	1:G:274:PRO:HD2	2.01	0.42
1:C:93:MET:HA	1:C:94:PRO:HA	1.84	0.42
1:C:273:ALA:HB1	1:C:274:PRO:HD2	2.01	0.42
1:F:76:ARG:HA	1:F:163:GLN:O	2.20	0.42
1:A:305:HIS:O	1:A:312:HIS:HE1	2.02	0.42
1:B:63:ILE:O	1:B:112:PHE:HA	2.19	0.42
1:D:119:LEU:HD11	1:D:126:LYS:HG2	2.02	0.42
1:E:63:ILE:O	1:E:112:PHE:HA	2.20	0.42
1:G:136:ASP:OD1	1:G:138:SER:OG	2.35	0.42
1:B:66:PRO:HA	1:B:215:GLY:HA3	2.01	0.42
1:C:305:HIS:O	1:C:312:HIS:HE1	2.03	0.41
1:D:305:HIS:O	1:D:312:HIS:HE1	2.03	0.41
1:F:305:HIS:O	1:F:312:HIS:HE1	2.02	0.41
1:G:66:PRO:HA	1:G:215:GLY:HA3	2.02	0.41
1:G:76:ARG:HA	1:G:163:GLN:O	2.20	0.41
1:H:305:HIS:O	1:H:312:HIS:HE1	2.03	0.41
1:B:142:VAL:HG21	1:B:182:VAL:HG22	2.02	0.41
1:D:63:ILE:O	1:D:112:PHE:HA	2.20	0.41
1:H:99:ARG:N	1:H:100:PRO:CD	2.83	0.41
1:E:76:ARG:HA	1:E:163:GLN:O	2.19	0.41
1:E:215:GLY:CA	1:E:254:ALA:O	2.69	0.41
1:F:157:GLU:H	1:F:163:GLN:NE2	2.16	0.41
1:F:202:ARG:HA	1:F:202:ARG:HD3	1.96	0.41
1:G:63:ILE:O	1:G:112:PHE:HA	2.19	0.41
1:H:273:ALA:HB1	1:H:274:PRO:HD2	2.02	0.41
1:B:215:GLY:HA2	1:B:254:ALA:O	2.19	0.41
1:G:99:ARG:N	1:G:100:PRO:CD	2.84	0.41
1:H:201:TRP:CD2	1:H:243:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HA	1:A:163:GLN:O	2.21	0.41
1:D:250:TRP:CE3	1:D:273:ALA:HA	2.55	0.41
1:C:302:LEU:HD13	1:C:306:ILE:HD13	2.03	0.41
1:G:40:THR:H	1:G:43:GLN:HE21	1.68	0.41
1:H:76:ARG:HA	1:H:163:GLN:O	2.20	0.41
1:H:197:TRP:HA	1:H:198:PRO:HD2	1.96	0.41
1:B:250:TRP:CE3	1:B:273:ALA:HA	2.56	0.41
1:D:66:PRO:HA	1:D:215:GLY:HA3	2.01	0.41
1:D:76:ARG:HA	1:D:163:GLN:O	2.21	0.41
1:G:305:HIS:O	1:G:312:HIS:HE1	2.04	0.41
1:D:142:VAL:HG21	1:D:182:VAL:HG22	2.03	0.41
1:E:250:TRP:CE3	1:E:273:ALA:HA	2.56	0.41
1:F:215:GLY:CA	1:F:254:ALA:O	2.69	0.41
1:E:215:GLY:HA2	1:E:254:ALA:O	2.19	0.41
1:E:305:HIS:O	1:E:312:HIS:HE1	2.03	0.41
1:B:232:THR:HG22	1:B:266:LEU:HD22	2.03	0.41
1:C:250:TRP:CE3	1:C:273:ALA:HA	2.56	0.41
1:E:142:VAL:HG21	1:E:182:VAL:HG22	2.02	0.41
1:B:99:ARG:N	1:B:100:PRO:CD	2.83	0.40
1:G:215:GLY:CA	1:G:254:ALA:O	2.69	0.40
1:H:250:TRP:CE3	1:H:273:ALA:HA	2.56	0.40
1:E:99:ARG:N	1:E:100:PRO:CD	2.84	0.40
1:H:157:GLU:H	1:H:163:GLN:NE2	2.15	0.40
1:A:215:GLY:CA	1:A:254:ALA:O	2.69	0.40
1:G:250:TRP:CE3	1:G:273:ALA:HA	2.57	0.40
1:H:24:GLN:HE22	1:H:295:ASP:CG	2.29	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	296/304 (97%)	282 (95%)	13 (4%)	1 (0%)	36	53
1	B	296/304 (97%)	282 (95%)	13 (4%)	1 (0%)	36	53
1	C	301/304 (99%)	288 (96%)	12 (4%)	1 (0%)	36	53
1	D	301/304 (99%)	289 (96%)	11 (4%)	1 (0%)	36	53
1	E	294/304 (97%)	282 (96%)	11 (4%)	1 (0%)	36	53
1	F	295/304 (97%)	283 (96%)	11 (4%)	1 (0%)	36	53
1	G	296/304 (97%)	284 (96%)	11 (4%)	1 (0%)	36	53
1	H	296/304 (97%)	283 (96%)	12 (4%)	1 (0%)	36	53
All	All	2375/2432 (98%)	2273 (96%)	94 (4%)	8 (0%)	36	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	192	ALA
1	B	192	ALA
1	C	192	ALA
1	D	192	ALA
1	F	192	ALA
1	G	192	ALA
1	H	192	ALA
1	A	192	ALA

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	249/251 (99%)	245 (98%)	4 (2%)	55	78
1	B	249/251 (99%)	245 (98%)	4 (2%)	55	78
1	C	250/251 (100%)	244 (98%)	6 (2%)	43	69
1	D	250/251 (100%)	244 (98%)	6 (2%)	43	69
1	E	247/251 (98%)	243 (98%)	4 (2%)	55	78
1	F	248/251 (99%)	242 (98%)	6 (2%)	43	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	249/251 (99%)	244 (98%)	5 (2%)	48 73
1	H	249/251 (99%)	243 (98%)	6 (2%)	43 69
All	All	1991/2008 (99%)	1950 (98%)	41 (2%)	47 72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	154	LYS
1	A	257	VAL
1	A	324	LEU
1	B	99	ARG
1	B	154	LYS
1	B	257	VAL
1	B	306	ILE
1	C	52	LEU
1	C	120	VAL
1	C	154	LYS
1	C	257	VAL
1	C	306	ILE
1	C	323	GLU
1	D	24	GLN
1	D	52	LEU
1	D	120	VAL
1	D	154	LYS
1	D	257	VAL
1	D	324	LEU
1	E	52	LEU
1	E	119	LEU
1	E	154	LYS
1	E	257	VAL
1	F	52	LEU
1	F	82	GLU
1	F	154	LYS
1	F	257	VAL
1	F	297	ASP
1	F	306	ILE
1	G	37	ARG
1	G	52	LEU
1	G	120	VAL
1	G	154	LYS

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Mol	Chain	Res	Type
1	G	257	VAL
1	H	52	LEU
1	H	154	LYS
1	H	257	VAL
1	H	300	ARG
1	H	323	GLU
1	H	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	163	GLN
1	A	246	GLN
1	A	312	HIS
1	B	43	GLN
1	B	163	GLN
1	B	230	HIS
1	B	312	HIS
1	B	314	GLN
1	C	24	GLN
1	C	43	GLN
1	C	163	GLN
1	C	241	GLN
1	C	312	HIS
1	C	314	GLN
1	D	43	GLN
1	D	163	GLN
1	D	246	GLN
1	D	312	HIS
1	D	314	GLN
1	E	43	GLN
1	E	241	GLN
1	E	246	GLN
1	E	312	HIS
1	E	314	GLN
1	F	43	GLN
1	F	163	GLN
1	F	230	HIS
1	F	246	GLN
1	F	312	HIS
1	F	314	GLN

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Mol	Chain	Res	Type
1	G	43	GLN
1	G	163	GLN
1	G	230	HIS
1	G	246	GLN
1	G	312	HIS
1	G	314	GLN
1	H	43	GLN
1	H	163	GLN
1	H	246	GLN
1	H	312	HIS
1	H	314	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	M9L	A	401	-	15,15,15	1.77	3 (20%)	19,20,20	2.33	8 (42%)
2	M9L	D	401	-	15,15,15	1.15	1 (6%)	19,20,20	1.38	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	M9L	C	401	-	15,15,15	0.83	0	19,20,20	1.62	5 (26%)
2	M9L	B	401	-	15,15,15	1.11	1 (6%)	19,20,20	1.51	3 (15%)
2	M9L	E	401	-	15,15,15	1.79	2 (13%)	19,20,20	1.22	2 (10%)
2	M9L	H	401	-	15,15,15	1.35	2 (13%)	19,20,20	1.66	4 (21%)
2	M9L	F	401	-	15,15,15	1.94	4 (26%)	19,20,20	2.06	6 (31%)
2	M9L	G	401	-	15,15,15	1.62	2 (13%)	19,20,20	1.58	4 (21%)

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	M9L	A	401	-	-	2/12/12/12	0/1/1/1
2	M9L	D	401	-	-	2/12/12/12	0/1/1/1
2	M9L	C	401	-	-	2/12/12/12	0/1/1/1
2	M9L	B	401	-	-	2/12/12/12	0/1/1/1
2	M9L	E	401	-	-	2/12/12/12	0/1/1/1
2	M9L	H	401	-	-	2/12/12/12	0/1/1/1
2	M9L	F	401	-	-	2/12/12/12	0/1/1/1
2	M9L	G	401	-	-	2/12/12/12	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	M9L	O13-C12	5.69	1.38	1.22
2	G	401	M9L	O13-C12	4.55	1.35	1.22
2	F	401	M9L	O14-C12	-4.34	1.16	1.30
2	A	401	M9L	O13-C12	3.97	1.33	1.22
2	A	401	M9L	O14-C12	-3.59	1.19	1.30
2	F	401	M9L	O1-C2	-3.39	1.19	1.24
2	H	401	M9L	C11-C5	3.22	1.44	1.39
2	F	401	M9L	C4-C12	-2.97	1.49	1.53
2	D	401	M9L	C4-C12	-2.91	1.49	1.53
2	F	401	M9L	O13-C12	2.66	1.30	1.22
2	G	401	M9L	O14-C12	-2.55	1.22	1.30
2	A	401	M9L	O1-C2	2.29	1.28	1.24
2	E	401	M9L	O14-C12	-2.15	1.23	1.30
2	H	401	M9L	C4-N3	2.14	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	M9L	C4-C12	-2.08	1.50	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	M9L	C5-C4-C12	4.91	118.83	109.44
2	F	401	M9L	O14-C12-C4	4.86	125.71	113.62
2	F	401	M9L	O1-C2-N15	-4.14	114.84	123.18
2	A	401	M9L	C11-C5-C4	3.92	127.07	120.78
2	G	401	M9L	O1-C2-N15	-3.78	115.57	123.18
2	H	401	M9L	O1-C2-N15	-3.77	115.58	123.18
2	D	401	M9L	O1-C2-N15	-3.71	115.72	123.18
2	F	401	M9L	O14-C12-O13	-3.71	115.67	124.08
2	B	401	M9L	O14-C12-C4	3.68	122.78	113.62
2	H	401	M9L	N15-C2-N3	3.64	124.77	116.77
2	D	401	M9L	C10-C11-C5	-3.31	117.88	121.18
2	G	401	M9L	O14-C12-C4	3.11	121.35	113.62
2	A	401	M9L	O14-C12-O13	-3.00	117.27	124.08
2	B	401	M9L	N15-C2-N3	3.00	123.35	116.77
2	A	401	M9L	C6-C5-C4	-2.96	116.03	120.78
2	A	401	M9L	C7-C6-C5	2.92	124.10	121.18
2	A	401	M9L	C5-C4-N3	-2.85	105.56	112.75
2	C	401	M9L	C11-C5-C6	2.83	121.81	118.30
2	H	401	M9L	O14-C12-C4	2.83	120.65	113.62
2	C	401	M9L	C10-C11-C5	-2.71	118.48	121.18
2	B	401	M9L	O14-C12-O13	-2.70	117.96	124.08
2	A	401	M9L	N15-C2-N3	-2.69	110.85	116.77
2	H	401	M9L	O14-C12-O13	-2.69	117.98	124.08
2	E	401	M9L	O14-C12-C4	2.66	120.23	113.62
2	C	401	M9L	C7-C6-C5	-2.57	118.61	121.18
2	F	401	M9L	C7-C6-C5	-2.56	118.63	121.18
2	G	401	M9L	C5-C4-N3	-2.39	106.72	112.75
2	E	401	M9L	O1-C2-N15	-2.34	118.47	123.18
2	C	401	M9L	O14-C12-O13	-2.32	118.82	124.08
2	A	401	M9L	O14-C12-C4	2.30	119.33	113.62
2	F	401	M9L	N15-C2-N3	2.25	121.70	116.77
2	C	401	M9L	O1-C2-N15	-2.24	118.67	123.18
2	F	401	M9L	C11-C10-C8	-2.21	117.54	119.88
2	G	401	M9L	O14-C12-O13	-2.01	119.53	124.08

There are no chirality outliers.

All (16) torsion outliers are listed below:

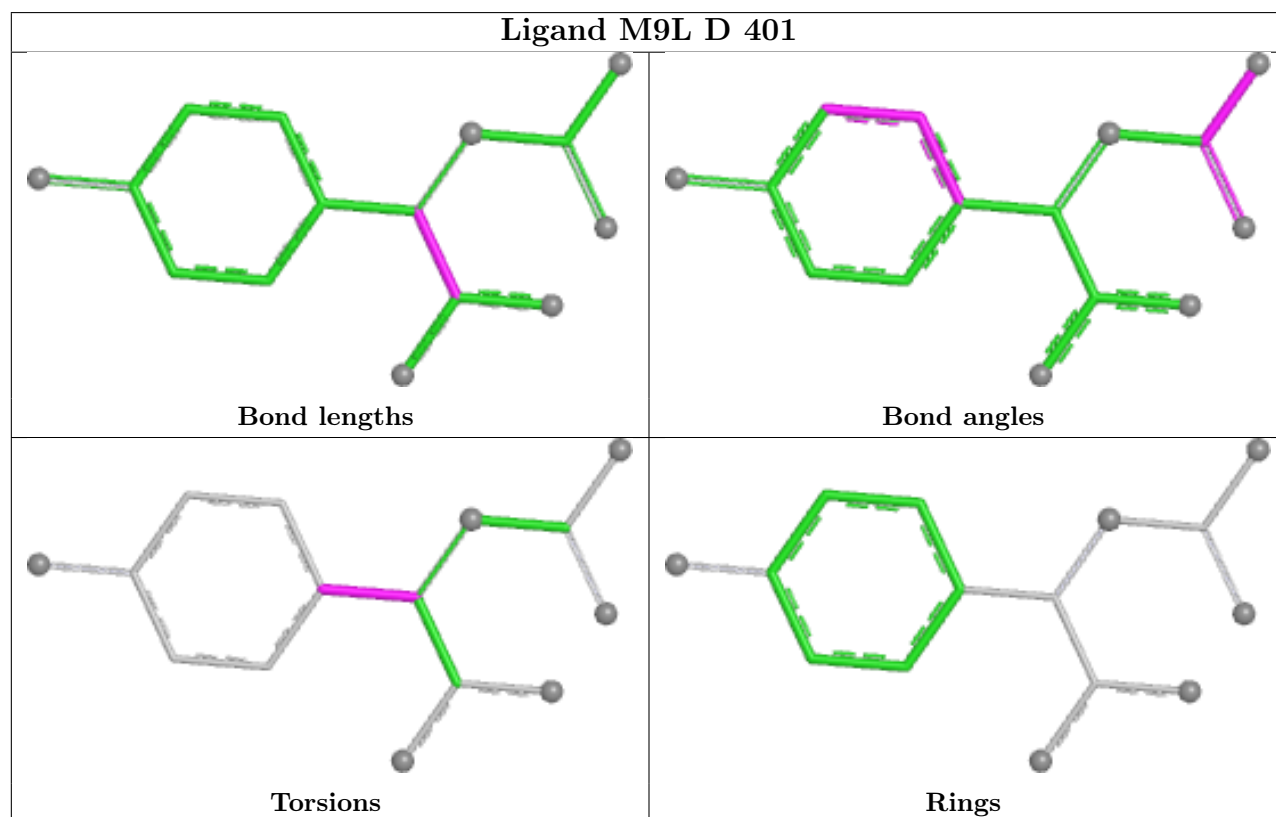
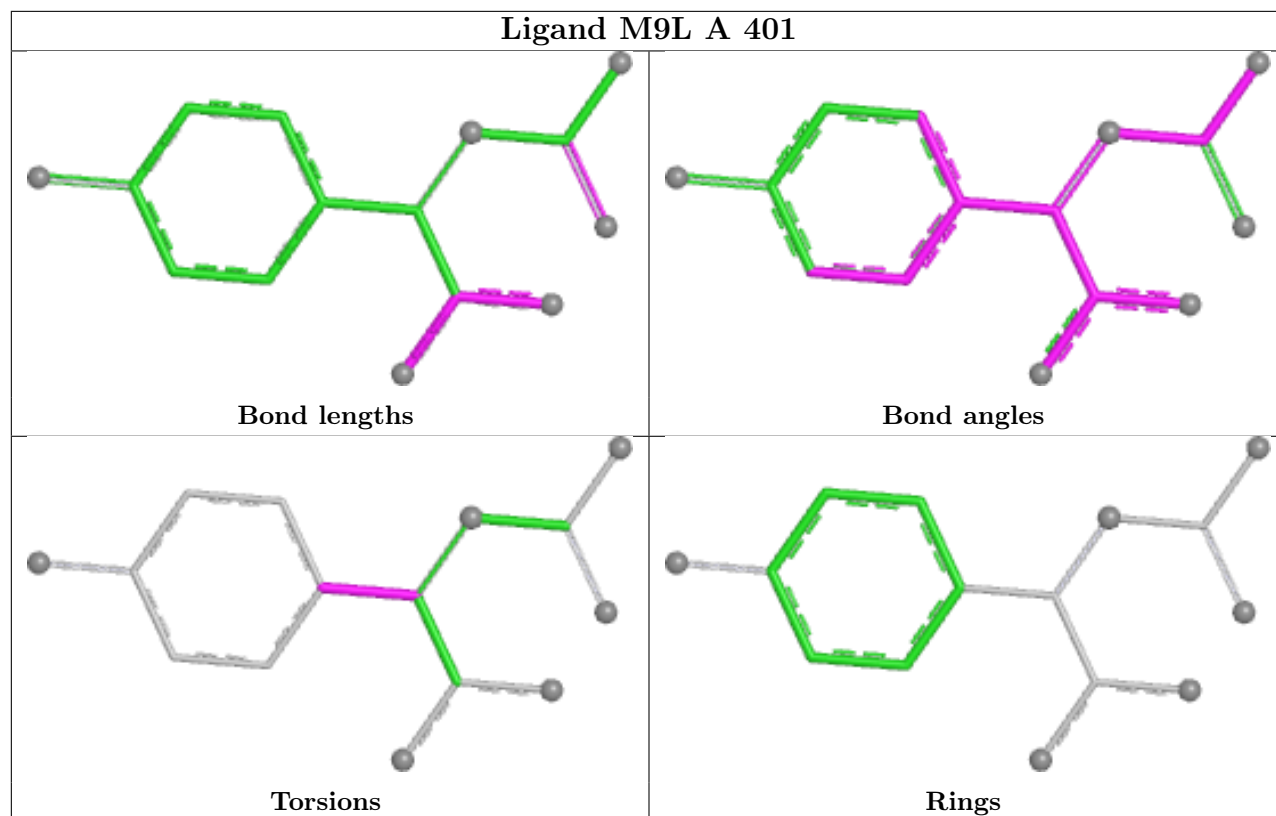
Mol	Chain	Res	Type	Atoms
2	A	401	M9L	C12-C4-C5-C6
2	H	401	M9L	C12-C4-C5-C6
2	A	401	M9L	C12-C4-C5-C11
2	B	401	M9L	C12-C4-C5-C6
2	B	401	M9L	C12-C4-C5-C11
2	D	401	M9L	C12-C4-C5-C6
2	D	401	M9L	C12-C4-C5-C11
2	H	401	M9L	C12-C4-C5-C11
2	E	401	M9L	C12-C4-C5-C11
2	F	401	M9L	C12-C4-C5-C6
2	E	401	M9L	C12-C4-C5-C6
2	C	401	M9L	C12-C4-C5-C11
2	G	401	M9L	C12-C4-C5-C11
2	F	401	M9L	C12-C4-C5-C11
2	C	401	M9L	C12-C4-C5-C6
2	G	401	M9L	C12-C4-C5-C6

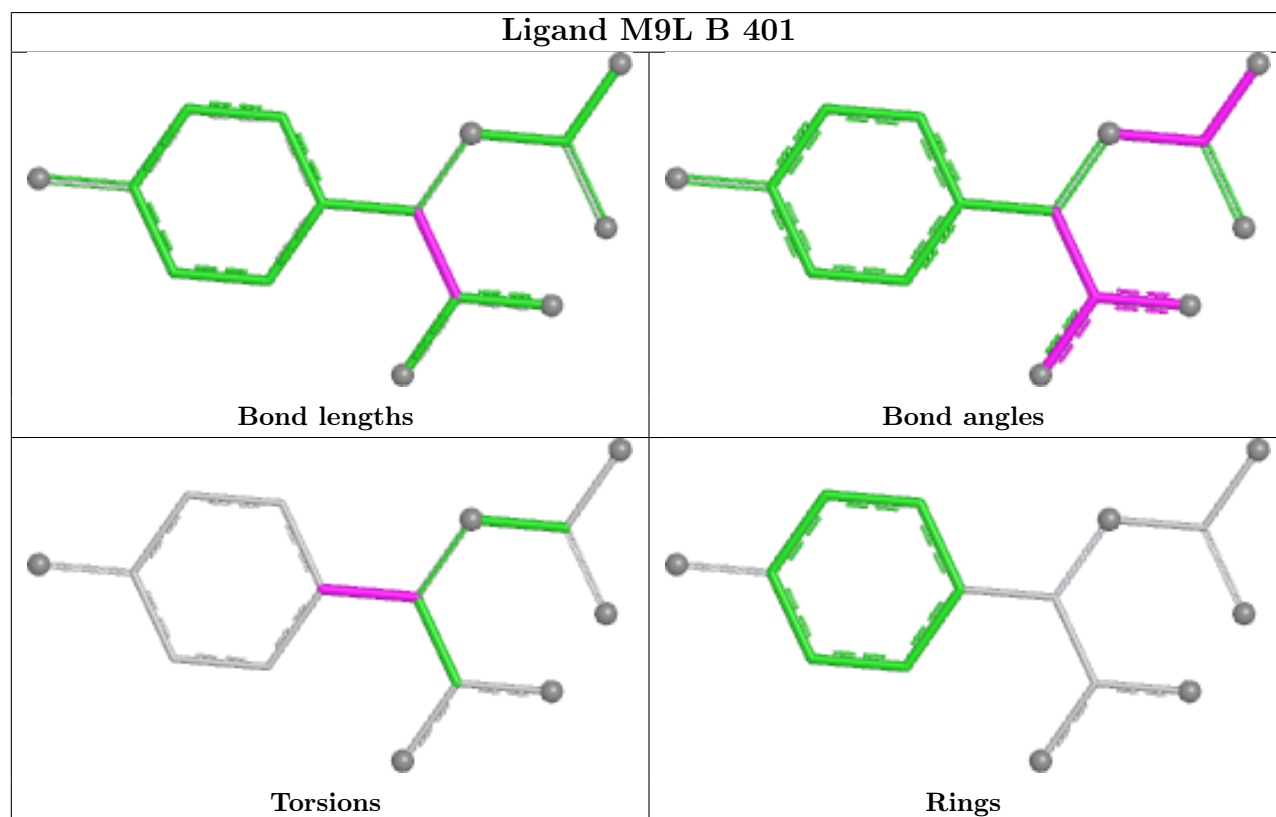
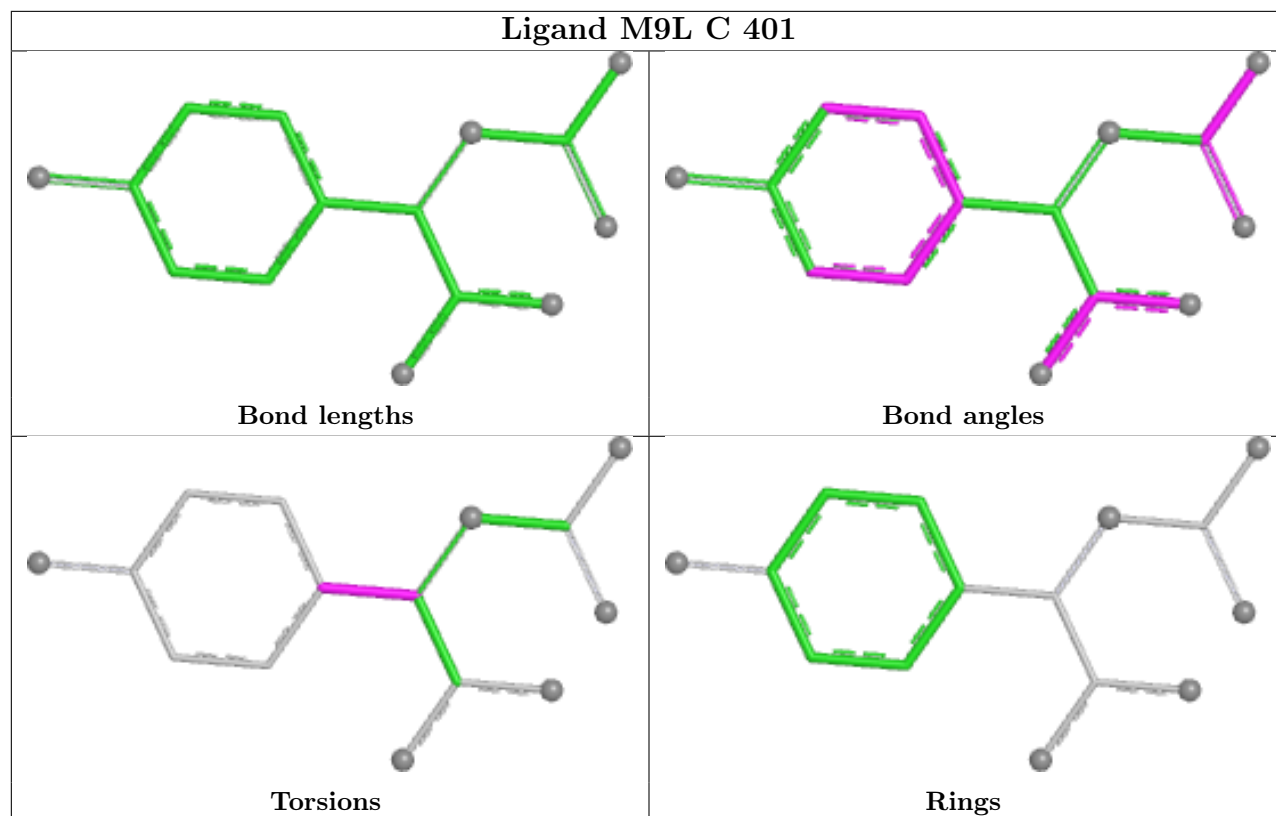
There are no ring outliers.

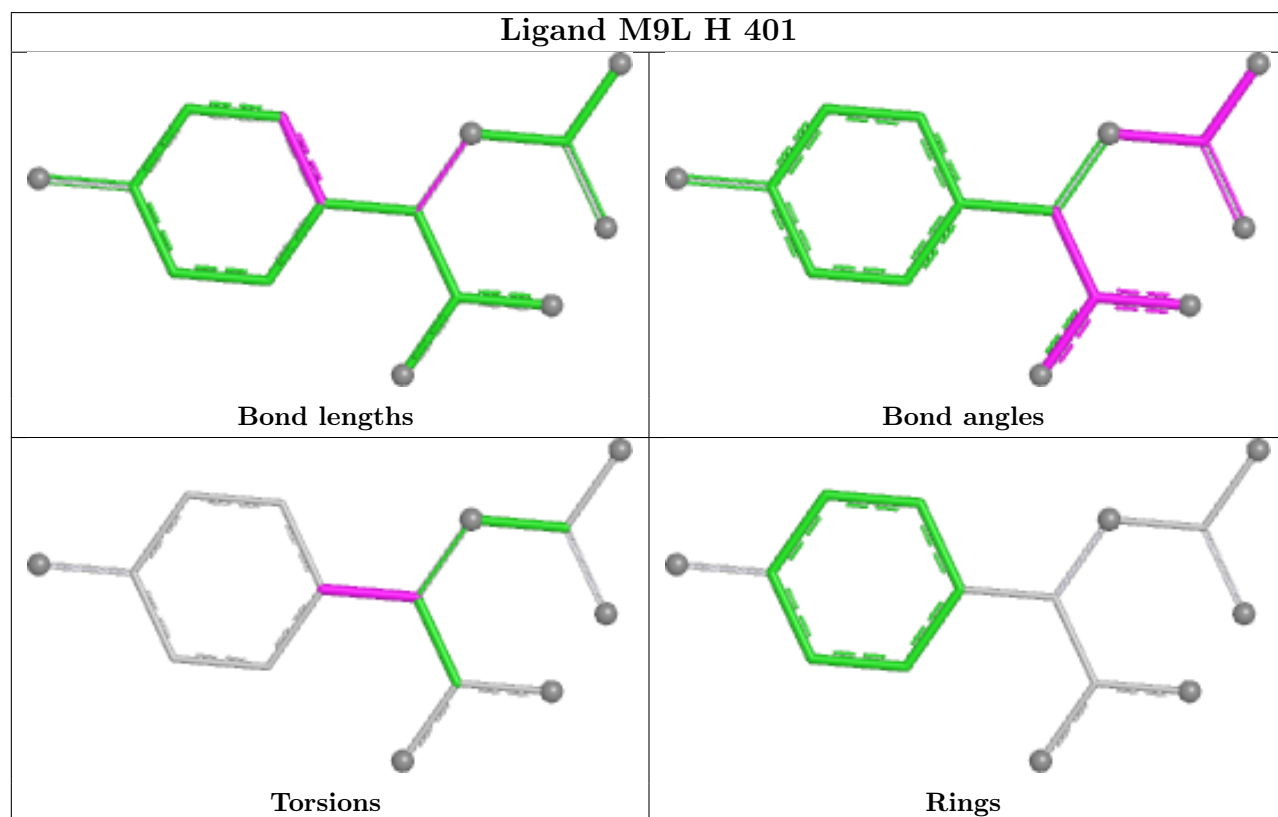
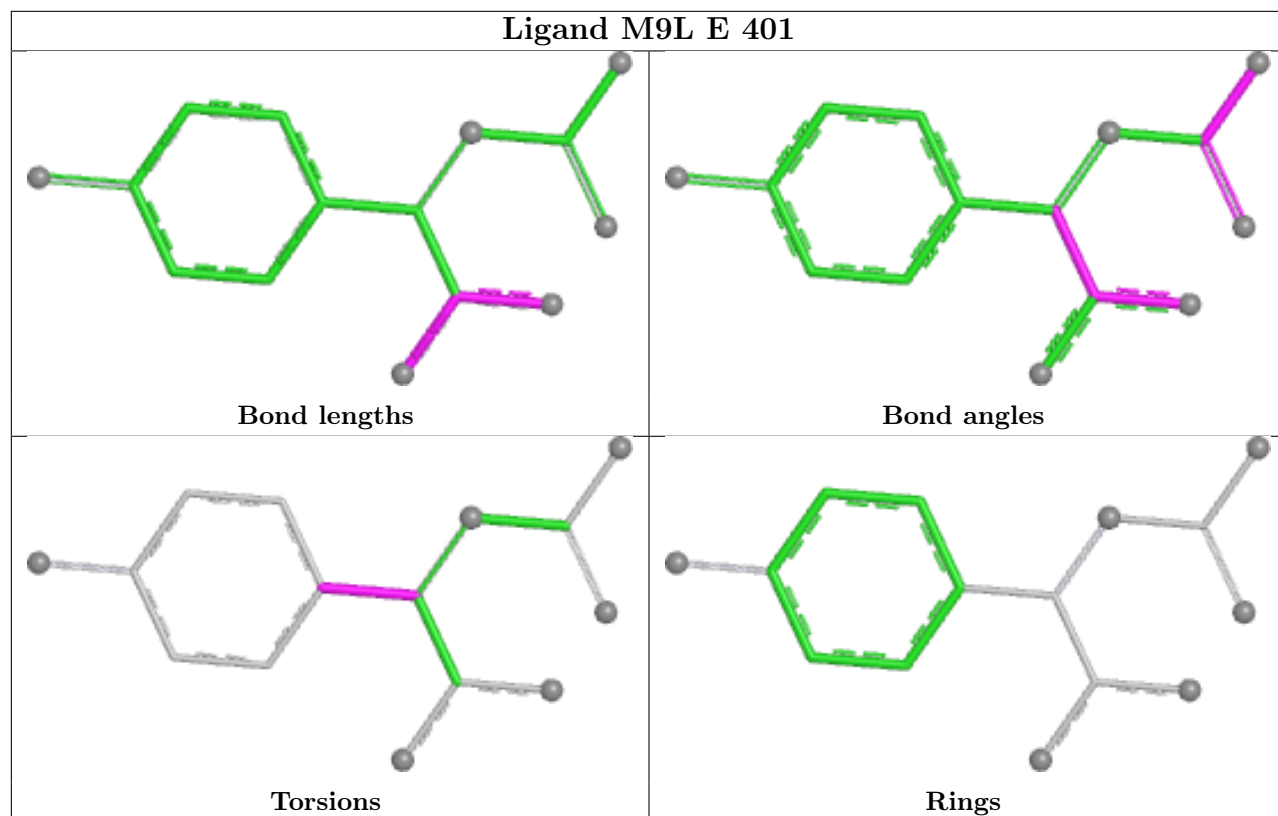
2 monomers are involved in 2 short contacts:

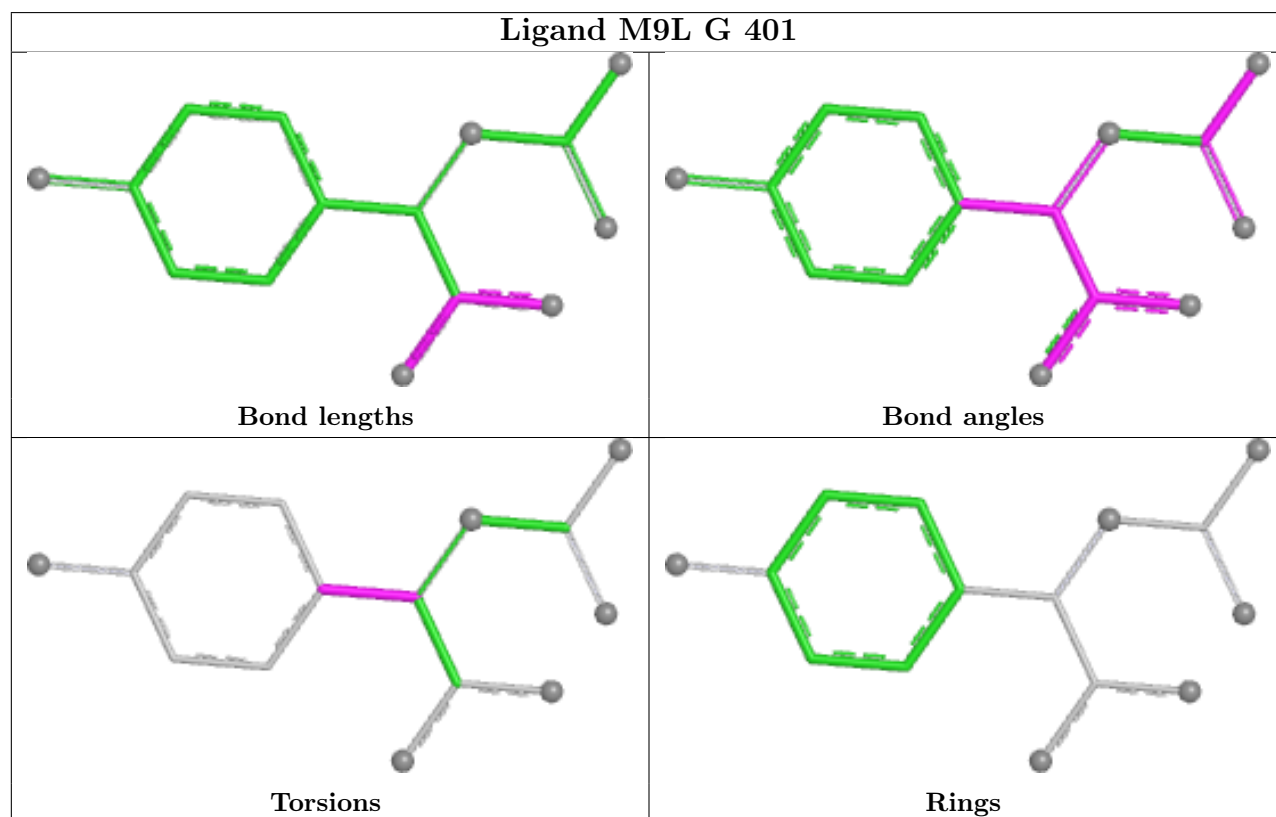
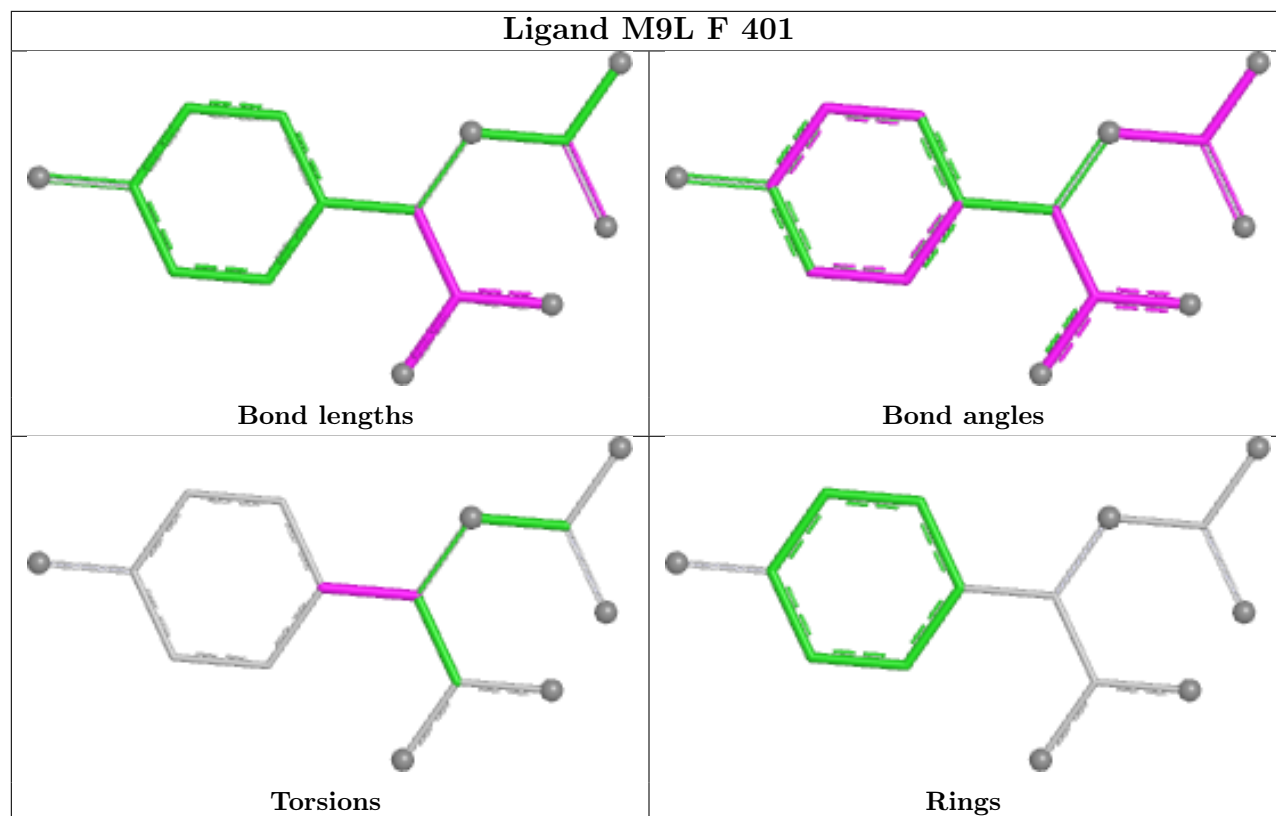
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	M9L	1	0
2	B	401	M9L	1	0

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 ⓘ

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	300/304 (98%)	0.15	3 (1%) 79 77	11, 23, 40, 57	0
1	B	300/304 (98%)	0.07	5 (1%) 69 66	10, 21, 37, 75	0
1	C	303/304 (99%)	0.04	4 (1%) 75 72	9, 19, 34, 79	0
1	D	303/304 (99%)	0.09	2 (0%) 84 82	9, 21, 39, 58	0
1	E	298/304 (98%)	0.17	6 (2%) 65 62	12, 21, 42, 83	0
1	F	299/304 (98%)	0.14	2 (0%) 84 82	12, 22, 39, 76	0
1	G	300/304 (98%)	0.08	6 (2%) 65 62	9, 20, 39, 66	0
1	H	300/304 (98%)	0.41	10 (3%) 49 46	14, 29, 53, 78	0
All	All	2403/2432 (98%)	0.14	38 (1%) 70 68	9, 22, 43, 83	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	126	LYS	4.1
1	E	120	VAL	3.9
1	B	121	VAL	3.8
1	B	122	GLU	3.6
1	G	83	ALA	3.3
1	C	162	PHE	3.1
1	G	22	THR	3.0
1	F	122	GLU	3.0
1	G	324	LEU	2.9
1	C	22	THR	2.8
1	G	126	LYS	2.8
1	A	324	LEU	2.8
1	H	22	THR	2.7
1	D	22	THR	2.7
1	E	22	THR	2.7
1	C	125	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	22	THR	2.5
1	H	97	VAL	2.4
1	H	121	VAL	2.4
1	G	139	GLY	2.4
1	H	162	PHE	2.3
1	B	22	THR	2.3
1	H	184	ALA	2.3
1	G	122	GLU	2.3
1	E	82	GLU	2.2
1	C	184	ALA	2.2
1	E	324	LEU	2.2
1	H	105	ALA	2.1
1	E	162	PHE	2.1
1	F	121	VAL	2.1
1	H	83	ALA	2.1
1	D	52	LEU	2.1
1	B	120	VAL	2.0
1	B	184	ALA	2.0
1	H	324	LEU	2.0
1	H	309	PHE	2.0
1	A	243	GLY	2.0
1	H	137	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 [i](#)

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

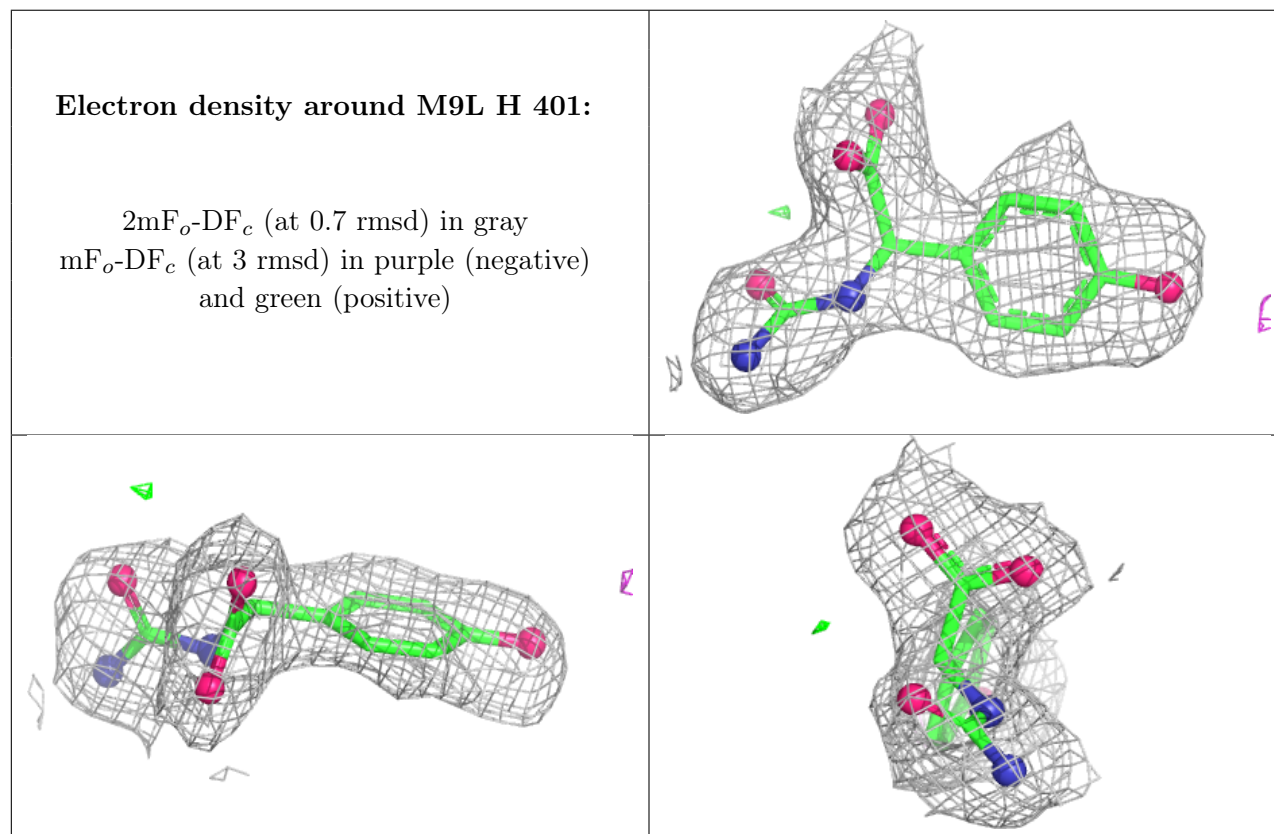
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	M9L	H	401	15/15	0.92	0.09	17,19,20,23	0

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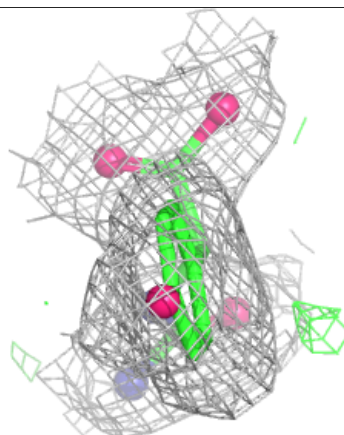
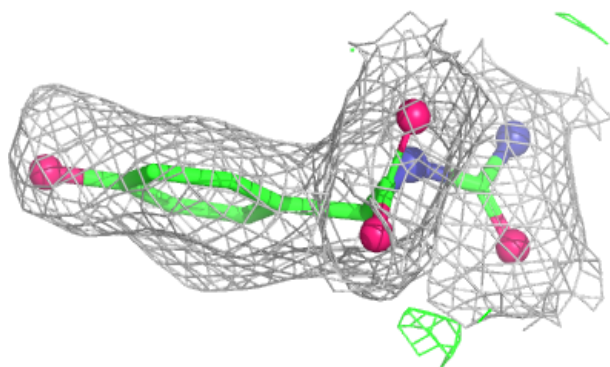
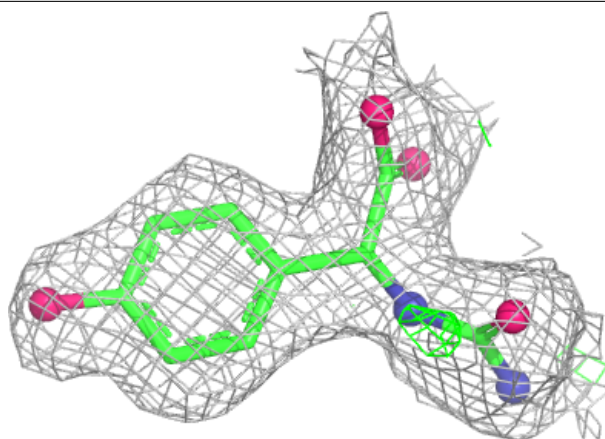
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	M9L	E	401	15/15	0.94	0.07	13,16,17,18	0
2	M9L	F	401	15/15	0.94	0.08	10,11,12,12	0
2	M9L	A	401	15/15	0.94	0.08	8,9,10,10	0
2	M9L	B	401	15/15	0.95	0.07	12,14,16,17	0
2	M9L	G	401	15/15	0.96	0.07	18,20,23,24	0
2	M9L	D	401	15/15	0.96	0.07	14,16,19,19	0
2	M9L	C	401	15/15	0.97	0.06	13,15,17,18	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.

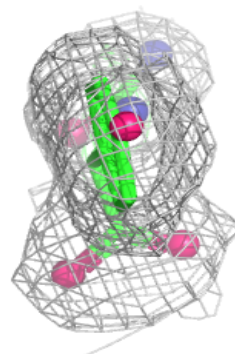
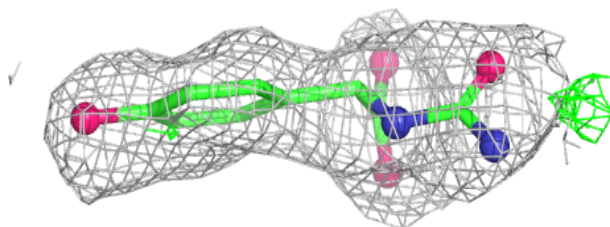
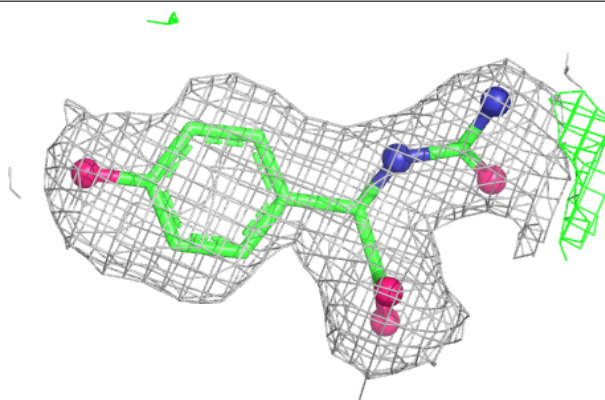


Electron density around M9L E 401:

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

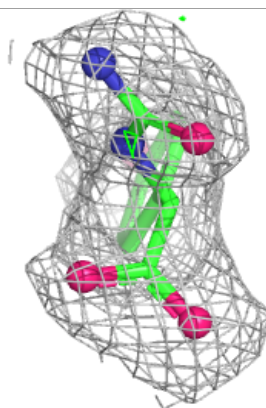
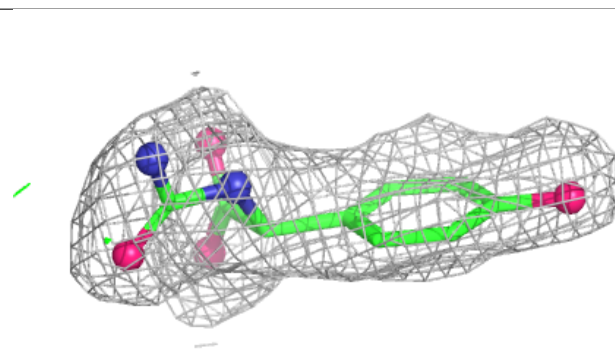
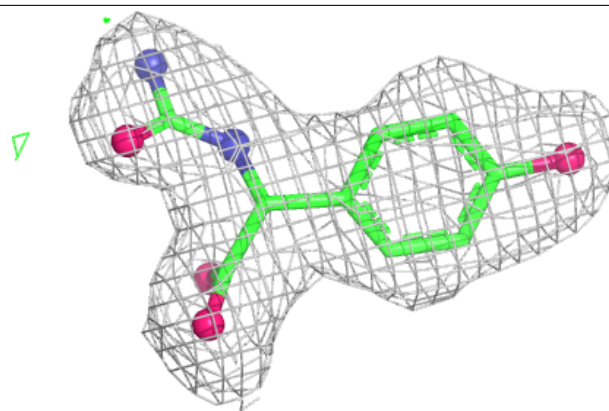
**Electron density around M9L F 401:**

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



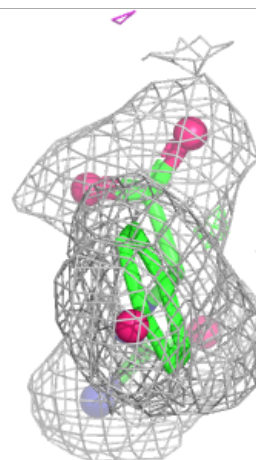
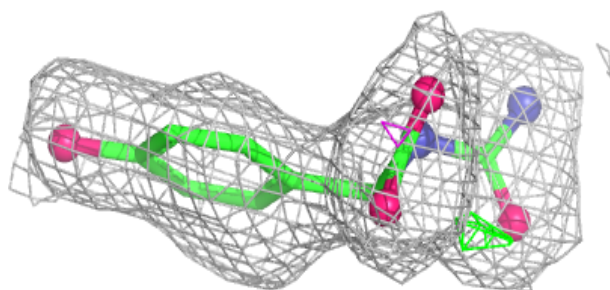
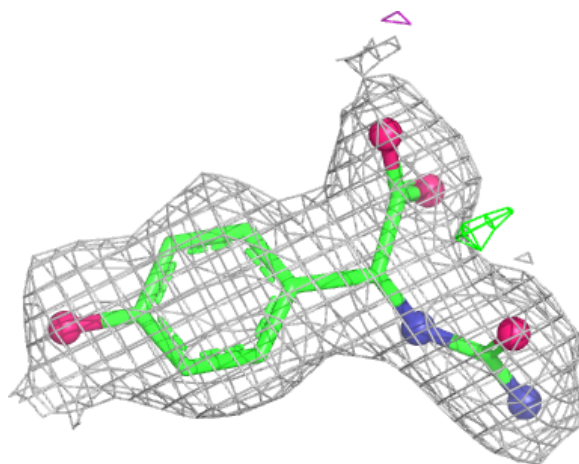
Electron density around M9L A 401:

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



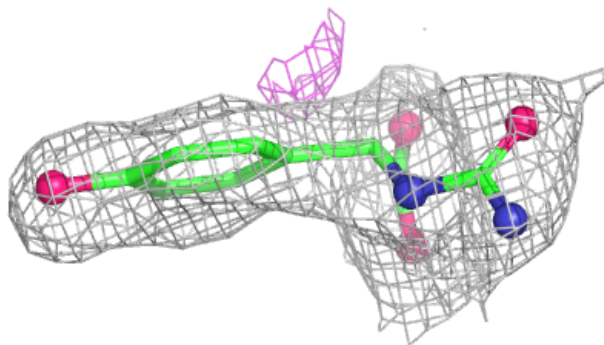
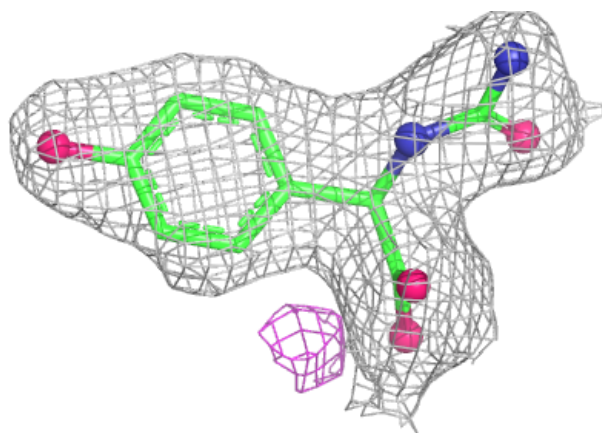
Electron density around M9L B 401:

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

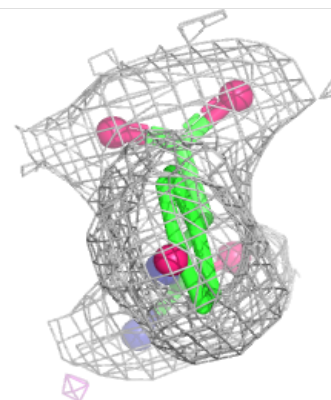
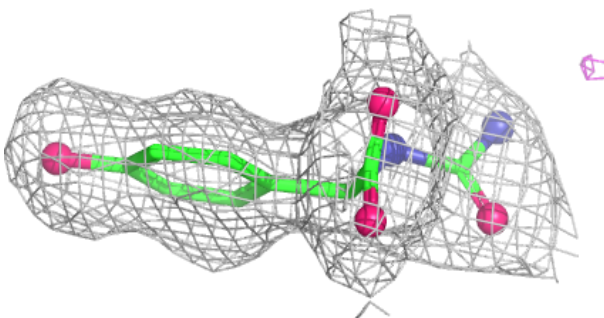
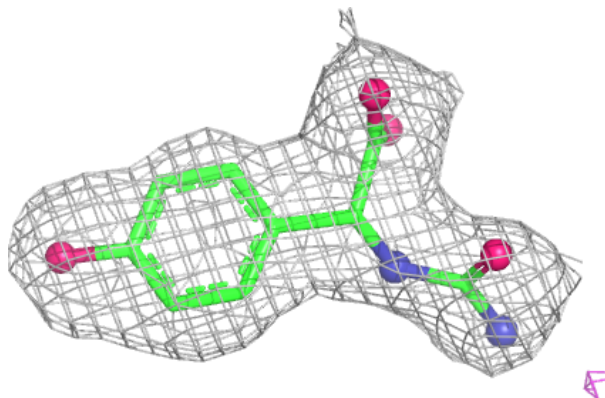


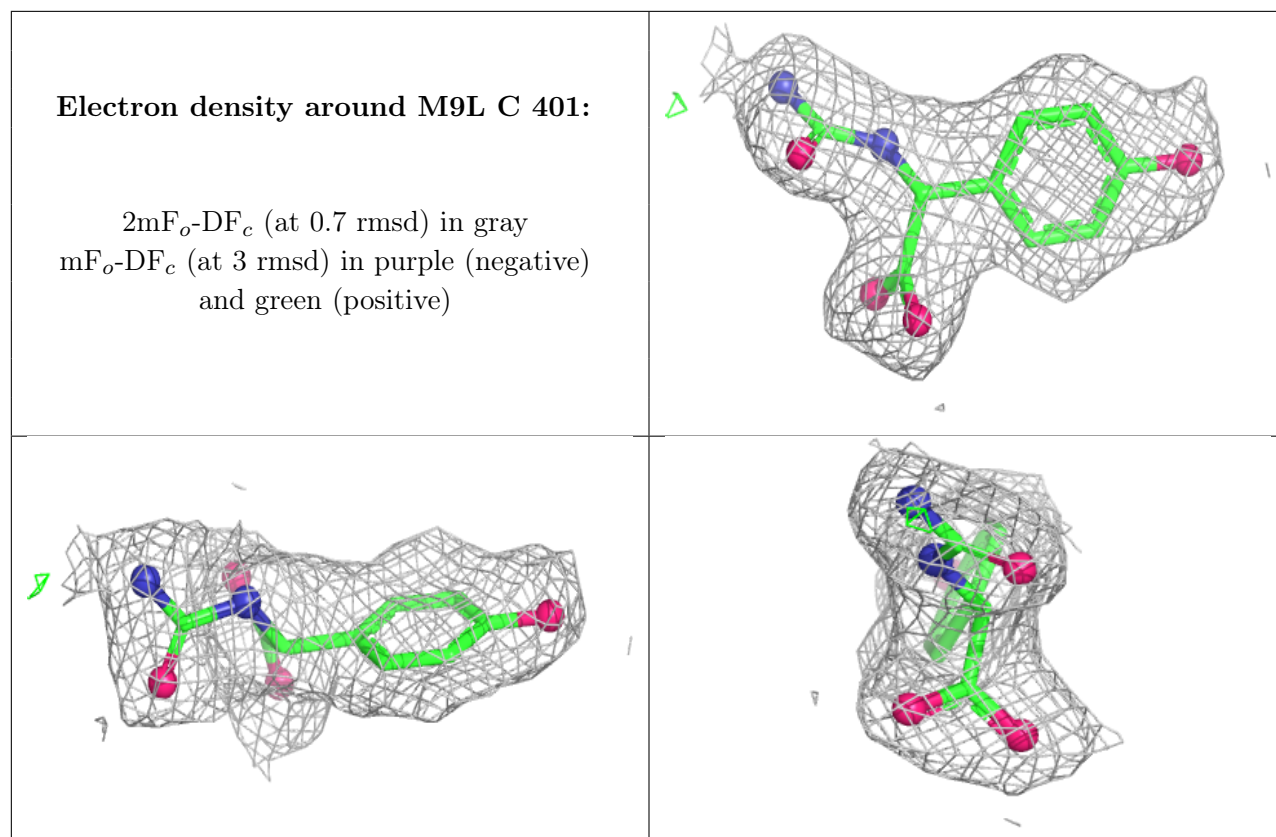
Electron density around M9L G 401:

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

**Electron density around M9L 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.