



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 03:05 AM EST

PDB ID : 4LRH
Title : Crystal structure of human folate receptor alpha in complex with folic acid
Authors : Ke, J.; Chen, C.; Zhou, X.E.; Yi, W.; Brunzelle, J.S.; Li, J.; Young, E.-L.; Xu, H.E.; Melcher, K.
Deposited on : 2013-07-19
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

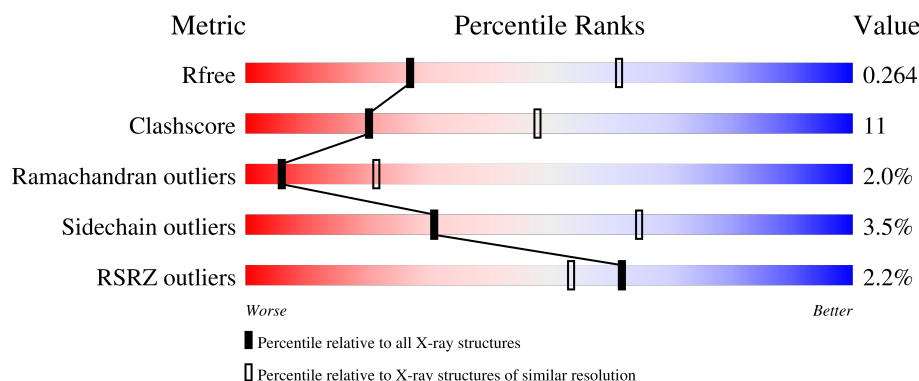
1 Overall quality at a glance

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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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	218	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 72%, green 22%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 72% 22% • 5% </div> </div>
1	B	218	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 69%, green 23%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 69% 23% • 6% </div> </div>
1	C	218	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 67%, green 28%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 67% 28% • • </div> </div>
1	D	218	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 68%, green 26%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 68% 26% • • </div> </div>
1	E	218	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 70%, green 23%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 70% 23% • 6% </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	218	<div><div><div></div><div></div><div></div></div><div>3%65%28%• 5%</div></div>
1	G	218	<div><div><div></div><div></div><div></div></div><div>2%68%23%• 6%</div></div>
1	H	218	<div><div><div></div><div></div><div></div></div><div>%69%22%• 6%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14328 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 Folate receptor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1697	1064	307	306	20			
1	B	204	Total	C	N	O	S	0	0	0
			1675	1052	301	302	20			
1	C	209	Total	C	N	O	S	0	0	0
			1712	1075	309	308	20			
1	D	210	Total	C	N	O	S	0	0	0
			1722	1083	311	308	20			
1	E	206	Total	C	N	O	S	0	0	0
			1691	1061	306	304	20			
1	F	208	Total	C	N	O	S	0	0	0
			1705	1070	308	307	20			
1	G	205	Total	C	N	O	S	0	0	0
			1686	1058	305	303	20			
1	H	204	Total	C	N	O	S	0	0	0
			1680	1055	304	301	20			

There are 40 discrepancies between the modelled and reference sequences:

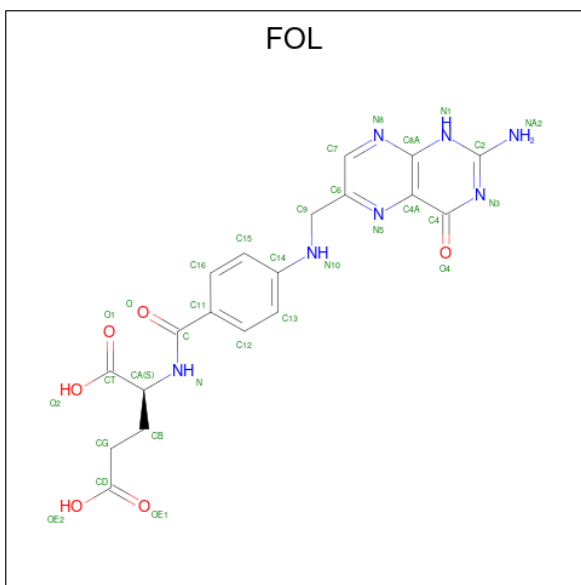
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	THR	-	expression tag	UNP P15328
A	215	LEU	-	expression tag	UNP P15328
A	216	VAL	-	expression tag	UNP P15328
A	217	PRO	-	expression tag	UNP P15328
A	218	ARG	-	expression tag	UNP P15328
B	214	THR	-	expression tag	UNP P15328
B	215	LEU	-	expression tag	UNP P15328
B	216	VAL	-	expression tag	UNP P15328
B	217	PRO	-	expression tag	UNP P15328
B	218	ARG	-	expression tag	UNP P15328
C	214	THR	-	expression tag	UNP P15328
C	215	LEU	-	expression tag	UNP P15328
C	216	VAL	-	expression tag	UNP P15328

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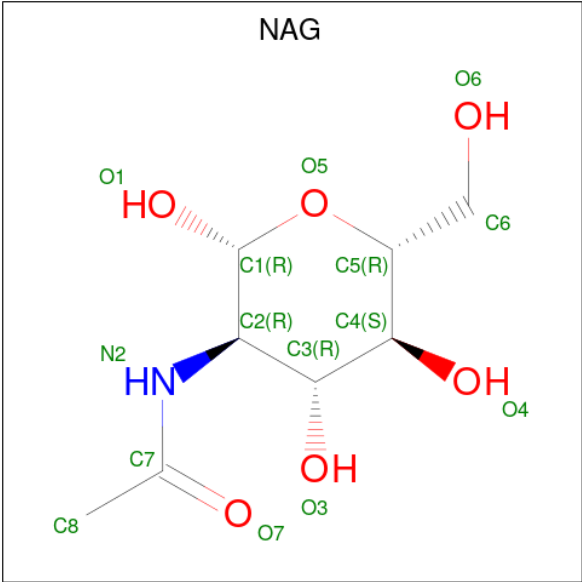
Chain	Residue	Modelled	Actual	Comment	Reference
C	217	PRO	-	expression tag	UNP P15328
C	218	ARG	-	expression tag	UNP P15328
D	214	THR	-	expression tag	UNP P15328
D	215	LEU	-	expression tag	UNP P15328
D	216	VAL	-	expression tag	UNP P15328
D	217	PRO	-	expression tag	UNP P15328
D	218	ARG	-	expression tag	UNP P15328
E	214	THR	-	expression tag	UNP P15328
E	215	LEU	-	expression tag	UNP P15328
E	216	VAL	-	expression tag	UNP P15328
E	217	PRO	-	expression tag	UNP P15328
E	218	ARG	-	expression tag	UNP P15328
F	214	THR	-	expression tag	UNP P15328
F	215	LEU	-	expression tag	UNP P15328
F	216	VAL	-	expression tag	UNP P15328
F	217	PRO	-	expression tag	UNP P15328
F	218	ARG	-	expression tag	UNP P15328
G	214	THR	-	expression tag	UNP P15328
G	215	LEU	-	expression tag	UNP P15328
G	216	VAL	-	expression tag	UNP P15328
G	217	PRO	-	expression tag	UNP P15328
G	218	ARG	-	expression tag	UNP P15328
H	214	THR	-	expression tag	UNP P15328
H	215	LEU	-	expression tag	UNP P15328
H	216	VAL	-	expression tag	UNP P15328
H	217	PRO	-	expression tag	UNP P15328
H	218	ARG	-	expression tag	UNP P15328

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 32	C 19	N 7	O 6	0	0
2	B	1	Total 32	C 19	N 7	O 6	0	0
2	C	1	Total 32	C 19	N 7	O 6	0	0
2	D	1	Total 32	C 19	N 7	O 6	0	0
2	E	1	Total 32	C 19	N 7	O 6	0	0
2	F	1	Total 32	C 19	N 7	O 6	0	0
2	G	1	Total 32	C 19	N 7	O 6	0	0
2	H	1	Total 32	C 19	N 7	O 6	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

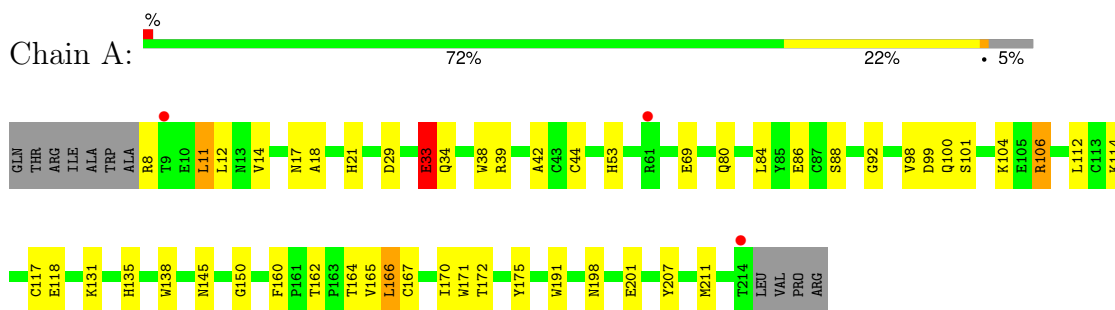
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	22	Total	O	0	0
			22	22		
4	C	21	Total	O	0	0
			21	21		
4	D	19	Total	O	0	0
			19	19		
4	E	21	Total	O	0	0
			21	21		
4	F	13	Total	O	0	0
			13	13		
4	G	20	Total	O	0	0
			20	20		
4	H	34	Total	O	0	0
			34	34		

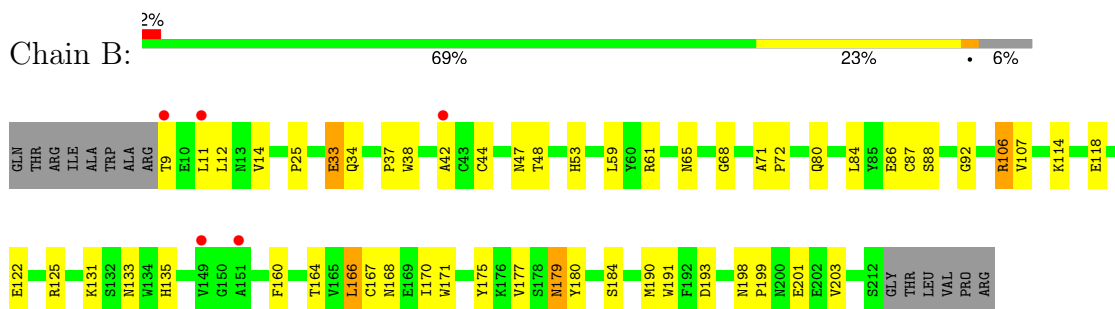
3 Residue-property plots [i](#)

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.

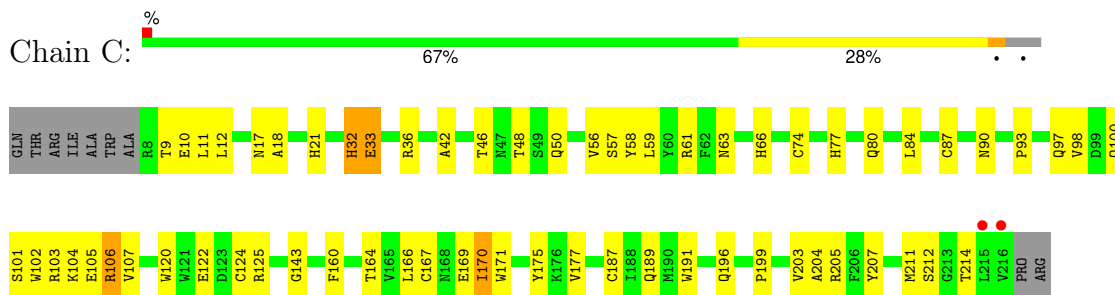
- Molecule 1: Folate receptor alpha



- Molecule 1: Folate receptor alpha

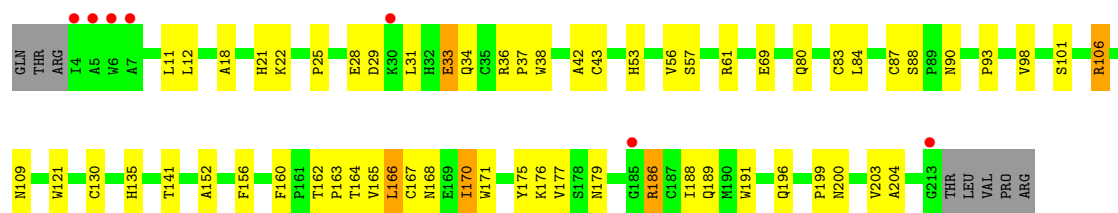


- Molecule 1: Folate receptor alpha

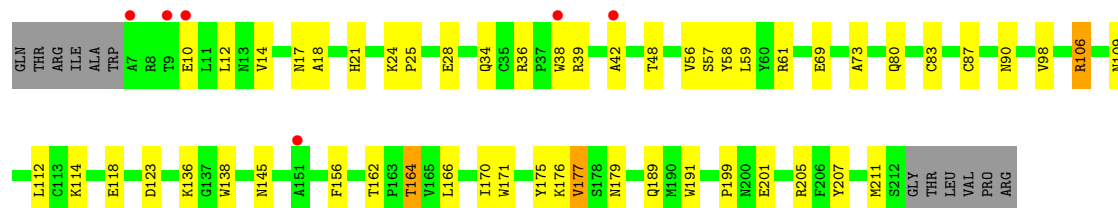


- Molecule 1: Folate receptor alpha

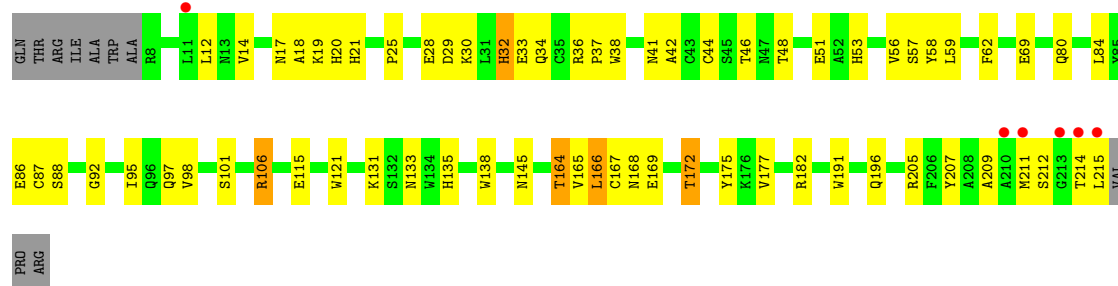




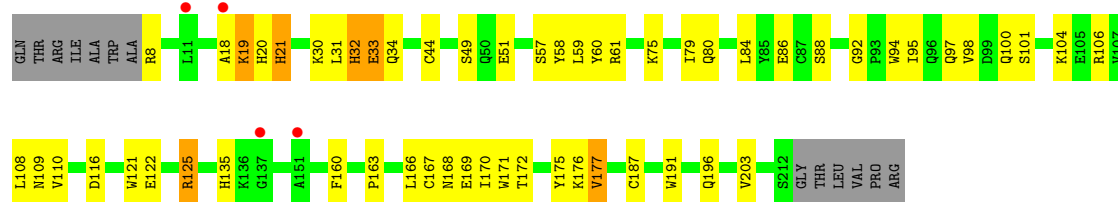
- Molecule 1: Folate receptor alpha



- Molecule 1: Folate receptor alpha



- Molecule 1: Folate receptor alpha



- Molecule 1: Folate receptor alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.02Å 144.59Å 216.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.80 49.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.00-2.80) 99.5 (49.00-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.227 , 0.267 0.227 , 0.264	Depositor DCC
R_{free} test set	5728 reflections (8.17%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14328	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.45	0/1755	0.61	0/2384
1	B	0.42	0/1733	0.56	0/2355
1	C	0.41	0/1770	0.54	0/2405
1	D	0.40	0/1782	0.56	0/2422
1	E	0.41	0/1749	0.56	0/2376
1	F	0.38	0/1763	0.56	0/2395
1	G	0.38	0/1744	0.54	0/2369
1	H	0.47	0/1738	0.60	0/2361
All	All	0.42	0/14034	0.57	0/19067

There are no bond length outliers.

There are no bond angle outliers.

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	1697	0	1551	31	0
1	B	1675	0	1528	33	0
1	C	1712	0	1573	45	0
1	D	1722	0	1576	37	0
1	E	1691	0	1546	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1705	0	1563	49	0
1	G	1686	0	1543	41	0
1	H	1680	0	1536	33	0
2	A	32	0	17	0	0
2	B	32	0	17	1	0
2	C	32	0	17	0	0
2	D	32	0	17	0	0
2	E	32	0	17	1	0
2	F	32	0	17	0	0
2	G	32	0	17	1	0
2	H	32	0	17	0	0
3	A	42	0	39	1	0
3	B	42	0	39	3	0
3	C	28	0	26	0	0
3	D	42	0	39	1	0
3	E	42	0	39	3	0
3	F	42	0	39	1	0
3	G	28	0	26	0	0
3	H	42	0	39	1	0
4	A	46	0	0	1	0
4	B	22	0	0	0	0
4	C	21	0	0	1	0
4	D	19	0	0	0	0
4	E	21	0	0	3	0
4	F	13	0	0	0	0
4	G	20	0	0	1	0
4	H	34	0	0	0	0
All	All	14328	0	12838	300	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 11.

All (300) 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:D:98:VAL:HG11	1:D:106:ARG:HD3	1.52	0.89
1:F:98:VAL:HG11	1:F:106:ARG:HD3	1.56	0.87
1:E:80:GLN:HG3	1:E:191:TRP:CZ2	2.10	0.86
1:E:98:VAL:HG11	1:E:106:ARG:HD3	1.58	0.82
1:D:186:ARG:HH11	1:D:186:ARG:HB3	1.46	0.81
1:C:80:GLN:HG3	1:C:191:TRP:CZ2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLU:HG3	1:C:12:LEU:H	1.47	0.79
1:B:80:GLN:HG3	1:B:191:TRP:CZ2	2.18	0.78
1:D:80:GLN:HG3	1:D:191:TRP:CH2	2.20	0.76
1:F:80:GLN:HG3	1:F:191:TRP:CZ2	2.22	0.74
1:G:98:VAL:HG11	1:G:106:ARG:HD3	1.68	0.74
1:B:80:GLN:HG3	1:B:191:TRP:CE2	2.25	0.71
1:D:80:GLN:HG3	1:D:191:TRP:CZ2	2.25	0.71
1:B:131:LYS:HE3	1:B:133:ASN:O	1.91	0.70
1:H:80:GLN:HG3	1:H:191:TRP:CE2	2.27	0.70
1:F:18:ALA:HB3	1:F:21:HIS:ND1	2.06	0.70
1:H:18:ALA:HB3	1:H:21:HIS:ND1	2.08	0.69
1:A:80:GLN:HG3	1:A:191:TRP:CZ2	2.27	0.69
1:H:80:GLN:HG3	1:H:191:TRP:CZ2	2.27	0.69
1:A:131:LYS:HB3	1:B:193:ASP:OD2	1.93	0.69
1:G:80:GLN:HG3	1:G:191:TRP:CZ2	2.28	0.68
1:D:33:GLU:HG3	1:D:34:GLN:H	1.59	0.68
1:F:215:LEU:HD12	1:H:13:ASN:HD22	1.60	0.67
1:F:34:GLN:HB2	1:F:53:HIS:NE2	2.09	0.67
1:H:98:VAL:HG11	1:H:106:ARG:HD3	1.79	0.65
1:E:109:ASN:HA	1:E:176:LYS:HB2	1.78	0.64
1:D:38:TRP:HB3	1:D:42:ALA:HB2	1.79	0.64
1:A:18:ALA:HB3	1:A:21:HIS:ND1	2.12	0.64
1:B:106:ARG:HG2	1:B:107:VAL:H	1.63	0.64
1:H:44:CYS:HB3	1:H:86:GLU:O	1.98	0.63
1:E:90:ASN:HD22	1:E:201:GLU:HA	1.65	0.62
1:C:164:THR:HA	1:C:177:VAL:HG21	1.80	0.62
3:E:303:NAG:H83	4:E:411:HOH:O	1.99	0.62
1:C:169:GLU:HB3	1:F:196:GLN:HE22	1.64	0.62
1:F:12:LEU:HD21	1:F:205:ARG:HG3	1.83	0.61
1:G:167:CYS:O	1:G:175:TYR:HB2	2.00	0.61
1:A:44:CYS:HB3	1:A:86:GLU:O	2.01	0.60
1:A:80:GLN:HG3	1:A:191:TRP:CE2	2.36	0.60
1:A:34:GLN:OE1	1:A:80:GLN:HG2	2.02	0.60
3:A:304:NAG:H83	4:A:429:HOH:O	2.01	0.60
1:B:44:CYS:HB3	1:B:86:GLU:O	2.02	0.59
1:G:57:SER:O	1:G:61:ARG:HA	2.02	0.59
1:G:125:ARG:HB2	1:G:125:ARG:HH11	1.67	0.59
1:E:179:ASN:HB2	3:E:304:NAG:N2	2.18	0.59
1:B:167:CYS:O	1:B:175:TYR:HB2	2.03	0.59
1:D:106:ARG:HH11	1:D:106:ARG:HB2	1.68	0.58
1:H:32:HIS:CG	1:H:33:GLU:H	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:GLY:HA2	1:G:95:ILE:HD12	1.85	0.58
1:C:160:PHE:CD2	1:C:166:LEU:HD23	2.39	0.58
1:E:10:GLU:HG2	1:E:14:VAL:HG11	1.86	0.58
1:C:12:LEU:HD21	1:C:205:ARG:HG2	1.85	0.57
1:H:160:PHE:CD1	1:H:166:LEU:HA	2.39	0.57
1:B:84:LEU:HD12	1:B:88:SER:HB2	1.86	0.57
1:C:169:GLU:HB3	1:F:196:GLN:NE2	2.20	0.56
1:D:34:GLN:OE1	1:D:80:GLN:HG2	2.04	0.56
1:F:32:HIS:CG	1:F:33:GLU:H	2.22	0.56
1:F:165:VAL:O	1:F:169:GLU:HB2	2.04	0.56
1:E:28:GLU:HB3	4:E:403:HOH:O	2.05	0.56
1:F:80:GLN:HG3	1:F:191:TRP:CH2	2.39	0.56
1:G:84:LEU:HD12	1:G:88:SER:HB2	1.87	0.56
1:G:92:GLY:HA2	1:G:95:ILE:CD1	2.35	0.56
1:G:60:TYR:HB3	2:G:301:FOL:H15	1.87	0.56
1:E:38:TRP:O	1:E:42:ALA:HB2	2.06	0.56
1:E:42:ALA:HB1	1:E:87:CYS:HB3	1.88	0.56
1:C:160:PHE:CG	1:C:166:LEU:HD23	2.40	0.55
1:G:18:ALA:HB3	1:G:21:HIS:ND1	2.21	0.55
1:C:32:HIS:CG	1:C:33:GLU:H	2.25	0.55
1:A:29:ASP:HA	1:A:39:ARG:HD3	1.86	0.55
1:F:168:ASN:OD1	1:F:177:VAL:HG23	2.07	0.55
1:D:28:GLU:O	1:D:31:LEU:HG	2.07	0.55
1:E:136:LYS:HA	2:E:301:FOL:O1	2.06	0.55
1:F:167:CYS:O	1:F:175:TYR:HB2	2.07	0.54
1:B:42:ALA:HB1	1:B:87:CYS:HB3	1.88	0.54
1:B:47:ASN:HD22	3:B:302:NAG:H82	1.72	0.54
1:E:189:GLN:NE2	1:E:199:PRO:HG3	2.23	0.54
1:E:61:ARG:HD3	4:E:409:HOH:O	2.07	0.54
1:B:11:LEU:O	1:B:92:GLY:HA3	2.08	0.54
1:C:77:HIS:CD2	1:C:120:TRP:HA	2.43	0.54
1:C:160:PHE:CZ	1:C:170:ILE:HD12	2.43	0.54
1:A:138:TRP:HB3	1:A:145:ASN:HB2	1.90	0.53
1:E:80:GLN:HG3	1:E:191:TRP:CH2	2.43	0.53
1:C:212:SER:OG	1:C:214:THR:HG22	2.09	0.53
1:E:12:LEU:HD21	1:E:205:ARG:HA	1.89	0.53
1:B:106:ARG:HG2	1:B:107:VAL:N	2.22	0.53
1:G:168:ASN:OD1	1:G:176:LYS:HA	2.09	0.53
1:A:207:TYR:O	1:A:211:MET:HG2	2.09	0.53
1:C:33:GLU:O	1:C:36:ARG:HB2	2.09	0.53
1:G:44:CYS:HB3	1:G:86:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:HG3	1:B:53:HIS:NE2	2.24	0.53
1:D:42:ALA:HB1	1:D:87:CYS:HB3	1.90	0.53
1:D:170:ILE:HG23	1:D:171:TRP:N	2.24	0.53
1:E:18:ALA:HB3	1:E:21:HIS:ND1	2.24	0.53
1:G:51:GLU:HG3	1:G:58:TYR:HB3	1.90	0.53
1:F:164:THR:HA	1:F:177:VAL:HG21	1.90	0.53
1:G:84:LEU:HD23	1:G:175:TYR:OH	2.09	0.52
1:C:42:ALA:HB1	1:C:87:CYS:HB3	1.92	0.52
1:D:56:VAL:CG1	1:D:61:ARG:HG3	2.39	0.52
1:A:160:PHE:CD1	1:A:166:LEU:HA	2.45	0.52
1:G:20:HIS:NE2	1:G:59:LEU:HA	2.24	0.52
1:C:80:GLN:HG3	1:C:191:TRP:CE2	2.45	0.52
1:C:167:CYS:O	1:C:175:TYR:HB2	2.10	0.51
1:D:168:ASN:OD1	1:D:177:VAL:HG23	2.10	0.51
1:E:56:VAL:HG12	1:E:61:ARG:HG3	1.91	0.51
1:F:167:CYS:HB2	1:F:177:VAL:HG22	1.92	0.51
1:B:9:THR:HG21	1:B:12:LEU:HD12	1.92	0.51
1:C:98:VAL:HG11	1:C:106:ARG:HD3	1.92	0.51
1:G:80:GLN:HG3	1:G:191:TRP:CE2	2.45	0.51
1:B:38:TRP:HB3	1:B:42:ALA:HB2	1.93	0.51
1:C:170:ILE:HG23	1:C:171:TRP:N	2.25	0.51
1:E:34:GLN:OE1	1:E:80:GLN:HG2	2.11	0.51
1:H:22:LYS:HG3	1:H:43:CYS:O	2.11	0.51
1:C:80:GLN:HG3	1:C:191:TRP:CH2	2.46	0.51
1:B:160:PHE:CD1	1:B:166:LEU:HA	2.46	0.51
1:F:38:TRP:O	1:F:42:ALA:HB2	2.11	0.51
1:F:121:TRP:HA	1:F:166:LEU:HD12	1.92	0.50
1:G:160:PHE:CD1	1:G:166:LEU:HA	2.47	0.50
3:E:303:NAG:H81	1:H:36:ARG:HH22	1.76	0.50
1:F:80:GLN:HG3	1:F:191:TRP:CE2	2.46	0.50
1:E:164:THR:HA	1:E:177:VAL:HG21	1.92	0.50
1:G:34:GLN:OE1	1:G:80:GLN:HG2	2.11	0.50
1:B:135:HIS:HD2	2:B:301:FOL:H13	1.76	0.50
1:E:48:THR:HG23	1:E:59:LEU:HD21	1.93	0.50
1:G:80:GLN:HG3	1:G:191:TRP:CH2	2.46	0.50
1:A:11:LEU:HD12	1:A:11:LEU:H	1.77	0.50
1:C:48:THR:HG23	1:C:59:LEU:HD21	1.94	0.50
1:F:215:LEU:HD12	1:H:13:ASN:ND2	2.24	0.50
1:A:98:VAL:HG11	1:A:106:ARG:HD3	1.93	0.50
1:D:167:CYS:O	1:D:175:TYR:HB2	2.11	0.50
1:G:168:ASN:ND2	1:G:177:VAL:HG23	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:HIS:CG	1:H:33:GLU:N	2.80	0.50
1:D:84:LEU:HD12	1:D:88:SER:HB2	1.94	0.50
1:E:114:LYS:O	1:E:118:GLU:HG3	2.11	0.49
1:C:10:GLU:HG2	4:C:419:HOH:O	2.11	0.49
1:D:90:ASN:HB3	1:D:204:ALA:HB2	1.94	0.49
1:H:207:TYR:O	1:H:211:MET:HG2	2.12	0.49
1:B:84:LEU:HD22	1:B:190:MET:HB3	1.94	0.49
1:G:187:CYS:O	1:G:203:VAL:HG21	2.13	0.49
1:F:84:LEU:HD12	1:F:88:SER:HB2	1.94	0.49
1:E:73:ALA:O	1:E:123:ASP:HB3	2.12	0.48
1:C:84:LEU:HD23	1:C:175:TYR:OH	2.13	0.48
1:E:58:TYR:HA	1:E:61:ARG:NH2	2.28	0.48
1:A:112:LEU:HD23	1:A:117:CYS:HB2	1.95	0.48
1:C:207:TYR:O	1:C:211:MET:HG2	2.13	0.48
1:G:32:HIS:CG	1:G:33:GLU:H	2.31	0.48
1:F:207:TYR:O	1:F:211:MET:HG2	2.13	0.48
1:A:12:LEU:HD12	1:A:12:LEU:N	2.29	0.48
1:E:90:ASN:HD21	1:E:201:GLU:HG2	1.79	0.47
1:G:59:LEU:C	1:G:61:ARG:H	2.17	0.47
1:C:56:VAL:HG12	1:C:61:ARG:HG3	1.96	0.47
1:C:61:ARG:HG2	1:C:143:GLY:O	2.14	0.47
1:D:196:GLN:HE21	1:G:169:GLU:HB3	1.78	0.47
1:F:58:TYR:CZ	3:F:302:NAG:H62	2.49	0.47
1:G:8:ARG:HB3	4:G:417:HOH:O	2.14	0.47
1:G:94:TRP:HB3	1:G:108:LEU:O	2.15	0.47
1:F:131:LYS:HE3	1:F:133:ASN:O	2.14	0.47
1:A:198:ASN:HB3	1:A:201:GLU:OE2	2.15	0.47
1:E:162:THR:OG1	1:E:164:THR:HG23	2.15	0.47
1:F:209:ALA:HB1	1:F:215:LEU:HA	1.97	0.47
1:H:32:HIS:O	1:H:36:ARG:HG3	2.14	0.47
1:B:164:THR:O	1:B:168:ASN:HB2	2.14	0.46
1:E:112:LEU:HD13	1:E:175:TYR:CE2	2.49	0.46
1:F:25:PRO:HB3	1:F:41:ASN:HD21	1.80	0.46
1:F:92:GLY:HA2	1:F:95:ILE:CD1	2.45	0.46
1:H:84:LEU:HD12	1:H:88:SER:HB2	1.96	0.46
1:A:114:LYS:O	1:A:118:GLU:HG3	2.15	0.46
1:D:56:VAL:HG12	1:D:61:ARG:HG3	1.95	0.46
1:B:48:THR:HG23	1:B:59:LEU:HD21	1.97	0.46
1:F:44:CYS:HB3	1:F:86:GLU:O	2.15	0.46
1:E:90:ASN:ND2	1:E:201:GLU:HA	2.30	0.46
1:H:168:ASN:OD1	1:H:177:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HG23	1:A:171:TRP:N	2.31	0.46
1:C:18:ALA:HB3	1:C:21:HIS:ND1	2.31	0.46
1:D:34:GLN:HB2	1:D:53:HIS:NE2	2.31	0.46
1:F:209:ALA:HB1	1:F:215:LEU:H	1.81	0.46
1:A:38:TRP:O	1:A:42:ALA:HB2	2.16	0.45
1:C:11:LEU:O	1:C:93:PRO:HD3	2.15	0.45
1:C:12:LEU:HD11	1:C:205:ARG:HA	1.99	0.45
1:D:22:LYS:HG3	1:D:43:CYS:O	2.16	0.45
1:E:57:SER:O	1:E:61:ARG:HA	2.15	0.45
1:C:100:GLN:O	1:C:102:TRP:N	2.50	0.45
1:G:109:ASN:HA	1:G:176:LYS:HB2	1.97	0.45
1:D:130:CYS:HB2	1:D:152:ALA:HB3	1.99	0.45
1:C:32:HIS:CD2	1:C:33:GLU:H	2.34	0.45
1:B:122:GLU:OE2	1:B:125:ARG:NH1	2.49	0.45
1:D:33:GLU:O	1:D:36:ARG:HB2	2.17	0.45
1:A:162:THR:OG1	1:A:165:VAL:HG23	2.16	0.45
1:H:38:TRP:O	1:H:42:ALA:HB2	2.17	0.45
1:A:84:LEU:HD12	1:A:88:SER:HB2	1.99	0.45
1:A:99:ASP:OD2	1:A:104:LYS:HG3	2.17	0.45
1:G:125:ARG:HH11	1:G:125:ARG:CB	2.30	0.45
1:G:168:ASN:HD21	1:G:177:VAL:HG23	1.82	0.45
1:C:58:TYR:HA	1:C:61:ARG:NH2	2.32	0.45
1:B:179:ASN:HB3	3:B:304:NAG:C7	2.47	0.44
1:C:63:ASN:HD21	1:C:66:HIS:HA	1.80	0.44
1:F:30:LYS:O	1:F:46:THR:HG23	2.17	0.44
1:G:122:GLU:OE2	1:G:125:ARG:NH1	2.50	0.44
1:B:34:GLN:OE1	1:B:80:GLN:HG2	2.16	0.44
1:C:17:ASN:H	1:C:105:GLU:HB2	1.81	0.44
1:C:189:GLN:NE2	1:C:199:PRO:HG3	2.33	0.44
1:D:121:TRP:CE3	1:D:163:PRO:HG3	2.52	0.44
1:E:138:TRP:HB3	1:E:145:ASN:HB2	2.00	0.44
1:A:80:GLN:HG3	1:A:191:TRP:CH2	2.52	0.44
1:B:34:GLN:HB2	1:B:53:HIS:NE2	2.32	0.44
1:D:38:TRP:CZ3	1:D:83:CYS:HB3	2.53	0.44
1:E:12:LEU:O	1:E:14:VAL:HG13	2.17	0.44
1:C:187:CYS:O	1:C:203:VAL:HG21	2.18	0.44
1:D:11:LEU:HD22	1:D:93:PRO:HA	1.99	0.44
1:F:135:HIS:HB2	1:F:172:THR:HG23	1.99	0.44
1:G:110:VAL:HB	1:G:175:TYR:HD2	1.82	0.44
1:F:48:THR:HG23	1:F:59:LEU:HD21	1.99	0.44
1:H:12:LEU:O	1:H:14:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLN:NE2	1:D:199:PRO:HG3	2.33	0.44
1:H:73:ALA:O	1:H:123:ASP:HB3	2.18	0.44
1:H:140:TRP:CZ2	1:H:145:ASN:HB3	2.52	0.44
1:C:122:GLU:OE2	1:C:125:ARG:NH1	2.48	0.43
1:H:34:GLN:HB3	1:H:80:GLN:HE21	1.83	0.43
1:H:112:LEU:HD23	1:H:117:CYS:HB2	2.01	0.43
1:A:34:GLN:HB2	1:A:53:HIS:NE2	2.33	0.43
1:D:57:SER:O	1:D:61:ARG:HA	2.18	0.43
1:G:31:LEU:HD22	1:G:49:SER:HB3	2.00	0.43
1:A:166:LEU:HD22	1:A:166:LEU:O	2.19	0.43
1:D:160:PHE:CD1	1:D:166:LEU:HA	2.54	0.43
1:D:166:LEU:HD22	1:D:166:LEU:O	2.18	0.43
1:G:98:VAL:HG23	1:G:100:GLN:HG2	2.00	0.43
1:D:160:PHE:CZ	1:D:170:ILE:HD12	2.53	0.43
1:D:199:PRO:O	1:D:203:VAL:HG23	2.18	0.43
1:H:160:PHE:CZ	1:H:170:ILE:HD12	2.53	0.43
1:F:115:GLU:HB2	1:F:182:ARG:CD	2.49	0.43
1:C:48:THR:HG23	1:C:59:LEU:CD2	2.48	0.43
1:A:135:HIS:HB2	1:A:172:THR:HG23	2.00	0.43
1:B:180:TYR:HB3	1:B:184:SER:OG	2.18	0.43
1:C:46:THR:O	1:C:50:GLN:HG3	2.19	0.43
1:D:18:ALA:HB3	1:D:21:HIS:ND1	2.33	0.43
1:F:42:ALA:HB1	1:F:87:CYS:HB3	2.00	0.43
1:H:32:HIS:CE1	1:H:33:GLU:HG3	2.54	0.43
1:H:46:THR:O	1:H:50:GLN:HG3	2.18	0.43
1:A:171:TRP:HA	1:A:171:TRP:CE3	2.53	0.43
1:E:36:ARG:O	1:E:39:ARG:HG3	2.19	0.43
1:H:58:TYR:CZ	3:H:302:NAG:H61	2.54	0.43
1:D:188:ILE:HG23	1:D:200:ASN:OD1	2.18	0.43
1:F:53:HIS:HD1	1:F:53:HIS:H	1.65	0.43
1:C:90:ASN:HB3	1:C:204:ALA:HB2	2.00	0.42
1:F:212:SER:C	1:F:214:THR:H	2.22	0.42
1:H:36:ARG:N	1:H:37:PRO:CD	2.81	0.42
1:A:11:LEU:O	1:A:92:GLY:HA3	2.18	0.42
1:A:33:GLU:HB2	1:A:34:GLN:H	1.68	0.42
1:A:167:CYS:O	1:A:175:TYR:HB2	2.20	0.42
1:C:57:SER:O	1:C:61:ARG:HA	2.18	0.42
1:F:48:THR:HG23	1:F:59:LEU:CD2	2.49	0.42
1:H:10:GLU:C	1:H:12:LEU:H	2.23	0.42
1:F:12:LEU:O	1:F:14:VAL:HG13	2.20	0.42
1:G:170:ILE:HG23	1:G:171:TRP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:TYR:O	1:E:211:MET:HG3	2.19	0.42
1:G:125:ARG:HB2	1:G:125:ARG:NH1	2.31	0.42
1:H:138:TRP:HB3	1:H:145:ASN:HB2	2.01	0.42
1:F:32:HIS:CG	1:F:33:GLU:N	2.87	0.42
1:B:198:ASN:O	1:B:201:GLU:HG3	2.19	0.42
1:F:51:GLU:HB3	1:F:57:SER:HB2	2.00	0.42
1:G:135:HIS:HB2	1:G:172:THR:HG23	2.01	0.42
1:H:189:GLN:HE21	1:H:192:PHE:HB3	1.84	0.42
1:F:25:PRO:HB3	1:F:41:ASN:ND2	2.34	0.41
1:D:109:ASN:HA	1:D:176:LYS:HB2	2.03	0.41
1:E:48:THR:HG23	1:E:59:LEU:CD2	2.50	0.41
1:F:115:GLU:HB2	1:F:182:ARG:HD2	2.02	0.41
1:F:56:VAL:HA	1:F:62:PHE:O	2.21	0.41
1:B:71:ALA:HA	1:B:72:PRO:HD3	1.97	0.41
1:B:199:PRO:O	1:B:203:VAL:HG23	2.20	0.41
1:E:171:TRP:HA	1:E:171:TRP:CE3	2.55	0.41
1:F:36:ARG:HB2	1:F:37:PRO:HD3	2.02	0.41
1:G:75:LYS:O	1:G:79:ILE:HG13	2.21	0.41
1:D:141:THR:HG21	3:D:303:NAG:H5	2.03	0.41
1:F:19:LYS:HE2	1:F:20:HIS:CE1	2.56	0.41
1:A:131:LYS:HB3	1:A:131:LYS:NZ	2.36	0.41
1:E:170:ILE:HG23	1:E:171:TRP:N	2.35	0.41
1:G:19:LYS:HE2	1:G:20:HIS:CE1	2.56	0.41
1:G:110:VAL:HB	1:G:175:TYR:CD2	2.55	0.41
1:B:114:LYS:O	1:B:118:GLU:HG3	2.21	0.41
1:C:18:ALA:HA	1:C:103:ARG:HB2	2.01	0.41
1:D:12:LEU:HD12	1:D:12:LEU:N	2.36	0.41
1:D:162:THR:OG1	1:D:165:VAL:HG23	2.20	0.41
1:G:121:TRP:CE3	1:G:163:PRO:HG3	2.55	0.41
1:H:176:LYS:O	1:H:177:VAL:C	2.59	0.41
1:B:12:LEU:O	1:B:14:VAL:HG13	2.21	0.41
1:F:30:LYS:HD3	1:F:30:LYS:HA	1.85	0.41
1:H:170:ILE:HG23	1:H:171:TRP:N	2.36	0.41
1:A:12:LEU:O	1:A:14:VAL:HG13	2.21	0.40
1:F:92:GLY:HA2	1:F:95:ILE:HD12	2.02	0.40
1:F:138:TRP:HB3	1:F:145:ASN:HB2	2.02	0.40
1:G:97:GLN:HG3	1:G:104:LYS:HG2	2.02	0.40
1:B:179:ASN:HB3	3:B:304:NAG:H82	2.03	0.40
1:E:38:TRP:CZ3	1:E:83:CYS:HB3	2.56	0.40
1:F:53:HIS:ND1	1:F:53:HIS:N	2.69	0.40
1:H:92:GLY:N	1:H:93:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:GLU:C	1:F:30:LYS:H	2.24	0.40
1:B:170:ILE:HG23	1:B:171:TRP:N	2.37	0.40
1:C:160:PHE:CD1	1:C:166:LEU:HA	2.57	0.40
1:B:65:ASN:HB3	1:B:68:GLY:O	2.22	0.40
1:C:74:CYS:HB2	1:C:124:CYS:HA	2.04	0.40
1:C:97:GLN:NE2	1:C:104:LYS:HE2	2.37	0.40
1:C:170:ILE:CG2	1:C:171:TRP:N	2.85	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	205/218 (94%)	183 (89%)	19 (9%)	3 (2%)	8	29
1	B	202/218 (93%)	181 (90%)	17 (8%)	4 (2%)	6	21
1	C	207/218 (95%)	179 (86%)	24 (12%)	4 (2%)	6	23
1	D	208/218 (95%)	180 (86%)	23 (11%)	5 (2%)	5	18
1	E	204/218 (94%)	175 (86%)	28 (14%)	1 (0%)	25	56
1	F	206/218 (94%)	178 (86%)	24 (12%)	4 (2%)	6	23
1	G	203/218 (93%)	181 (89%)	16 (8%)	6 (3%)	3	13
1	H	202/218 (93%)	178 (88%)	19 (9%)	5 (2%)	4	17
All	All	1637/1744 (94%)	1435 (88%)	170 (10%)	32 (2%)	6	21

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	B	33	GLU
1	C	9	THR

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Mol	Chain	Res	Type
1	C	33	GLU
1	C	101	SER
1	D	33	GLU
1	H	9	THR
1	H	101	SER
1	D	101	SER
1	F	29	ASP
1	G	19	LYS
1	G	21	HIS
1	G	32	HIS
1	H	32	HIS
1	A	101	SER
1	A	150	GLY
1	B	25	PRO
1	C	32	HIS
1	F	101	SER
1	G	33	GLU
1	G	101	SER
1	H	33	GLU
1	B	177	VAL
1	D	29	ASP
1	E	25	PRO
1	F	32	HIS
1	F	172	THR
1	D	25	PRO
1	D	37	PRO
1	G	177	VAL
1	H	177	VAL
1	B	37	PRO

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	184/193 (95%)	175 (95%)	9 (5%)	21	52
1	B	182/193 (94%)	178 (98%)	4 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	186/193 (96%)	182 (98%)	4 (2%)	47	79
1	D	185/193 (96%)	176 (95%)	9 (5%)	21	52
1	E	183/193 (95%)	175 (96%)	8 (4%)	24	56
1	F	185/193 (96%)	179 (97%)	6 (3%)	34	68
1	G	183/193 (95%)	179 (98%)	4 (2%)	47	79
1	H	182/193 (94%)	174 (96%)	8 (4%)	24	56
All	All	1470/1544 (95%)	1418 (96%)	52 (4%)	31	65

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	11	LEU
1	A	17	ASN
1	A	33	GLU
1	A	69	GLU
1	A	100	GLN
1	A	106	ARG
1	A	164	THR
1	A	166	LEU
1	B	61	ARG
1	B	106	ARG
1	B	166	LEU
1	B	179	ASN
1	C	106	ARG
1	C	107	VAL
1	C	170	ILE
1	C	196	GLN
1	D	69	GLU
1	D	106	ARG
1	D	135	HIS
1	D	156	PHE
1	D	164	THR
1	D	166	LEU
1	D	170	ILE
1	D	179	ASN
1	D	186	ARG
1	E	17	ASN
1	E	24	LYS
1	E	69	GLU

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Mol	Chain	Res	Type
1	E	106	ARG
1	E	156	PHE
1	E	164	THR
1	E	166	LEU
1	E	177	VAL
1	F	17	ASN
1	F	69	GLU
1	F	97	GLN
1	F	106	ARG
1	F	164	THR
1	F	166	LEU
1	G	30	LYS
1	G	116	ASP
1	G	125	ARG
1	G	196	GLN
1	H	10	GLU
1	H	17	ASN
1	H	69	GLU
1	H	106	ARG
1	H	156	PHE
1	H	164	THR
1	H	166	LEU
1	H	174	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	80	GLN
1	A	189	GLN
1	B	17	ASN
1	B	63	ASN
1	B	196	GLN
1	C	32	HIS
1	C	80	GLN
1	C	97	GLN
1	C	154	GLN
1	C	189	GLN
1	D	17	ASN
1	D	80	GLN
1	D	119	GLN
1	D	189	GLN

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Mol	Chain	Res	Type
1	D	196	GLN
1	E	90	ASN
1	E	119	GLN
1	F	41	ASN
1	F	90	ASN
1	F	97	GLN
1	F	119	GLN
1	F	189	GLN
1	F	196	GLN
1	G	13	ASN
1	G	32	HIS
1	G	41	ASN
1	G	96	GLN
1	G	154	GLN
1	G	189	GLN
1	H	17	ASN
1	H	63	ASN
1	H	80	GLN
1	H	90	ASN
1	H	97	GLN
1	H	135	HIS
1	H	189	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 ⓘ

30 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	303	1	14,14,15	0.64	0	17,19,21	0.72	1 (5%)
2	FOL	H	301	-	34,34,34	1.36	3 (8%)	43,47,47	2.05	10 (23%)
2	FOL	G	301	-	34,34,34	1.61	5 (14%)	43,47,47	2.08	12 (27%)
3	NAG	H	302	1	14,14,15	0.66	0	17,19,21	0.69	0
3	NAG	G	303	1	14,14,15	0.67	0	17,19,21	0.78	0
2	FOL	E	301	-	34,34,34	1.72	9 (26%)	43,47,47	2.12	11 (25%)
3	NAG	B	302	1	14,14,15	0.52	0	17,19,21	0.88	1 (5%)
2	FOL	A	301	-	34,34,34	1.44	7 (20%)	43,47,47	2.05	9 (20%)
3	NAG	A	302	1	14,14,15	0.52	0	17,19,21	0.78	0
3	NAG	F	302	1	14,14,15	0.63	0	17,19,21	0.69	0
3	NAG	E	303	1	14,14,15	0.65	0	17,19,21	0.82	1 (5%)
2	FOL	F	301	-	34,34,34	1.60	5 (14%)	43,47,47	2.13	11 (25%)
3	NAG	A	303	1	14,14,15	0.58	0	17,19,21	0.72	0
3	NAG	B	303	1	14,14,15	0.68	0	17,19,21	0.77	0
3	NAG	H	304	1	14,14,15	1.05	1 (7%)	17,19,21	0.84	0
3	NAG	G	302	1	14,14,15	0.55	0	17,19,21	0.76	0
3	NAG	D	304	1	14,14,15	0.74	0	17,19,21	0.84	0
2	FOL	D	301	-	34,34,34	1.62	7 (20%)	43,47,47	2.09	10 (23%)
3	NAG	E	302	1	14,14,15	0.64	0	17,19,21	0.73	0
3	NAG	H	303	1	14,14,15	0.70	0	17,19,21	0.71	1 (5%)
3	NAG	E	304	1	14,14,15	0.85	1 (7%)	17,19,21	0.66	0
3	NAG	D	302	1	14,14,15	0.52	0	17,19,21	0.73	0
3	NAG	C	302	1	14,14,15	0.51	0	17,19,21	0.81	1 (5%)
3	NAG	A	304	1	14,14,15	0.94	1 (7%)	17,19,21	0.69	0
2	FOL	C	301	-	34,34,34	1.65	7 (20%)	43,47,47	2.13	11 (25%)
3	NAG	B	304	1	14,14,15	1.15	1 (7%)	17,19,21	0.72	0
3	NAG	F	304	1	14,14,15	0.77	0	17,19,21	0.73	0
2	FOL	B	301	-	34,34,34	1.75	6 (17%)	43,47,47	2.19	11 (25%)
3	NAG	C	303	1	14,14,15	0.62	0	17,19,21	0.90	0
3	NAG	D	303	1	14,14,15	0.74	0	17,19,21	0.87	1 (5%)

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	NAG	F	303	1	-	2/6/23/26	0/1/1/1
2	FOL	H	301	-	-	9/22/22/22	0/3/3/3
2	FOL	G	301	-	-	7/22/22/22	0/3/3/3
3	NAG	H	302	1	-	2/6/23/26	0/1/1/1
3	NAG	G	303	1	-	4/6/23/26	0/1/1/1
2	FOL	E	301	-	-	6/22/22/22	0/3/3/3
3	NAG	B	302	1	-	2/6/23/26	0/1/1/1
2	FOL	A	301	-	-	9/22/22/22	0/3/3/3
3	NAG	A	302	1	-	0/6/23/26	0/1/1/1
3	NAG	F	302	1	-	2/6/23/26	0/1/1/1
3	NAG	E	303	1	-	4/6/23/26	0/1/1/1
2	FOL	F	301	-	-	8/22/22/22	0/3/3/3
3	NAG	A	303	1	-	3/6/23/26	0/1/1/1
3	NAG	B	303	1	-	4/6/23/26	0/1/1/1
3	NAG	H	304	1	-	2/6/23/26	0/1/1/1
3	NAG	G	302	1	-	2/6/23/26	0/1/1/1
3	NAG	D	304	1	-	5/6/23/26	0/1/1/1
2	FOL	D	301	-	-	9/22/22/22	0/3/3/3
3	NAG	E	302	1	-	3/6/23/26	0/1/1/1
3	NAG	H	303	1	-	2/6/23/26	0/1/1/1
3	NAG	E	304	1	-	2/6/23/26	0/1/1/1
3	NAG	D	302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	304	1	-	3/6/23/26	0/1/1/1
2	FOL	C	301	-	-	9/22/22/22	0/3/3/3
3	NAG	B	304	1	-	2/6/23/26	0/1/1/1
3	NAG	F	304	1	-	2/6/23/26	0/1/1/1
2	FOL	B	301	-	-	6/22/22/22	0/3/3/3
3	NAG	C	303	1	-	3/6/23/26	0/1/1/1
3	NAG	D	303	1	-	5/6/23/26	0/1/1/1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	FOL	C4A-C4	5.46	1.50	1.41
2	C	301	FOL	C4A-C4	5.29	1.50	1.41
2	E	301	FOL	C4A-C4	5.07	1.50	1.41
2	G	301	FOL	C4A-C4	4.78	1.49	1.41
2	F	301	FOL	C4A-C4	4.69	1.49	1.41
2	D	301	FOL	C4A-C4	4.41	1.49	1.41
2	H	301	FOL	C4A-C4	3.68	1.47	1.41
3	B	304	NAG	C1-C2	3.55	1.57	1.52
3	H	304	NAG	C1-C2	3.05	1.56	1.52
2	B	301	FOL	C4-N3	2.98	1.38	1.33
2	G	301	FOL	C12-C11	2.87	1.43	1.39
2	A	301	FOL	C4A-C4	2.83	1.46	1.41
2	C	301	FOL	C4-N3	2.79	1.37	1.33
2	F	301	FOL	C16-C11	2.75	1.43	1.39
2	E	301	FOL	C7-N8	2.75	1.36	1.31
2	E	301	FOL	C4A-C8A	2.71	1.45	1.40
2	D	301	FOL	C4-N3	2.70	1.37	1.33
2	B	301	FOL	C15-C14	2.67	1.43	1.39
2	B	301	FOL	C2-NA2	2.66	1.39	1.33
2	G	301	FOL	C16-C11	2.64	1.43	1.39
2	G	301	FOL	C15-C14	2.62	1.43	1.39
3	A	304	NAG	C1-C2	2.57	1.55	1.52
2	D	301	FOL	C16-C11	2.52	1.43	1.39
2	B	301	FOL	C16-C11	2.50	1.43	1.39
2	E	301	FOL	C15-C14	2.50	1.43	1.39
2	B	301	FOL	C12-C11	2.48	1.43	1.39
2	A	301	FOL	C7-N8	2.41	1.35	1.31
2	F	301	FOL	C7-N8	2.41	1.35	1.31
2	E	301	FOL	C12-C11	2.38	1.43	1.39
2	F	301	FOL	C15-C14	2.38	1.43	1.39
2	D	301	FOL	C12-C11	2.38	1.43	1.39
2	D	301	FOL	C7-N8	2.35	1.35	1.31
2	C	301	FOL	C15-C14	2.34	1.43	1.39
3	E	304	NAG	C1-C2	2.33	1.55	1.52
2	D	301	FOL	C15-C14	2.32	1.43	1.39
2	A	301	FOL	C15-C14	2.31	1.43	1.39
2	E	301	FOL	C8A-N1	2.29	1.41	1.36
2	E	301	FOL	C16-C11	2.29	1.42	1.39
2	H	301	FOL	C4-N3	2.27	1.36	1.33
2	C	301	FOL	C7-N8	2.27	1.35	1.31
2	D	301	FOL	C8A-N1	2.19	1.41	1.36
2	A	301	FOL	C12-C11	2.19	1.42	1.39
2	E	301	FOL	C7-C6	2.18	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	FOL	C7-N8	2.16	1.35	1.31
2	E	301	FOL	C4-N3	2.16	1.36	1.33
2	A	301	FOL	C4A-C8A	2.14	1.44	1.40
2	C	301	FOL	C8A-N1	2.13	1.41	1.36
2	A	301	FOL	C4-N3	2.12	1.36	1.33
2	A	301	FOL	C16-C11	2.10	1.42	1.39
2	F	301	FOL	C4A-C8A	2.08	1.44	1.40
2	C	301	FOL	C4A-C8A	2.08	1.44	1.40
2	H	301	FOL	C16-C11	2.06	1.42	1.39
2	C	301	FOL	C12-C11	2.02	1.42	1.39

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	FOL	N8-C8A-N1	6.16	122.48	115.77
2	F	301	FOL	N8-C8A-N1	6.03	122.34	115.77
2	C	301	FOL	N8-C8A-N1	6.01	122.32	115.77
2	D	301	FOL	N8-C8A-N1	5.99	122.30	115.77
2	G	301	FOL	N8-C8A-N1	5.93	122.23	115.77
2	A	301	FOL	N8-C8A-N1	5.91	122.20	115.77
2	H	301	FOL	N8-C8A-N1	5.86	122.16	115.77
2	B	301	FOL	N8-C8A-N1	5.60	121.88	115.77
2	B	301	FOL	C2-N1-C8A	5.44	121.35	115.48
2	C	301	FOL	C2-N1-C8A	5.00	120.87	115.48
2	F	301	FOL	C8A-C4A-C4	-4.99	116.87	119.96
2	G	301	FOL	C2-N1-C8A	4.88	120.75	115.48
2	D	301	FOL	C2-N1-C8A	4.87	120.74	115.48
2	E	301	FOL	C2-N3-C4	4.67	122.46	115.96
2	C	301	FOL	C2-N3-C4	4.66	122.44	115.96
2	E	301	FOL	C2-N1-C8A	4.65	120.50	115.48
2	E	301	FOL	C8A-C4A-C4	-4.65	117.08	119.96
2	F	301	FOL	C2-N1-C8A	4.63	120.47	115.48
2	H	301	FOL	C2-N1-C8A	4.62	120.47	115.48
2	F	301	FOL	C2-N3-C4	4.58	122.33	115.96
2	A	301	FOL	C8A-C4A-C4	-4.56	117.14	119.96
2	B	301	FOL	C2-N3-C4	4.51	122.23	115.96
2	A	301	FOL	C2-N3-C4	4.49	122.21	115.96
2	A	301	FOL	C2-N1-C8A	4.48	120.31	115.48
2	D	301	FOL	C2-N3-C4	4.46	122.16	115.96
2	G	301	FOL	C8A-C4A-C4	-4.36	117.26	119.96
2	H	301	FOL	C2-N3-C4	4.33	121.99	115.96
2	G	301	FOL	C2-N3-C4	4.32	121.97	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	FOL	C8A-C4A-C4	-4.30	117.30	119.96
2	B	301	FOL	N1-C2-N3	-4.28	121.77	127.21
2	H	301	FOL	N1-C2-N3	-4.15	121.93	127.21
2	B	301	FOL	C4A-C4-N3	-4.03	118.03	123.42
2	D	301	FOL	N1-C2-N3	-4.03	122.09	127.21
2	C	301	FOL	C8A-C4A-C4	-4.00	117.48	119.96
2	B	301	FOL	C8A-C4A-C4	-3.99	117.49	119.96
2	C	301	FOL	C4A-C4-N3	-3.94	118.15	123.42
2	C	301	FOL	N1-C2-N3	-3.90	122.26	127.21
2	H	301	FOL	C8A-C4A-C4	-3.80	117.61	119.96
2	A	301	FOL	N1-C2-N3	-3.79	122.39	127.21
2	B	301	FOL	C6-C7-N8	-3.75	119.54	123.14
2	G	301	FOL	N1-C2-N3	-3.74	122.46	127.21
2	C	301	FOL	C6-C7-N8	-3.67	119.62	123.14
2	E	301	FOL	N1-C2-N3	-3.59	122.65	127.21
2	F	301	FOL	N1-C2-N3	-3.56	122.69	127.21
2	E	301	FOL	C4A-C4-N3	-3.56	118.67	123.42
2	F	301	FOL	C4A-C4-N3	-3.48	118.77	123.42
2	A	301	FOL	C4A-C4-N3	-3.47	118.78	123.42
2	H	301	FOL	C4A-C4-N3	-3.43	118.83	123.42
2	G	301	FOL	C4A-C4-N3	-3.43	118.83	123.42
2	A	301	FOL	C6-C7-N8	-3.41	119.86	123.14
2	D	301	FOL	C4A-C4-N3	-3.41	118.86	123.42
2	G	301	FOL	C6-C7-N8	-3.37	119.90	123.14
2	H	301	FOL	C6-C7-N8	-3.30	119.97	123.14
2	F	301	FOL	C6-C7-N8	-3.29	119.98	123.14
2	D	301	FOL	C6-C7-N8	-3.28	119.99	123.14
2	E	301	FOL	C6-C7-N8	-3.22	120.05	123.14
2	B	301	FOL	C8A-C4A-N5	-3.07	119.02	122.30
2	B	301	FOL	C7-N8-C8A	2.87	121.20	117.20
2	C	301	FOL	C8A-C4A-N5	-2.71	119.41	122.30
2	A	301	FOL	C7-N8-C8A	2.70	120.96	117.20
2	G	301	FOL	C7-N8-C8A	2.68	120.94	117.20
2	F	301	FOL	C7-N8-C8A	2.60	120.82	117.20
2	C	301	FOL	C7-N8-C8A	2.56	120.77	117.20
2	D	301	FOL	C7-N8-C8A	2.56	120.76	117.20
2	H	301	FOL	C7-N8-C8A	2.55	120.75	117.20
2	G	301	FOL	C8A-C4A-N5	-2.54	119.58	122.30
3	E	303	NAG	C2-N2-C7	-2.51	119.53	122.90
2	B	301	FOL	O2-CT-O1	-2.44	118.55	124.08
2	F	301	FOL	C8A-C4A-N5	-2.41	119.73	122.30
3	B	302	NAG	C2-N2-C7	-2.37	119.73	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FOL	C6-N5-C4A	2.36	121.03	118.45
2	E	301	FOL	C8A-C4A-N5	-2.33	119.81	122.30
2	E	301	FOL	O2-CT-O1	-2.33	118.80	124.08
2	F	301	FOL	O2-CT-CA	2.30	121.29	113.51
2	E	301	FOL	C7-N8-C8A	2.27	120.36	117.20
2	G	301	FOL	O2-CT-O1	-2.26	118.94	124.08
3	D	303	NAG	C2-N2-C7	-2.23	119.92	122.90
2	D	301	FOL	C8A-C4A-N5	-2.18	119.97	122.30
2	F	301	FOL	O2-CT-O1	-2.18	119.13	124.08
2	D	301	FOL	O2-CT-O1	-2.18	119.13	124.08
2	B	301	FOL	C6-N5-C4A	2.17	120.83	118.45
2	E	301	FOL	O2-CT-CA	2.14	120.76	113.51
2	G	301	FOL	O2-CT-CA	2.11	120.65	113.51
2	H	301	FOL	C8A-C4A-N5	-2.09	120.07	122.30
2	G	301	FOL	C6-N5-C4A	2.08	120.73	118.45
2	C	301	FOL	O2-CT-O1	-2.08	119.36	124.08
3	F	303	NAG	C2-N2-C7	-2.08	120.11	122.90
2	H	301	FOL	O2-CT-O1	-2.06	119.40	124.08
3	H	303	NAG	C2-N2-C7	-2.05	120.16	122.90
2	A	301	FOL	O2-CT-O1	-2.03	119.47	124.08
3	C	302	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	NAG	C8-C7-N2-C2
3	A	303	NAG	O7-C7-N2-C2
3	A	304	NAG	C1-C2-N2-C7
3	B	302	NAG	C8-C7-N2-C2
3	B	302	NAG	O7-C7-N2-C2
3	C	302	NAG	C8-C7-N2-C2
3	C	302	NAG	O7-C7-N2-C2
3	C	303	NAG	C8-C7-N2-C2
3	C	303	NAG	O7-C7-N2-C2
3	D	302	NAG	C8-C7-N2-C2
3	D	302	NAG	O7-C7-N2-C2
3	D	303	NAG	C3-C2-N2-C7
3	D	303	NAG	C8-C7-N2-C2
3	D	303	NAG	O7-C7-N2-C2
3	D	304	NAG	C8-C7-N2-C2
3	D	304	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	E	302	NAG	C8-C7-N2-C2
3	E	302	NAG	O7-C7-N2-C2
3	F	304	NAG	C8-C7-N2-C2
3	F	304	NAG	O7-C7-N2-C2
3	G	302	NAG	C8-C7-N2-C2
3	G	302	NAG	O7-C7-N2-C2
3	G	303	NAG	C8-C7-N2-C2
3	G	303	NAG	O7-C7-N2-C2
3	H	303	NAG	C8-C7-N2-C2
3	H	303	NAG	O7-C7-N2-C2
3	H	304	NAG	C8-C7-N2-C2
3	H	304	NAG	O7-C7-N2-C2
3	E	303	NAG	O7-C7-N2-C2
3	F	302	NAG	O5-C5-C6-O6
2	F	301	FOL	CB-CA-CT-O2
3	E	304	NAG	O5-C5-C6-O6
3	E	303	NAG	C4-C5-C6-O6
3	E	303	NAG	C8-C7-N2-C2
3	F	303	NAG	C8-C7-N2-C2
3	F	303	NAG	O7-C7-N2-C2
3	B	303	NAG	C4-C5-C6-O6
3	F	302	NAG	C4-C5-C6-O6
2	G	301	FOL	C13-C14-N10-C9
3	E	304	NAG	C4-C5-C6-O6
3	E	303	NAG	O5-C5-C6-O6
2	G	301	FOL	C15-C14-N10-C9
2	F	301	FOL	N-CA-CB-CG
3	B	303	NAG	O5-C5-C6-O6
3	B	304	NAG	C8-C7-N2-C2
2	A	301	FOL	N-CA-CB-CG
2	B	301	FOL	N-CA-CB-CG
2	A	301	FOL	N-CA-CT-O1
2	A	301	FOL	N-CA-CT-O2
2	C	301	FOL	N-CA-CB-CG
2	D	301	FOL	N-CA-CB-CG
2	E	301	FOL	N-CA-CB-CG
2	G	301	FOL	N-CA-CB-CG
2	H	301	FOL	N-CA-CB-CG
2	B	301	FOL	CT-CA-CB-CG
2	C	301	FOL	CT-CA-CB-CG
2	F	301	FOL	CT-CA-CB-CG
3	B	304	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	F	301	FOL	C13-C14-N10-C9
3	B	303	NAG	C8-C7-N2-C2
2	C	301	FOL	C13-C14-N10-C9
2	F	301	FOL	CB-CA-CT-O1
3	E	302	NAG	O5-C5-C6-O6
2	F	301	FOL	C15-C14-N10-C9
2	A	301	FOL	CT-CA-CB-CG
2	D	301	FOL	CT-CA-CB-CG
2	E	301	FOL	CT-CA-CB-CG
2	G	301	FOL	CT-CA-CB-CG
2	H	301	FOL	CT-CA-CB-CG
2	E	301	FOL	N-CA-CT-O2
2	F	301	FOL	N-CA-CT-O2
2	A	301	FOL	C13-C14-N10-C9
2	C	301	FOL	C15-C14-N10-C9
2	E	301	FOL	N-CA-CT-O1
2	E	301	FOL	C13-C14-N10-C9
3	D	304	NAG	C4-C5-C6-O6
2	A	301	FOL	C15-C14-N10-C9
2	E	301	FOL	C15-C14-N10-C9
3	B	303	NAG	O7-C7-N2-C2
3	H	302	NAG	C8-C7-N2-C2
2	B	301	FOL	C13-C14-N10-C9
3	H	302	NAG	O7-C7-N2-C2
2	F	301	FOL	N-CA-CT-O1
2	B	301	FOL	C15-C14-N10-C9
2	D	301	FOL	C13-C14-N10-C9
3	A	304	NAG	O5-C5-C6-O6
2	H	301	FOL	C13-C14-N10-C9
3	G	303	NAG	C4-C5-C6-O6
3	D	304	NAG	C3-C2-N2-C7
2	A	301	FOL	CB-CA-CT-O2
2	B	301	FOL	CB-CA-CT-O2
2	A	301	FOL	CB-CA-CT-O1
2	B	301	FOL	CB-CA-CT-O1
3	D	302	NAG	C4-C5-C6-O6
2	D	301	FOL	C15-C14-N10-C9
3	D	303	NAG	C4-C5-C6-O6
2	H	301	FOL	C15-C14-N10-C9
3	D	302	NAG	O5-C5-C6-O6
2	C	301	FOL	N-CA-CT-O1
3	C	303	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	D	301	FOL	N-CA-CT-O1
2	H	301	FOL	N-CA-CT-O1
2	H	301	FOL	N-CA-CT-O2
2	C	301	FOL	CB-CA-CT-O1
3	A	304	NAG	C3-C2-N2-C7
3	A	303	NAG	C4-C5-C6-O6
2	C	301	FOL	N-CA-CT-O2
2	D	301	FOL	N-CA-CT-O2
2	D	301	FOL	CB-CA-CT-O1
2	G	301	FOL	CB-CA-CT-O2
2	H	301	FOL	CB-CA-CT-O1
2	C	301	FOL	CB-CA-CT-O2
2	D	301	FOL	CB-CA-CT-O2
2	H	301	FOL	CB-CA-CT-O2
3	G	303	NAG	O5-C5-C6-O6
2	G	301	FOL	CB-CA-CT-O1
3	D	304	NAG	O5-C5-C6-O6
3	D	303	NAG	O5-C5-C6-O6
2	A	301	FOL	N5-C6-C9-N10
2	C	301	FOL	N5-C6-C9-N10
2	D	301	FOL	N5-C6-C9-N10
2	G	301	FOL	N5-C6-C9-N10
2	H	301	FOL	N5-C6-C9-N10

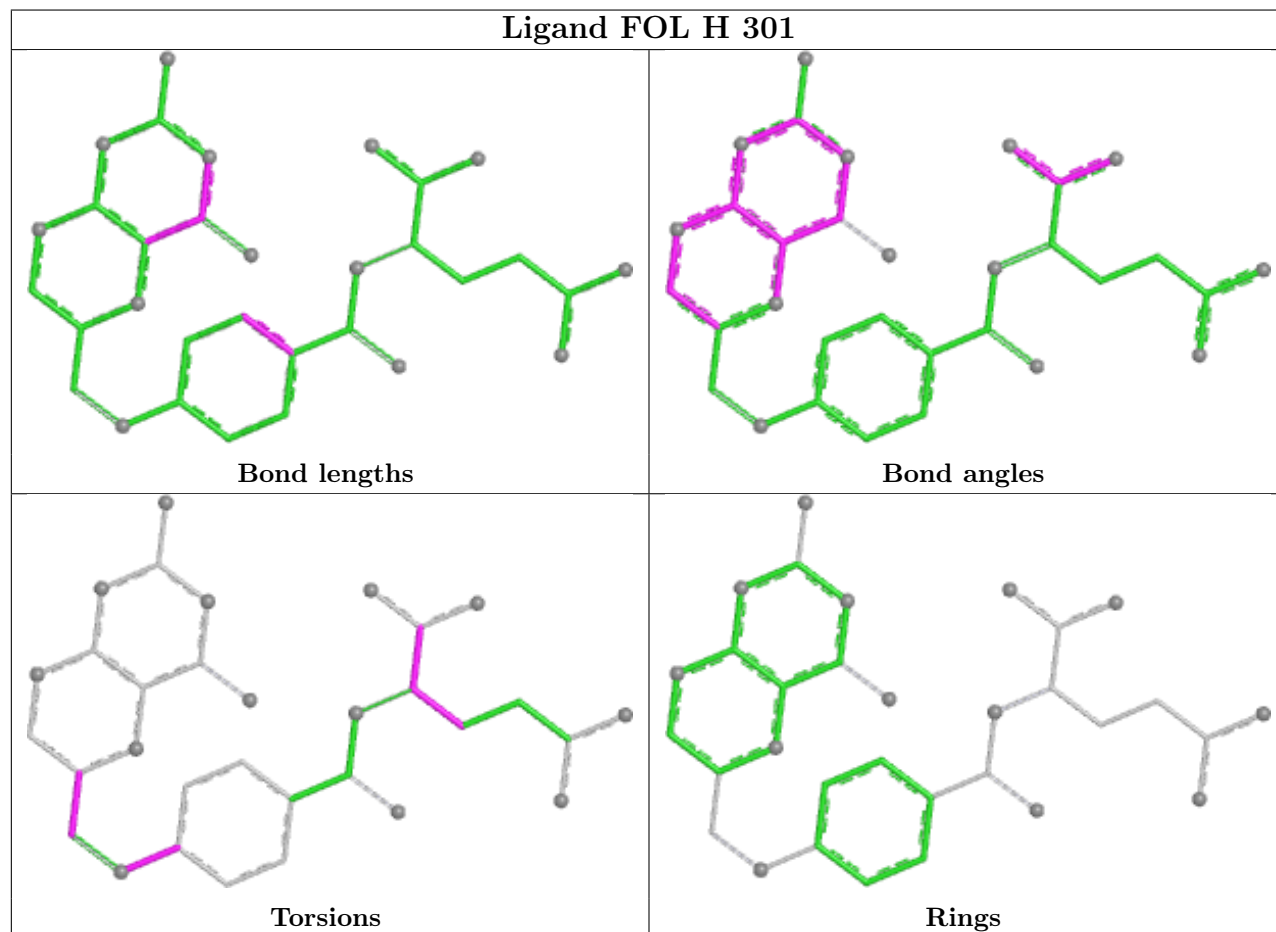
There are no ring outliers.

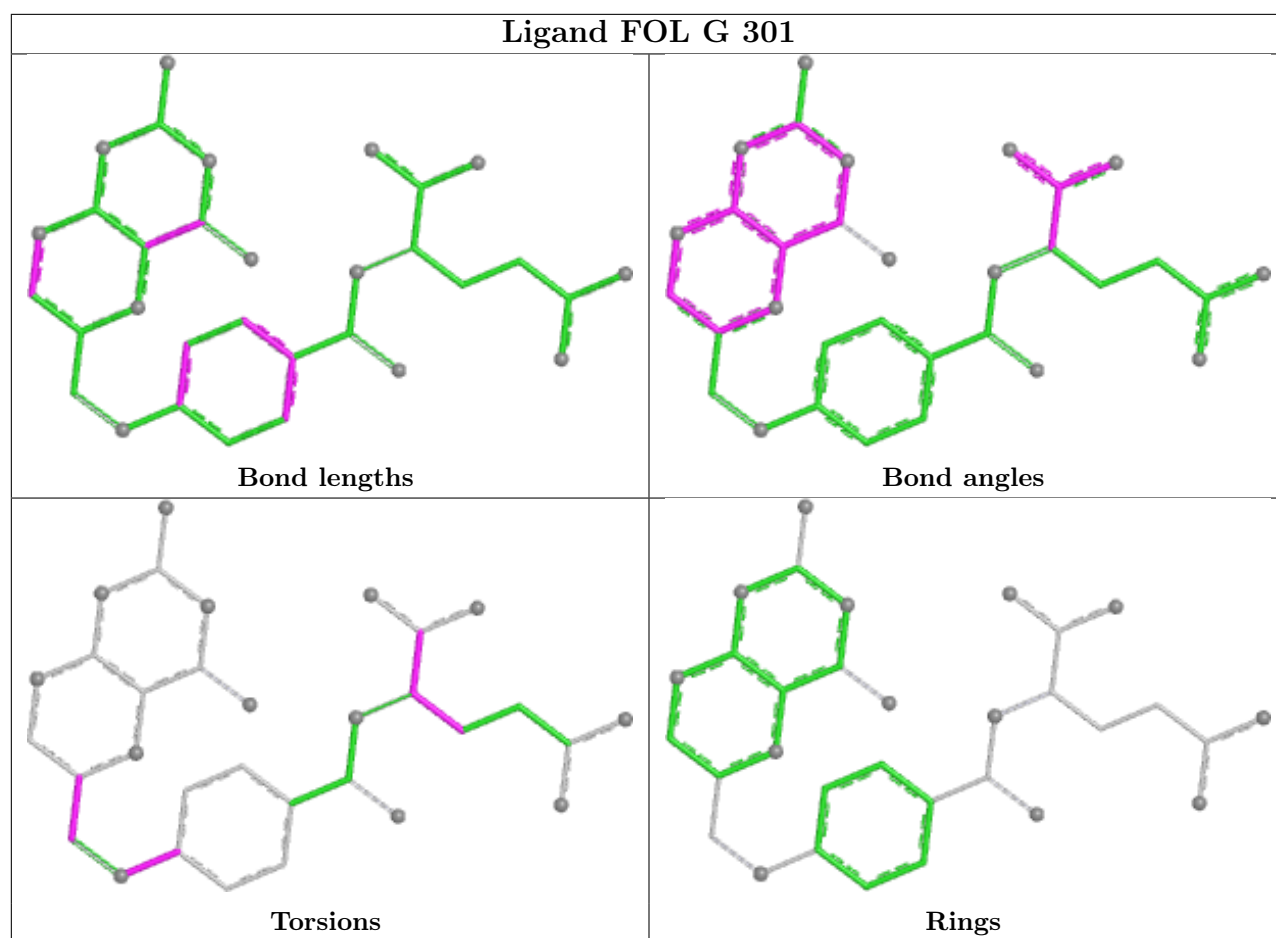
11 monomers are involved in 13 short contacts:

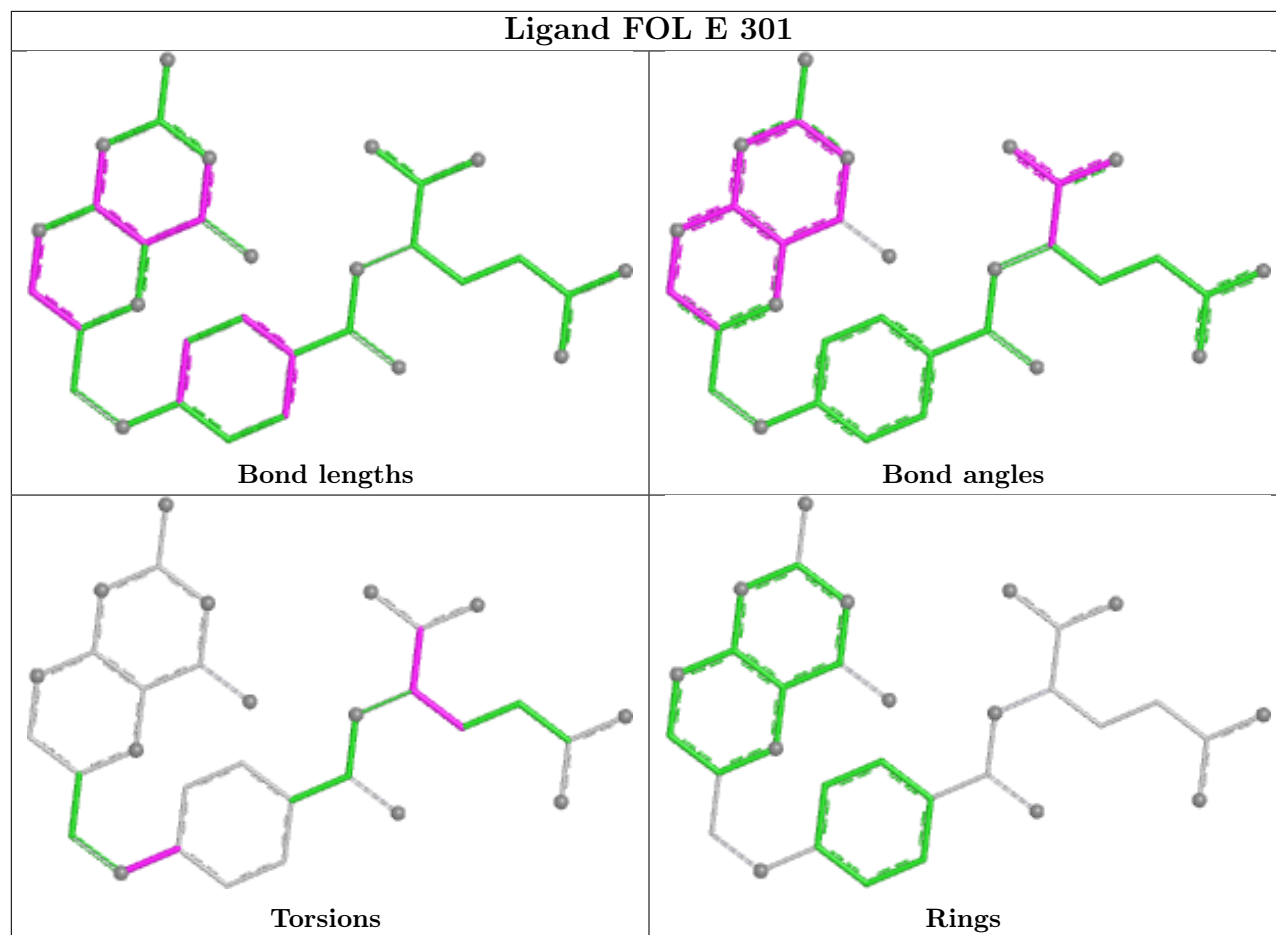
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	FOL	1	0
3	H	302	NAG	1	0
2	E	301	FOL	1	0
3	B	302	NAG	1	0
3	F	302	NAG	1	0
3	E	303	NAG	2	0
3	E	304	NAG	1	0
3	A	304	NAG	1	0
3	B	304	NAG	2	0
2	B	301	FOL	1	0
3	D	303	NAG	1	0

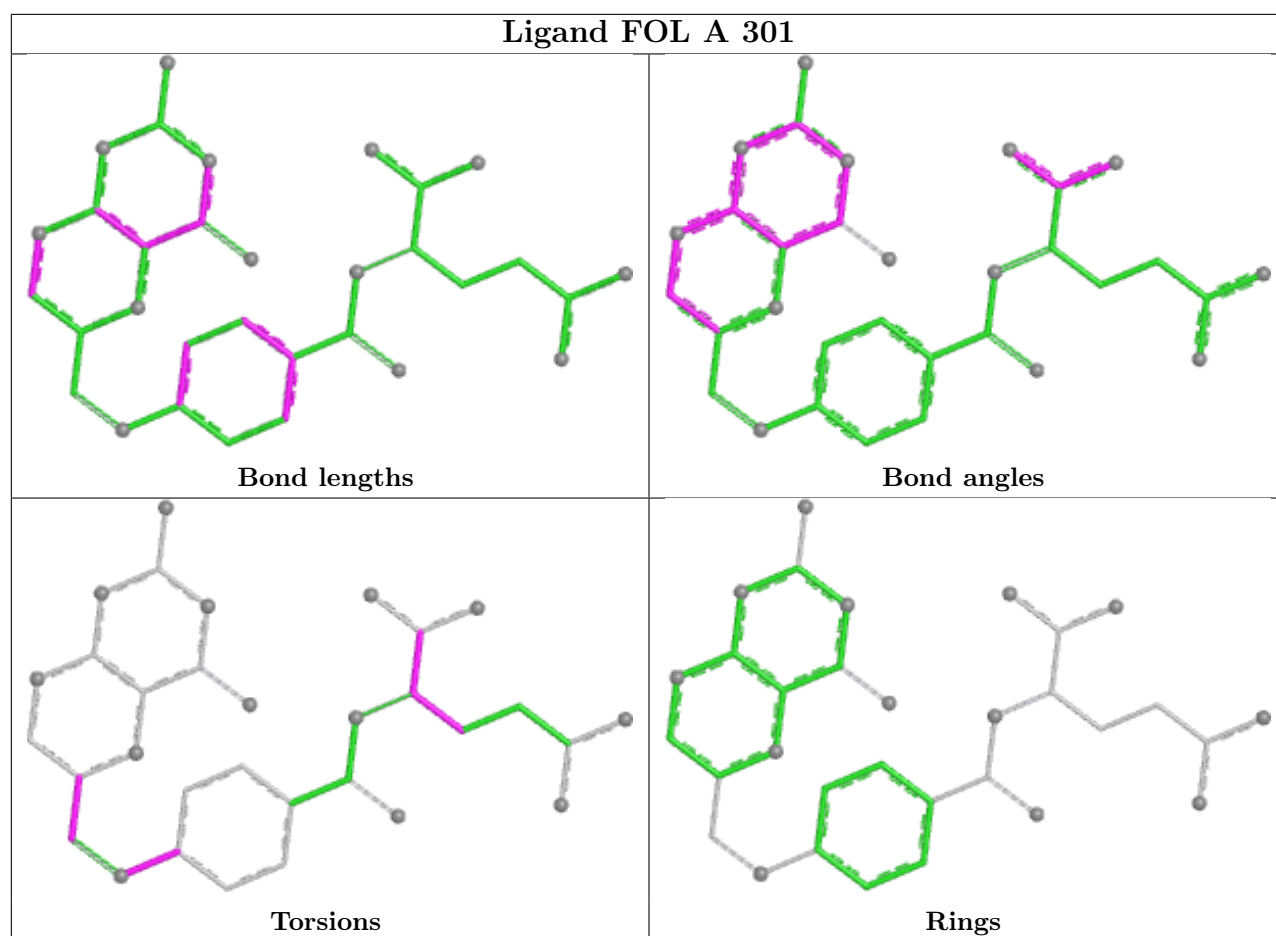
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

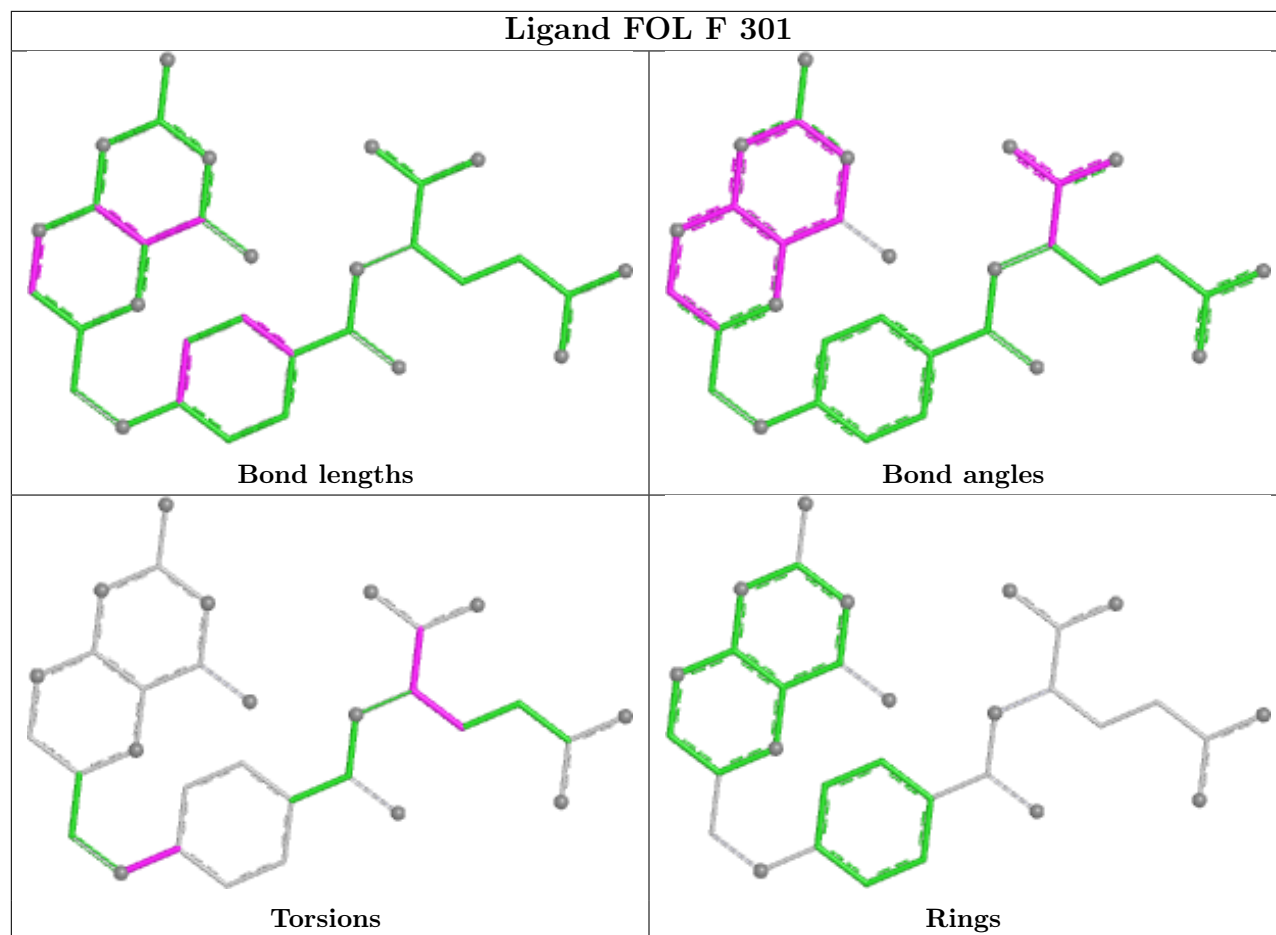




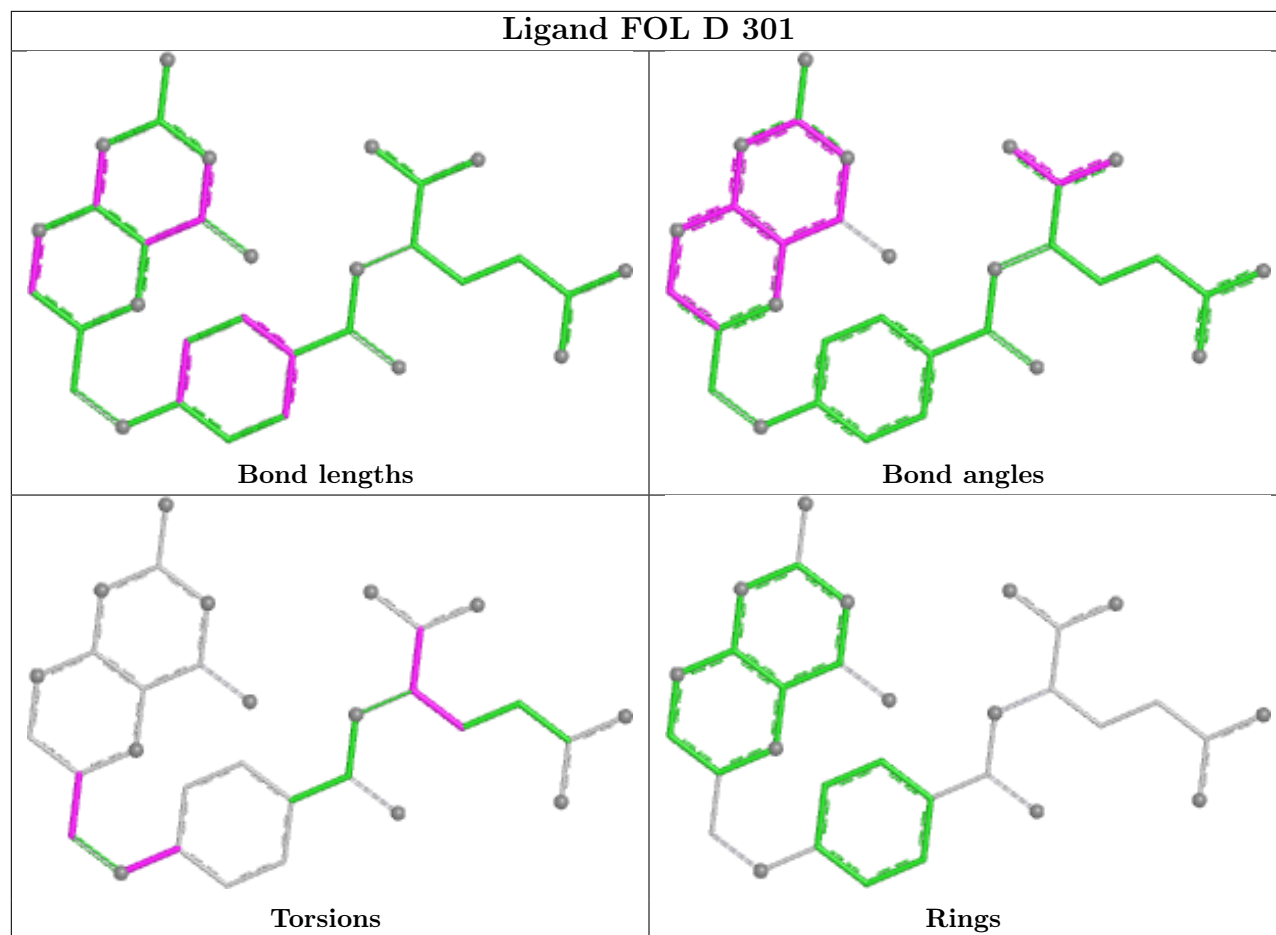




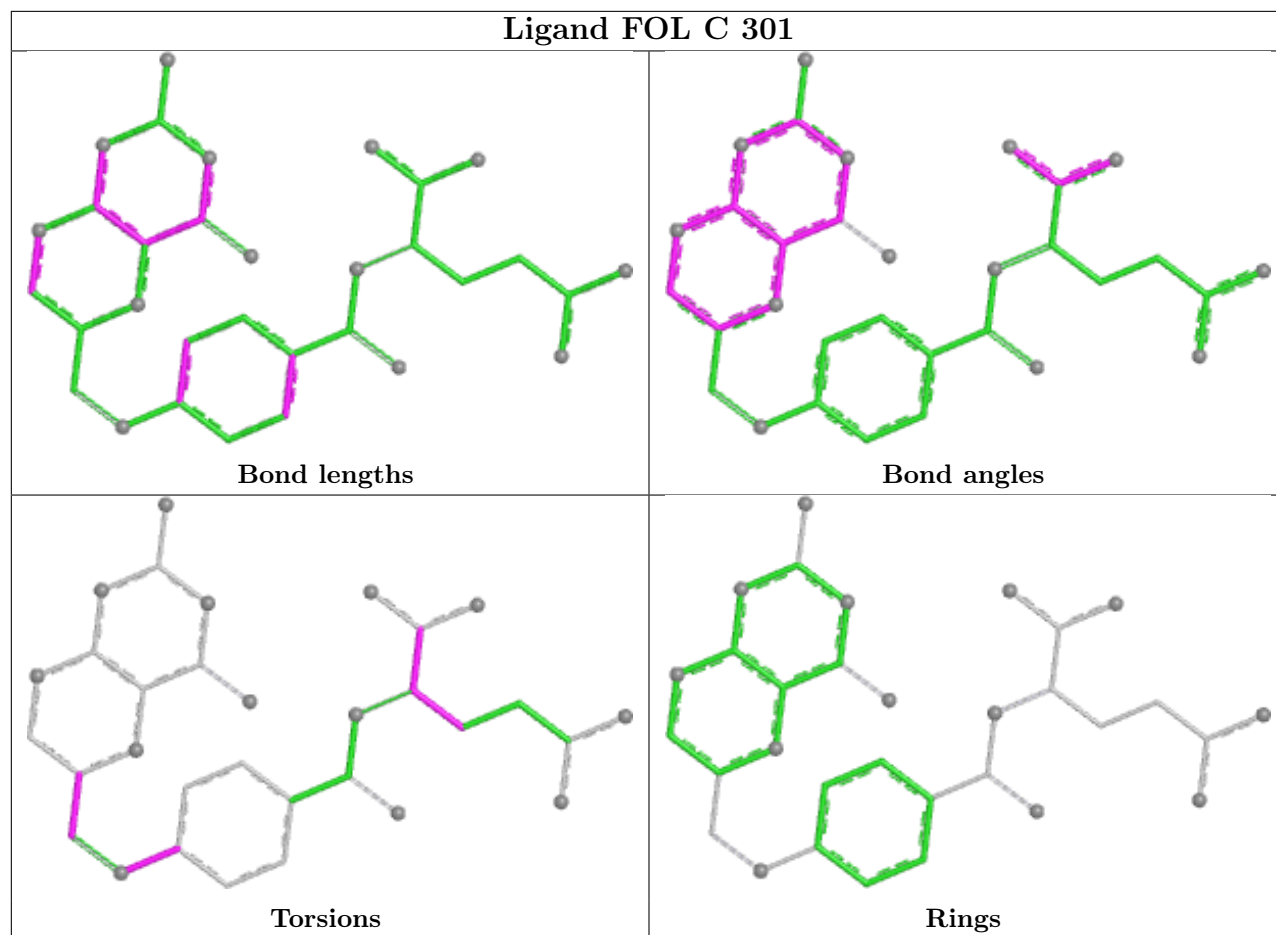
Ligand FOL F 301

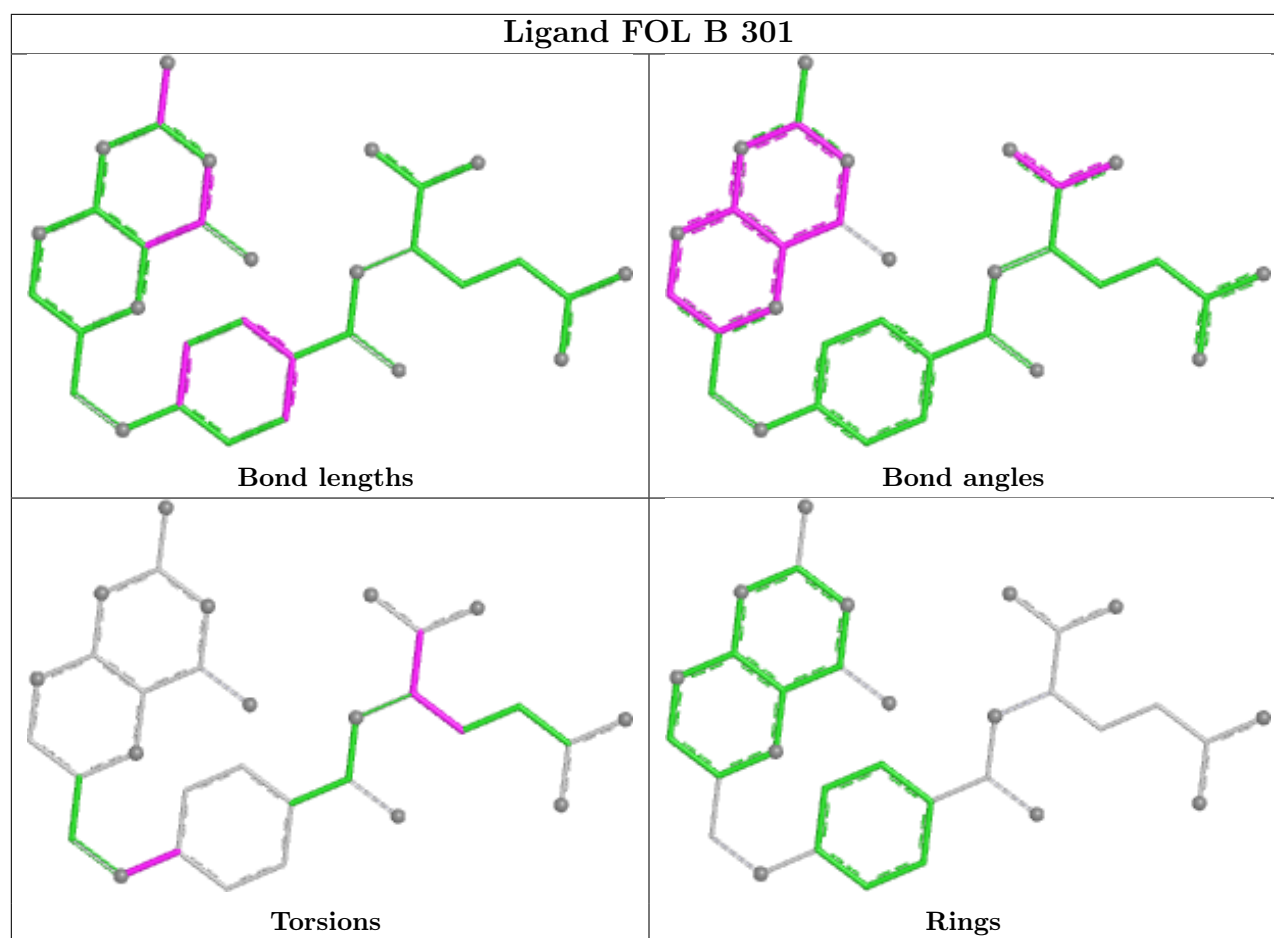


Ligand FOL D 301



Ligand FOL C 301





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	207/218 (94%)	-0.03	3 (1%) 73 66	35, 54, 78, 125	0
1	B	204/218 (93%)	0.30	5 (2%) 58 49	43, 69, 93, 112	0
1	C	209/218 (95%)	0.22	2 (0%) 79 73	48, 69, 91, 115	0
1	D	210/218 (96%)	0.40	7 (3%) 49 41	51, 70, 98, 132	0
1	E	206/218 (94%)	0.47	6 (2%) 54 45	45, 71, 97, 109	0
1	F	208/218 (95%)	0.43	6 (2%) 54 45	51, 73, 97, 123	0
1	G	205/218 (94%)	0.53	4 (1%) 64 56	49, 78, 110, 132	0
1	H	204/218 (93%)	0.05	3 (1%) 71 64	31, 56, 77, 112	0
All	All	1653/1744 (94%)	0.30	36 (2%) 62 53	31, 67, 98, 132	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	ILE	4.9
1	F	215	LEU	4.0
1	D	6	TRP	3.6
1	D	7	ALA	3.4
1	D	213	GLY	3.3
1	E	7	ALA	3.1
1	B	9	THR	2.9
1	D	5	ALA	2.9
1	C	216	VAL	2.9
1	F	214	THR	2.8
1	H	9	THR	2.8
1	A	214	THR	2.7
1	G	137	GLY	2.6
1	A	9	THR	2.6
1	H	10	GLU	2.5
1	D	30	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	210	ALA	2.5
1	D	185	GLY	2.4
1	G	11	LEU	2.3
1	G	151	ALA	2.3
1	F	211	MET	2.3
1	H	11	LEU	2.3
1	G	18	ALA	2.3
1	E	9	THR	2.3
1	B	149	VAL	2.2
1	F	213	GLY	2.2
1	A	61	ARG	2.2
1	B	151	ALA	2.1
1	B	11	LEU	2.1
1	E	42	ALA	2.1
1	F	11	LEU	2.1
1	C	215	LEU	2.1
1	E	10	GLU	2.1
1	B	42	ALA	2.0
1	E	38	TRP	2.0
1	E	151	ALA	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 monosaccharides 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
3	NAG	B	304	14/15	-0.03	0.22	109,112,113,114	0
3	NAG	D	304	14/15	0.21	0.18	113,117,120,121	0
3	NAG	H	304	14/15	0.25	0.24	112,116,118,118	0

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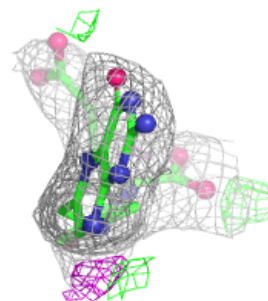
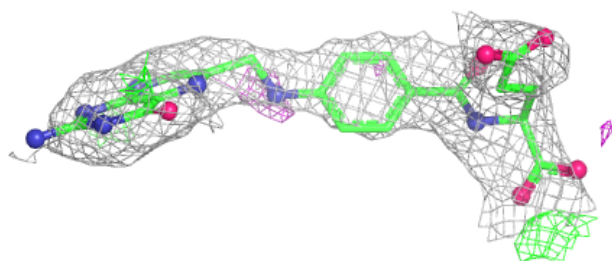
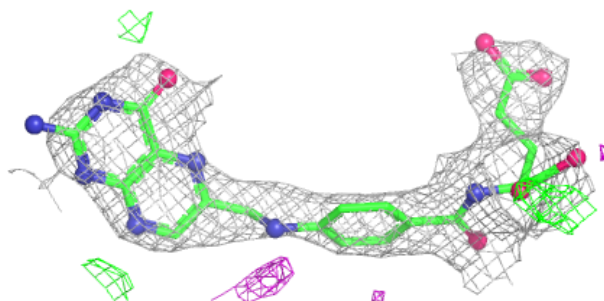
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	304	14/15	0.26	0.18	113,116,117,117	0
3	NAG	F	304	14/15	0.37	0.19	112,115,116,117	0
3	NAG	A	304	14/15	0.63	0.15	97,102,105,106	0
3	NAG	G	303	14/15	0.63	0.15	93,94,96,97	0
3	NAG	D	303	14/15	0.63	0.15	91,96,98,99	0
3	NAG	E	303	14/15	0.75	0.11	81,83,85,87	0
3	NAG	H	303	14/15	0.76	0.14	68,72,74,74	0
3	NAG	B	303	14/15	0.76	0.13	82,83,84,85	0
3	NAG	G	302	14/15	0.77	0.14	91,92,95,96	0
3	NAG	E	302	14/15	0.77	0.14	92,94,99,99	0
3	NAG	C	303	14/15	0.78	0.13	85,86,89,89	0
3	NAG	A	303	14/15	0.79	0.13	81,83,89,89	0
3	NAG	F	303	14/15	0.85	0.12	81,83,86,88	0
3	NAG	C	302	14/15	0.86	0.10	77,79,81,82	0
3	NAG	B	302	14/15	0.88	0.10	75,76,81,82	0
3	NAG	F	302	14/15	0.88	0.09	66,72,75,76	0
3	NAG	D	302	14/15	0.88	0.12	84,85,88,89	0
2	FOL	G	301	32/32	0.88	0.18	95,96,99,101	0
2	FOL	B	301	32/32	0.89	0.14	51,70,79,79	0
2	FOL	F	301	32/32	0.91	0.13	66,70,78,82	0
2	FOL	C	301	32/32	0.91	0.12	60,63,76,78	0
2	FOL	D	301	32/32	0.92	0.13	67,69,79,81	0
2	FOL	E	301	32/32	0.92	0.13	55,72,89,90	0
2	FOL	A	301	32/32	0.93	0.11	45,57,67,70	0
3	NAG	A	302	14/15	0.93	0.09	47,50,51,52	0
2	FOL	H	301	32/32	0.95	0.09	40,50,58,61	0
3	NAG	H	302	14/15	0.96	0.07	45,46,47,48	0

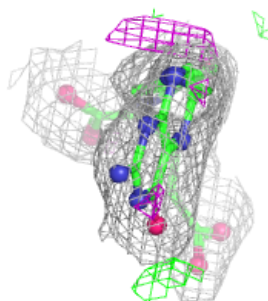
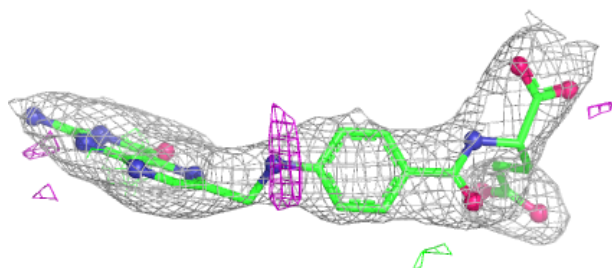
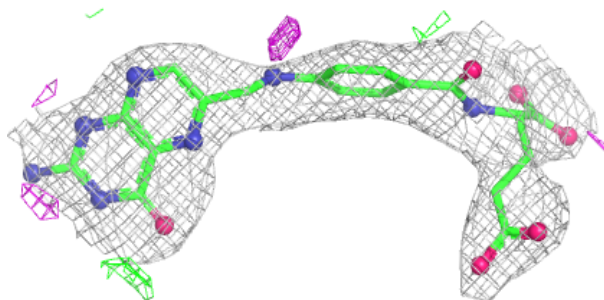
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FOL G 301:

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

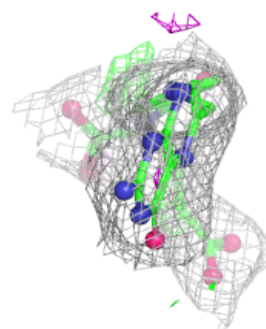
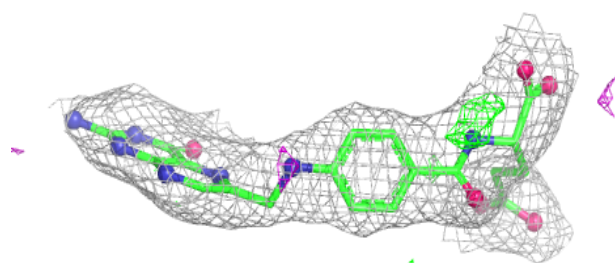
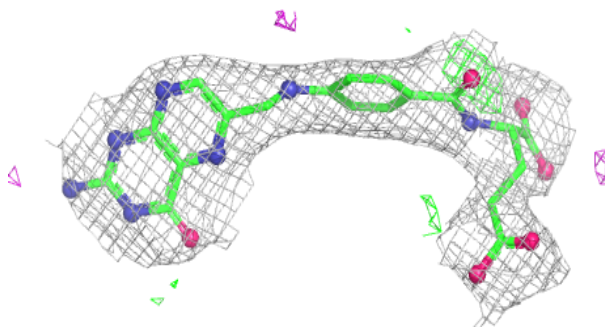
**Electron density around FOL B 301:**

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

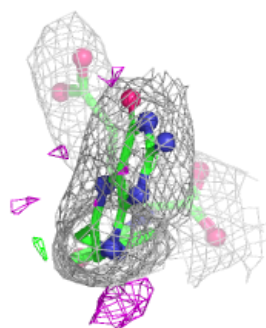
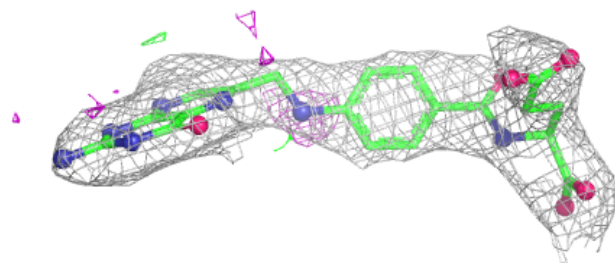
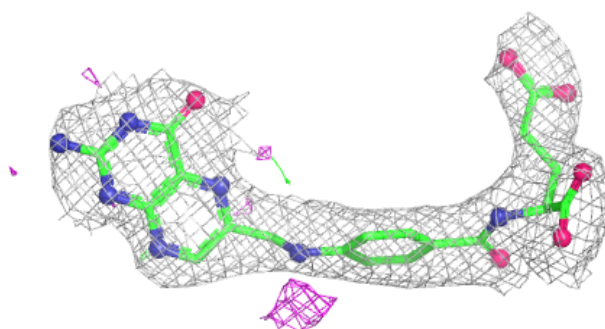


Electron density around FOL F 301:

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

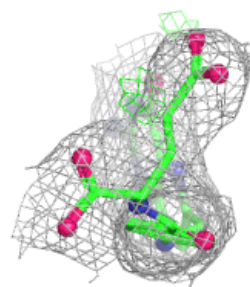
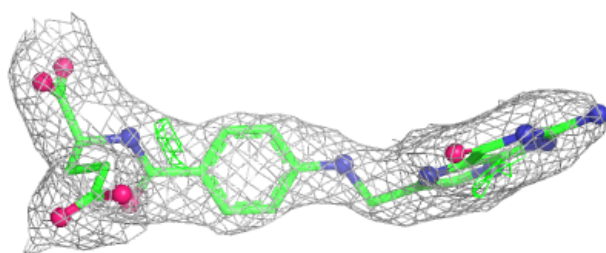
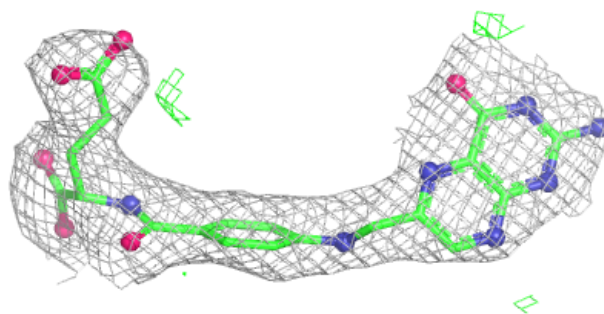
**Electron density around FOL C 301:**

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

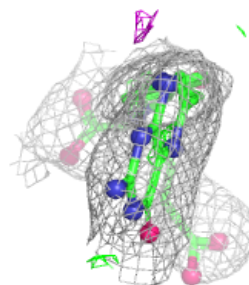
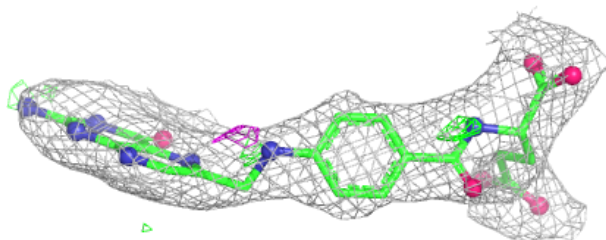
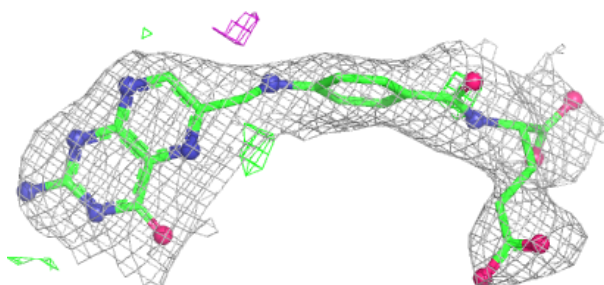


Electron density around FOL D 301:

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

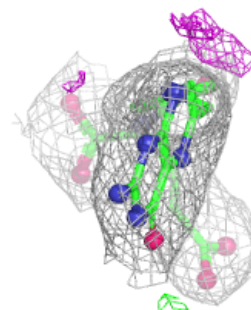
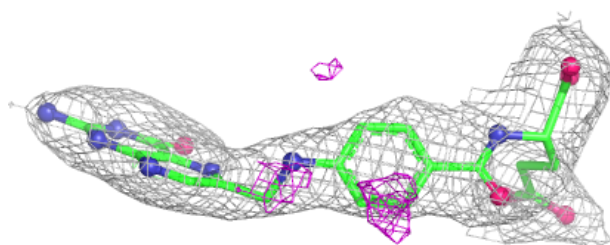
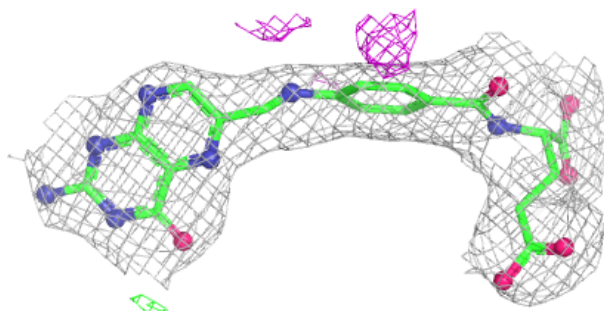
**Electron density around FOL E 301:**

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

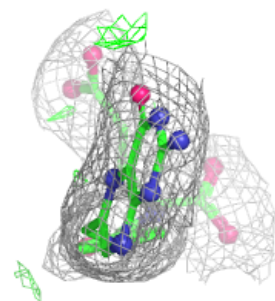
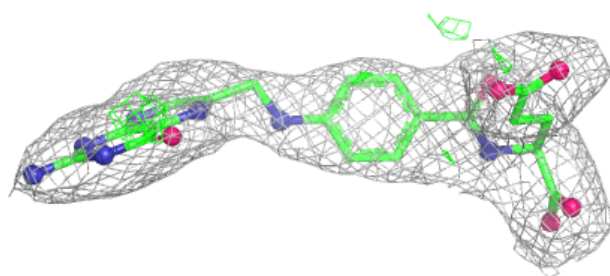
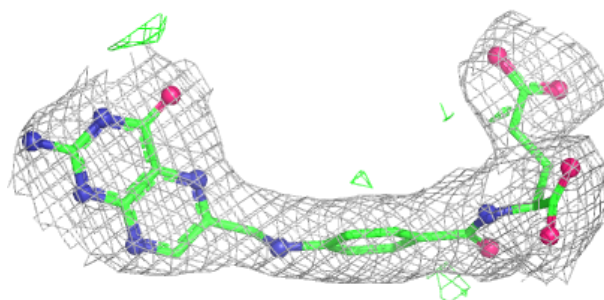


Electron density around FOL A 301:

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

**Electron density around FOL H 301:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.