



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:09 PM BST

PDB ID : 4HW2
Title : Discovery of potent Mcl-1 inhibitors using fragment-based methods and structure-based design
Authors : Zhao, B.
Deposited on : 2012-11-07
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

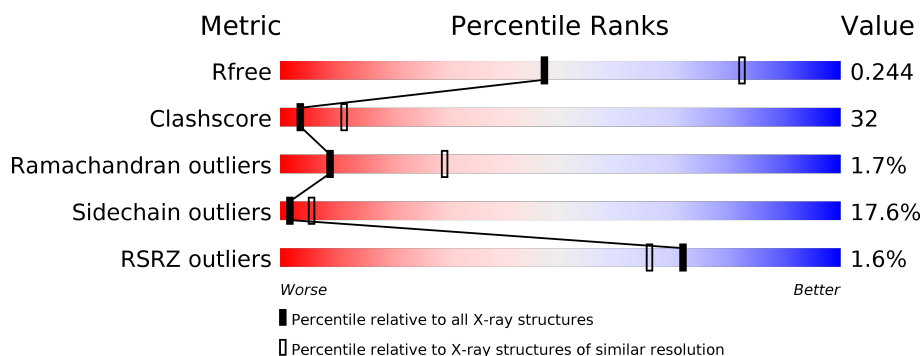
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	153	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>8%</div> <div>••</div> </div> </div>
1	B	153	<div> <div></div> <div> <div>52%</div> <div>33%</div> <div>14%</div> <div>•</div> </div> </div>
1	C	153	<div> <div>0%</div> <div> <div></div> <div>44%</div> <div>39%</div> <div>15%</div> <div>•</div> </div> </div>
1	D	153	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>7%</div> <div>••</div> </div> </div>
1	E	153	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>39%</div> <div>9%</div> <div>•</div> </div> </div>
1	F	153	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>32%</div> <div>15%</div> <div>••</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7376 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.

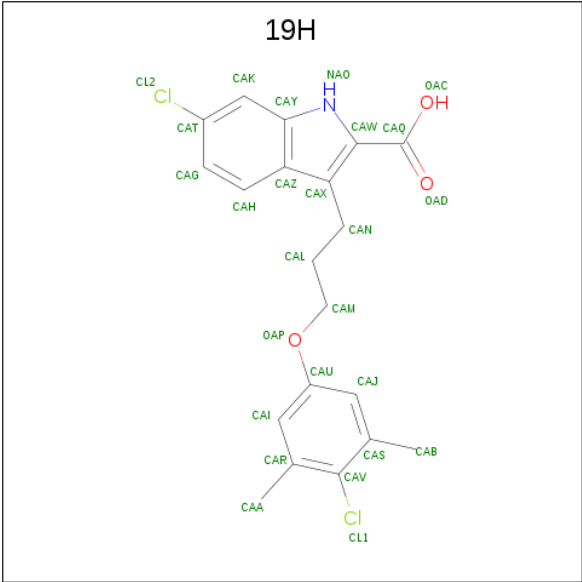
- Molecule 1 is a protein called Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1186	745	217	221	3			
1	B	151	Total	C	N	O	S	0	0	0
			1212	761	224	223	4			
1	C	150	Total	C	N	O	S	0	0	0
			1185	745	218	218	4			
1	D	151	Total	C	N	O	S	0	0	0
			1203	757	221	221	4			
1	E	151	Total	C	N	O	S	0	0	0
			1209	760	224	221	4			
1	F	150	Total	C	N	O	S	0	0	0
			1191	747	218	222	4			

There are 6 discrepancies between the modelled and reference sequences:

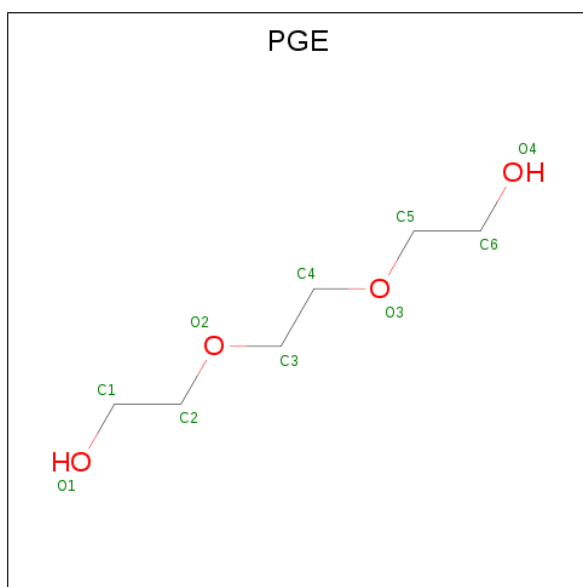
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	EXPRESSION TAG	UNP Q07820
B	171	GLY	-	EXPRESSION TAG	UNP Q07820
C	171	GLY	-	EXPRESSION TAG	UNP Q07820
D	171	GLY	-	EXPRESSION TAG	UNP Q07820
E	171	GLY	-	EXPRESSION TAG	UNP Q07820
F	171	GLY	-	EXPRESSION TAG	UNP Q07820

- Molecule 2 is 6-chloro-3-[3-(4-chloro-3,5-dimethylphenoxy)propyl]-1H-indole-2-carboxylic acid (three-letter code: 19H) (formula: C₂₀H₁₉Cl₂NO₃).



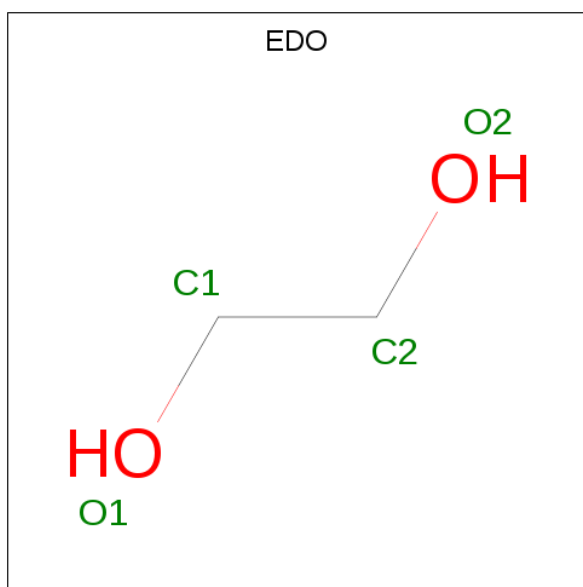
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	B	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	C	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	D	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	E	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		
2	F	1	Total	C	Cl	N	O	0	0
			26	20	2	1	3		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

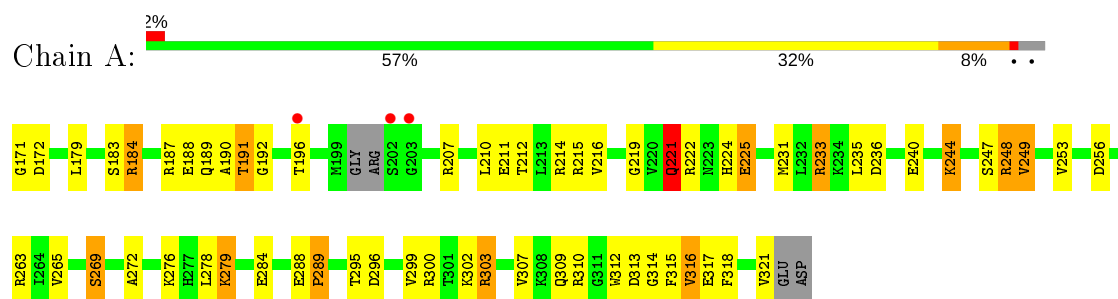


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

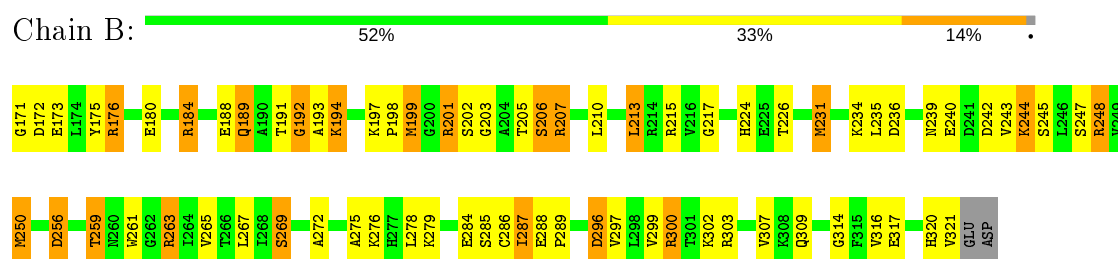
3 Residue-property plots

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

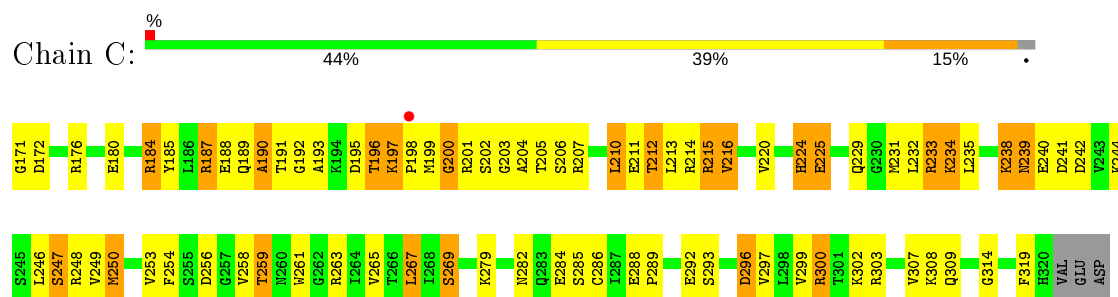
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



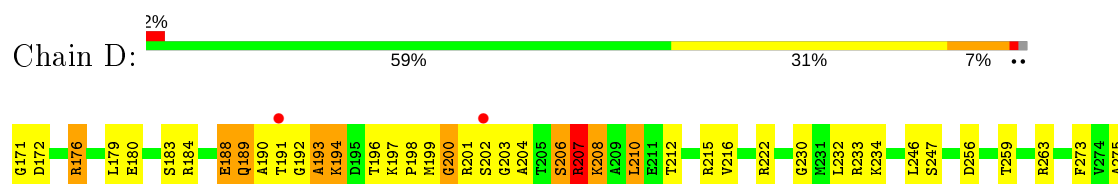
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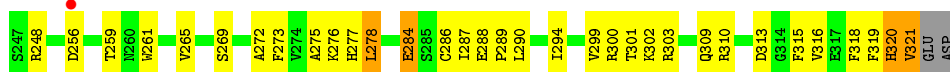


- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1





- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.00 Å 134.33 Å 62.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 38.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 97.3 (38.92-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.217 , 0.245 0.219 , 0.244	Depositor DCC
R_{free} test set	2491 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7376	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: PGE, EDO, 19H

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	1.29	9/1205 (0.7%)	0.87	0/1623
1	B	1.23	4/1232 (0.3%)	0.85	1/1656 (0.1%)
1	C	1.17	6/1205 (0.5%)	0.87	1/1623 (0.1%)
1	D	0.95	5/1223 (0.4%)	0.79	1/1645 (0.1%)
1	E	1.05	4/1229 (0.3%)	0.80	1/1652 (0.1%)
1	F	1.04	8/1211 (0.7%)	0.97	2/1631 (0.1%)
All	All	1.13	36/7305 (0.5%)	0.86	6/9830 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	F	0	2
All	All	0	4

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	269	SER	CB-OG	-6.00	1.34	1.42
1	C	216	VAL	CB-CG1	-5.92	1.40	1.52
1	F	184	ARG	CZ-NH1	-5.91	1.25	1.33
1	E	233	ARG	CZ-NH2	-5.80	1.25	1.33
1	A	233	ARG	CZ-NH1	-5.78	1.25	1.33
1	D	188	GLU	CD-OE1	-5.71	1.19	1.25
1	A	184	ARG	CZ-NH1	-5.70	1.25	1.33
1	F	211	GLU	CG-CD	-5.68	1.43	1.51
1	C	247	SER	CB-OG	-5.67	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	ARG	CZ-NH1	-5.66	1.25	1.33
1	A	247	SER	CB-OG	-5.64	1.34	1.42
1	B	316	VAL	CB-CG1	-5.64	1.41	1.52
1	A	316	VAL	CB-CG1	-5.61	1.41	1.52
1	D	184	ARG	CZ-NH1	-5.61	1.25	1.33
1	A	249	VAL	CB-CG2	-5.54	1.41	1.52
1	A	207	ARG	CZ-NH1	-5.53	1.25	1.33
1	D	208	LYS	CD-CE	-5.50	1.37	1.51
1	B	300	ARG	CZ-NH2	-5.49	1.25	1.33
1	C	300	ARG	CZ-NH1	-5.44	1.25	1.33
1	D	247	SER	CB-OG	-5.39	1.35	1.42
1	F	211	GLU	CD-OE1	-5.35	1.19	1.25
1	B	317	GLU	CG-CD	-5.34	1.44	1.51
1	F	300	ARG	CZ-NH1	-5.34	1.26	1.33
1	F	247	SER	CB-OG	-5.32	1.35	1.42
1	F	269	SER	CB-OG	-5.28	1.35	1.42
1	F	300	ARG	CZ-NH2	-5.27	1.26	1.33
1	C	225	GLU	CD-OE1	-5.24	1.19	1.25
1	B	215	ARG	CB-CG	-5.22	1.38	1.52
1	C	216	VAL	CB-CG2	-5.20	1.42	1.52
1	A	233	ARG	CZ-NH2	-5.20	1.26	1.33
1	A	221	GLN	CD-OE1	-5.19	1.12	1.24
1	D	207	ARG	CZ-NH1	-5.13	1.26	1.33
1	F	206	SER	CB-OG	-5.11	1.35	1.42
1	E	216	VAL	CB-CG2	-5.06	1.42	1.52
1	A	225	GLU	CG-CD	-5.02	1.44	1.51
1	E	216	VAL	CB-CG1	-5.00	1.42	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	215	ARG	NE-CZ-NH2	-16.69	111.95	120.30
1	F	215	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	E	200	GLY	N-CA-C	8.26	133.76	113.10
1	B	194	LYS	N-CA-CB	5.65	120.77	110.60
1	C	190	ALA	N-CA-C	-5.27	96.77	111.00
1	D	222	ARG	NE-CZ-NH1	-5.15	117.72	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	248	ARG	Sidechain
1	C	215	ARG	Sidechain
1	F	176	ARG	Sidechain
1	F	215	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1186	0	1177	59	0
1	B	1212	0	1223	68	0
1	C	1185	0	1177	79	0
1	D	1203	0	1210	57	0
1	E	1209	0	1221	90	0
1	F	1191	0	1181	117	0
2	A	26	0	18	1	0
2	B	26	0	18	0	0
2	C	26	0	18	5	0
2	D	26	0	18	1	0
2	E	26	0	18	1	0
2	F	26	0	18	1	0
3	A	10	0	14	4	0
3	B	20	0	28	2	0
4	B	4	0	6	1	0
All	All	7376	0	7345	467	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 32.

All (467) 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:171:GLY:HA2	1:B:303:ARG:NH2	1.42	1.31
1:D:193:ALA:CB	1:D:194:LYS:HA	1.50	1.31
1:C:171:GLY:HA2	1:C:303:ARG:NH2	1.50	1.27
1:D:193:ALA:HB1	1:D:194:LYS:CA	1.70	1.21
1:E:318:PHE:HD2	1:E:319:PHE:CE1	1.59	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:GLY:CA	1:F:303:ARG:HH12	1.58	1.13
1:B:193:ALA:HB1	1:B:194:LYS:HB3	1.21	1.12
1:F:258:VAL:HG13	1:F:259:THR:H	1.08	1.11
1:E:318:PHE:CD2	1:E:319:PHE:HE1	1.68	1.10
1:C:191:THR:HG21	1:C:193:ALA:HB2	1.20	1.09
1:F:211:GLU:HA	1:F:211:GLU:OE1	1.52	1.08
1:F:189:GLN:NE2	1:F:189:GLN:HA	1.67	1.07
1:B:203:GLY:O	1:B:207:ARG:HG3	1.56	1.06
1:F:258:VAL:HG13	1:F:259:THR:N	1.67	1.05
1:C:191:THR:HG22	1:C:193:ALA:N	1.72	1.05
1:F:171:GLY:HA2	1:F:303:ARG:NH1	1.73	1.04
1:B:171:GLY:CA	1:B:303:ARG:HH22	1.70	1.03
1:F:189:GLN:HA	1:F:189:GLN:HE21	1.15	1.03
1:B:173:GLU:CD	1:B:201:ARG:HD3	1.79	1.02
1:F:313:ASP:O	1:F:316:VAL:HG12	1.59	1.01
1:F:171:GLY:CA	1:F:303:ARG:NH1	2.23	1.00
1:B:171:GLY:HA2	1:B:303:ARG:HH22	0.90	0.98
1:C:171:GLY:CA	1:C:303:ARG:HH22	1.76	0.98
1:E:171:GLY:CA	1:E:303:ARG:NH2	2.26	0.97
1:F:258:VAL:O	1:F:259:THR:HB	1.62	0.97
1:C:171:GLY:CA	1:C:303:ARG:NH2	2.28	0.96
1:D:171:GLY:HA3	1:D:303:ARG:NH2	1.82	0.95
1:F:171:GLY:HA3	1:F:303:ARG:HH12	1.31	0.94
1:B:250:MET:CE	1:B:297:VAL:HG21	1.97	0.94
1:F:191:THR:HG22	1:F:279:LYS:HE2	1.49	0.94
1:A:224:HIS:CE1	3:A:402:PGE:H1	2.02	0.93
1:E:318:PHE:CD2	1:E:319:PHE:CE1	2.50	0.93
1:B:250:MET:HE2	1:B:297:VAL:HG21	1.49	0.92
1:C:184:ARG:HH12	1:C:195:ASP:CB	1.81	0.92
1:E:171:GLY:HA3	1:E:303:ARG:NH2	1.82	0.92
1:A:171:GLY:HA3	1:A:303:ARG:HH22	1.34	0.92
1:A:224:HIS:NE2	3:A:402:PGE:H1	1.84	0.92
1:E:278:LEU:HD23	1:E:286:CYS:HB2	1.52	0.92
1:D:320:HIS:O	1:D:321:VAL:HG12	1.67	0.92
1:F:196:THR:O	1:F:197:LYS:O	1.87	0.92
1:F:320:HIS:O	1:F:320:HIS:ND1	2.02	0.92
1:C:191:THR:HG22	1:C:192:GLY:N	1.85	0.91
1:F:201:ARG:O	1:F:202:SER:OG	1.86	0.91
1:B:171:GLY:CA	1:B:303:ARG:NH2	2.29	0.91
1:F:259:THR:OG1	1:F:302:LYS:HE3	1.70	0.91
1:B:173:GLU:OE2	1:B:201:ARG:HD3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ALA:O	1:C:191:THR:HB	1.67	0.91
1:C:171:GLY:HA2	1:C:303:ARG:HH22	1.08	0.90
1:F:236:ASP:OD1	1:F:236:ASP:O	1.90	0.90
1:C:202:SER:O	1:C:205:THR:HG22	1.70	0.90
1:A:187:ARG:O	1:A:191:THR:HG22	1.72	0.90
1:F:212:THR:HG23	1:F:215:ARG:NH2	1.88	0.89
1:E:278:LEU:CD2	1:E:286:CYS:HB2	2.03	0.89
1:F:171:GLY:HA2	1:F:303:ARG:HH12	1.31	0.89
1:E:216:VAL:HG21	1:E:319:PHE:HD2	1.36	0.87
1:A:313:ASP:O	1:A:317:GLU:HG2	1.74	0.87
1:F:258:VAL:CG1	1:F:259:THR:H	1.66	0.86
1:C:191:THR:HG22	1:C:193:ALA:H	1.35	0.86
1:E:171:GLY:HA2	1:E:303:ARG:NH2	1.89	0.85
1:E:171:GLY:CA	1:E:303:ARG:HH22	1.89	0.85
1:C:229:GLN:O	1:C:229:GLN:NE2	2.10	0.84
1:F:212:THR:HG23	1:F:215:ARG:HH21	1.42	0.84
1:C:288:GLU:O	1:C:292:GLU:HG3	1.78	0.84
1:F:221:GLN:O	1:F:225:GLU:HG2	1.79	0.83
1:D:193:ALA:HB1	1:D:194:LYS:HA	0.86	0.83
1:B:224:HIS:HA	4:B:404:EDO:H22	1.60	0.82
1:E:171:GLY:HA3	1:E:303:ARG:HH22	1.41	0.81
1:D:188:GLU:HG3	1:D:193:ALA:HB3	1.62	0.81
1:A:196:THR:CG2	1:C:284:GLU:OE2	2.28	0.80
1:C:191:THR:HG21	1:C:193:ALA:CB	2.07	0.80
1:E:318:PHE:HD2	1:E:319:PHE:HE1	0.87	0.80
1:A:303:ARG:O	1:A:307:VAL:HG23	1.80	0.80
1:C:191:THR:CG2	1:C:193:ALA:HB2	2.10	0.80
1:F:171:GLY:HA3	1:F:303:ARG:NH1	1.93	0.80
1:F:191:THR:OG1	1:F:192:GLY:N	2.15	0.79
1:F:258:VAL:HG22	1:F:259:THR:N	1.96	0.79
1:A:196:THR:HG21	1:C:284:GLU:OE2	1.83	0.79
1:E:232:LEU:O	1:E:232:LEU:HD12	1.81	0.79
1:F:222:ARG:NH1	1:F:223:ASN:OD1	2.16	0.79
1:F:248:ARG:HH11	1:F:248:ARG:HG3	1.47	0.79
1:C:184:ARG:NH1	1:C:195:ASP:CB	2.46	0.79
1:F:258:VAL:CG1	1:F:259:THR:N	2.33	0.79
1:B:197:LYS:HG2	1:B:198:PRO:HD2	1.65	0.78
1:A:171:GLY:CA	1:A:303:ARG:HH22	1.97	0.78
1:B:193:ALA:HB1	1:B:194:LYS:CB	2.10	0.78
1:F:259:THR:HG22	1:F:305:TRP:CE2	2.19	0.77
1:A:248:ARG:HG3	1:A:248:ARG:HH11	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:THR:O	1:C:197:LYS:CB	2.30	0.77
1:F:211:GLU:OE1	1:F:211:GLU:CA	2.30	0.76
1:F:187:ARG:HA	1:F:190:ALA:HB3	1.67	0.76
1:E:216:VAL:HG21	1:E:319:PHE:CD2	2.21	0.76
1:F:259:THR:HG21	1:F:305:TRP:CD2	2.21	0.75
1:C:216:VAL:HG12	1:C:265:VAL:HG11	1.67	0.75
1:E:229:GLN:HE21	1:E:229:GLN:C	1.90	0.75
1:F:191:THR:HG22	1:F:279:LYS:CE	2.15	0.75
1:F:279:LYS:HB2	1:F:284:GLU:OE2	1.87	0.74
1:F:239:ASN:HB3	1:F:283:GLN:OE1	1.88	0.74
1:E:313:ASP:O	1:E:316:VAL:HG12	1.88	0.73
1:A:295:THR:O	1:A:299:VAL:HG23	1.87	0.73
1:B:173:GLU:OE2	1:B:176:ARG:NH2	2.21	0.73
1:F:199:MET:HG3	1:F:199:MET:O	1.87	0.73
1:B:189:GLN:HG2	1:B:272:ALA:HB1	1.69	0.72
1:C:250:MET:HE3	1:C:297:VAL:HG21	1.71	0.72
1:B:261:TRP:O	1:B:265:VAL:HG23	1.89	0.72
1:E:321:VAL:O	1:E:321:VAL:HG12	1.88	0.72
1:B:303:ARG:O	1:B:307:VAL:HG23	1.89	0.72
1:C:212:THR:HG23	1:C:215:ARG:HH12	1.55	0.72
1:F:196:THR:OG1	1:F:197:LYS:N	2.20	0.72
1:B:189:GLN:CG	1:B:272:ALA:HB1	2.20	0.71
1:E:299:VAL:O	1:E:303:ARG:HB2	1.91	0.71
1:F:184:ARG:NH2	1:F:195:ASP:HB2	2.05	0.71
1:F:259:THR:CG2	1:F:305:TRP:CE2	2.73	0.71
1:B:171:GLY:HA3	1:B:175:TYR:HB2	1.73	0.71
1:C:191:THR:CG2	1:C:192:GLY:N	2.53	0.71
1:B:250:MET:CE	1:B:297:VAL:CG2	2.69	0.70
1:B:321:VAL:O	1:B:321:VAL:HG12	1.90	0.70
1:F:279:LYS:CB	1:F:284:GLU:OE2	2.39	0.70
1:A:171:GLY:HA3	1:A:303:ARG:NH2	2.07	0.70
1:E:205:THR:HG21	1:E:313:ASP:OD1	1.91	0.70
1:E:184:ARG:NH2	1:E:197:LYS:O	2.25	0.70
1:D:171:GLY:CA	1:D:303:ARG:NH2	2.54	0.69
1:E:229:GLN:NE2	1:E:229:GLN:O	2.25	0.69
1:A:253:VAL:HG12	2:A:401:19H:H9	1.75	0.69
1:D:321:VAL:HG13	1:D:321:VAL:O	1.92	0.69
1:A:235:LEU:O	1:A:236:ASP:HB2	1.91	0.69
1:B:224:HIS:HE2	3:B:403:PGE:H12	1.57	0.69
1:F:258:VAL:O	1:F:259:THR:CB	2.39	0.69
1:F:232:LEU:HD21	1:F:277:HIS:CG	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:HIS:O	1:E:321:VAL:HB	1.92	0.69
1:A:299:VAL:HG12	1:A:303:ARG:HH21	1.57	0.68
1:F:248:ARG:HH11	1:F:248:ARG:CG	2.06	0.68
1:C:296:ASP:O	1:C:300:ARG:HB2	1.93	0.68
1:C:191:THR:CG2	1:C:193:ALA:N	2.53	0.68
1:D:278:LEU:HD23	1:D:287:ILE:HD13	1.74	0.68
1:E:318:PHE:C	1:E:319:PHE:HD1	1.97	0.68
1:E:181:ILE:HG23	1:E:210:LEU:HD12	1.74	0.67
1:F:186:LEU:O	1:F:190:ALA:HB2	1.95	0.67
1:D:212:THR:O	1:D:216:VAL:HG22	1.94	0.67
1:E:199:MET:HB2	1:E:203:GLY:HA3	1.77	0.67
1:D:232:LEU:HD11	1:D:277:HIS:CD2	2.30	0.66
1:E:229:GLN:CA	1:E:229:GLN:HE21	2.05	0.66
1:F:250:MET:CE	1:F:294:ILE:HA	2.25	0.66
1:B:256:ASP:O	1:B:263:ARG:NH2	2.29	0.66
1:F:201:ARG:C	1:F:202:SER:HG	1.93	0.66
1:F:212:THR:HG21	1:F:319:PHE:HB2	1.78	0.66
1:C:265:VAL:O	1:C:269:SER:HB2	1.96	0.66
1:D:193:ALA:CB	1:D:194:LYS:CA	2.40	0.66
1:D:246:LEU:HD13	2:D:400:19H:CL1	2.32	0.66
1:B:184:ARG:O	1:B:188:GLU:HG3	1.96	0.66
1:C:190:ALA:O	1:C:191:THR:CB	2.42	0.66
1:F:199:MET:HE3	1:F:207:ARG:HD2	1.78	0.66
1:E:185:TYR:CZ	1:E:189:GLN:NE2	2.65	0.65
1:C:241:ASP:HA	1:C:244:LYS:HD3	1.77	0.65
1:C:191:THR:CG2	1:C:193:ALA:H	2.05	0.65
1:E:185:TYR:HE1	1:E:214:ARG:HA	1.61	0.65
1:C:188:GLU:OE2	1:C:214:ARG:NE	2.29	0.65
1:F:196:THR:O	1:F:197:LYS:C	2.34	0.64
1:B:207:ARG:HH11	1:B:207:ARG:HB2	1.61	0.64
1:D:317:GLU:HG2	1:D:317:GLU:O	1.95	0.64
1:F:259:THR:CG2	1:F:305:TRP:CD2	2.79	0.64
1:A:190:ALA:O	1:A:191:THR:HG22	1.97	0.64
1:F:240:GLU:O	1:F:244:LYS:HG3	1.97	0.64
1:D:203:GLY:HA2	1:D:206:SER:HB2	1.80	0.64
1:D:189:GLN:HG3	1:D:276:LYS:NZ	2.12	0.64
1:F:183:SER:O	1:F:187:ARG:HG3	1.97	0.64
1:A:248:ARG:CG	1:A:248:ARG:HH11	2.11	0.63
1:A:219:GLY:O	1:A:222:ARG:HB3	1.98	0.63
1:F:221:GLN:OE1	1:F:276:LYS:NZ	2.31	0.62
1:E:232:LEU:HD21	1:E:277:HIS:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:VAL:CG1	1:A:303:ARG:HH21	2.13	0.62
1:B:265:VAL:O	1:B:269:SER:HB2	1.98	0.62
1:E:290:LEU:O	1:E:294:ILE:HG13	2.00	0.61
1:E:191:THR:HG22	1:E:191:THR:O	2.00	0.61
1:A:189:GLN:HG2	1:A:272:ALA:HB1	1.82	0.61
1:D:298:LEU:HD11	1:D:306:LEU:HD11	1.82	0.61
1:A:279:LYS:HG2	1:A:284:GLU:HG2	1.83	0.61
1:C:239:ASN:HD22	1:C:241:ASP:HB2	1.66	0.61
1:D:171:GLY:HA3	1:D:303:ARG:HH22	1.65	0.61
1:F:216:VAL:HG11	1:F:319:PHE:CD1	2.35	0.61
1:A:299:VAL:CG1	1:A:303:ARG:NH2	2.64	0.61
1:B:288:GLU:HB3	1:B:289:PRO:HD3	1.83	0.60
1:A:171:GLY:CA	1:A:303:ARG:NH2	2.62	0.60
1:D:256:ASP:O	1:D:263:ARG:NH2	2.25	0.60
1:D:197:LYS:HG2	1:D:198:PRO:HD2	1.84	0.60
1:C:215:ARG:NH2	1:C:319:PHE:O	2.34	0.60
1:B:256:ASP:OD1	1:B:256:ASP:N	2.27	0.60
1:D:180:GLU:OE2	1:D:199:MET:HG2	2.01	0.60
1:A:309:GLN:O	1:A:310:ARG:HB2	2.00	0.59
1:A:196:THR:HG23	1:C:284:GLU:OE2	2.00	0.59
1:B:203:GLY:HA2	1:B:206:SER:HB2	1.83	0.59
1:B:296:ASP:O	1:B:300:ARG:HB2	2.02	0.59
1:E:232:LEU:HD21	1:E:277:HIS:CG	2.37	0.59
1:B:180:GLU:O	1:B:184:ARG:HG2	2.03	0.59
1:E:318:PHE:HD2	1:E:319:PHE:CD1	2.15	0.59
1:F:258:VAL:CG2	1:F:259:THR:N	2.54	0.59
1:E:301:THR:O	1:E:302:LYS:HD3	2.02	0.59
1:B:180:GLU:HG2	1:B:199:MET:HE3	1.82	0.59
1:E:211:GLU:OE1	1:E:214:ARG:NH1	2.36	0.59
1:F:284:GLU:N	1:F:284:GLU:OE1	2.36	0.58
1:D:193:ALA:HB3	1:D:194:LYS:HA	1.69	0.58
1:F:313:ASP:O	1:F:316:VAL:CG1	2.46	0.58
1:E:278:LEU:CD2	1:E:286:CYS:CB	2.81	0.58
1:A:212:THR:OG1	1:A:316:VAL:HG13	2.03	0.57
1:B:173:GLU:OE1	1:B:201:ARG:HD3	2.05	0.57
1:C:212:THR:CG2	1:C:215:ARG:HH12	2.17	0.57
1:D:176:ARG:HH12	1:D:201:ARG:CB	2.17	0.57
1:E:259:THR:HG23	1:E:302:LYS:NZ	2.20	0.57
1:E:321:VAL:CG1	1:E:321:VAL:O	2.51	0.57
1:F:189:GLN:CA	1:F:189:GLN:HE21	2.03	0.57
1:A:183:SER:OG	1:A:187:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ASN:N	1:E:239:ASN:OD1	2.37	0.57
1:C:202:SER:O	1:C:205:THR:CG2	2.47	0.57
1:D:216:VAL:HG11	1:D:319:PHE:CD1	2.38	0.57
1:B:197:LYS:CG	1:B:198:PRO:HD2	2.34	0.57
1:F:190:ALA:O	1:F:279:LYS:HD2	2.04	0.57
1:F:236:ASP:O	1:F:236:ASP:CG	2.43	0.57
1:A:240:GLU:HG3	1:A:244:LYS:HE3	1.85	0.56
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.70	0.56
1:D:197:LYS:CG	1:D:198:PRO:HD2	2.36	0.56
1:A:212:THR:O	1:A:216:VAL:HG13	2.05	0.56
1:B:180:GLU:OE2	1:B:199:MET:HG3	2.04	0.56
1:B:250:MET:HE3	1:B:297:VAL:HG21	1.85	0.56
1:C:212:THR:HG23	1:C:215:ARG:NH1	2.18	0.56
1:F:275:ALA:HB1	1:F:287:ILE:HD13	1.86	0.56
1:B:320:HIS:O	1:B:321:VAL:HB	2.05	0.56
1:C:197:LYS:N	1:C:198:PRO:HD3	2.20	0.56
1:A:221:GLN:NE2	1:A:276:LYS:HE3	2.21	0.56
1:F:250:MET:HE1	1:F:294:ILE:HA	1.86	0.56
1:C:187:ARG:HH11	1:C:187:ARG:CG	2.18	0.56
1:D:320:HIS:O	1:D:321:VAL:CG1	2.48	0.55
1:E:286:CYS:C	1:E:289:PRO:HD2	2.27	0.55
1:A:211:GLU:HG3	1:A:212:THR:N	2.19	0.55
1:F:188:GLU:CD	1:F:214:ARG:HE	2.09	0.55
1:A:299:VAL:HG12	1:A:303:ARG:NH2	2.20	0.55
1:A:188:GLU:OE2	1:A:214:ARG:NE	2.40	0.55
1:D:288:GLU:HB3	1:D:289:PRO:HD3	1.89	0.55
1:E:215:ARG:HG2	1:E:216:VAL:N	2.21	0.55
1:E:228:PHE:HB3	1:E:273:PHE:HD2	1.71	0.55
1:B:309:GLN:O	1:B:314:GLY:HA3	2.07	0.55
1:E:228:PHE:HB3	1:E:273:PHE:CD2	2.42	0.55
1:C:212:THR:CG2	1:C:215:ARG:NH1	2.69	0.55
1:B:207:ARG:HH11	1:B:207:ARG:CB	2.19	0.55
1:D:204:ALA:HA	1:D:207:ARG:NH2	2.22	0.55
1:F:189:GLN:HG3	1:F:276:LYS:HE3	1.88	0.55
1:F:191:THR:HG1	1:F:192:GLY:H	1.48	0.54
1:F:191:THR:HG22	1:F:279:LYS:NZ	2.21	0.54
1:F:318:PHE:HD2	1:F:319:PHE:CE2	2.24	0.54
1:D:179:LEU:O	1:D:183:SER:HB3	2.08	0.54
1:F:211:GLU:OE1	1:F:214:ARG:HB2	2.07	0.54
1:C:261:TRP:O	1:C:265:VAL:HG23	2.07	0.54
1:E:208:LYS:HB3	1:E:316:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:THR:C	1:E:302:LYS:HD3	2.28	0.54
1:C:188:GLU:HA	1:C:193:ALA:HB3	1.90	0.54
1:E:185:TYR:CE1	1:E:189:GLN:NE2	2.76	0.54
1:F:250:MET:HE3	1:F:294:ILE:HA	1.87	0.54
1:C:233:ARG:HG3	1:C:234:LYS:N	2.23	0.54
1:D:212:THR:CG2	1:D:319:PHE:HB2	2.38	0.53
1:E:173:GLU:OE2	1:E:176:ARG:NH2	2.42	0.53
1:E:199:MET:SD	1:E:206:SER:HB3	2.48	0.53
1:F:211:GLU:OE1	1:F:214:ARG:HD2	2.08	0.53
1:B:250:MET:HE2	1:B:297:VAL:CG2	2.31	0.53
1:C:187:ARG:HH11	1:C:187:ARG:HG2	1.71	0.53
1:B:180:GLU:HG2	1:B:199:MET:CE	2.39	0.53
1:C:250:MET:O	1:C:253:VAL:HG12	2.08	0.53
1:C:256:ASP:OD1	1:C:256:ASP:N	2.28	0.53
1:F:176:ARG:NH1	1:F:201:ARG:CB	2.72	0.53
1:F:284:GLU:O	1:F:286:CYS:N	2.41	0.53
1:B:240:GLU:O	1:B:244:LYS:HG2	2.09	0.52
1:C:309:GLN:O	1:C:314:GLY:HA3	2.09	0.52
1:D:171:GLY:CA	1:D:303:ARG:HH22	2.20	0.52
1:E:183:SER:OG	1:E:187:ARG:NH2	2.41	0.52
1:E:232:LEU:C	1:E:232:LEU:HD12	2.29	0.52
1:F:258:VAL:HG22	1:F:259:THR:O	2.09	0.52
1:A:188:GLU:CD	1:A:214:ARG:HE	2.13	0.52
1:A:190:ALA:HB2	1:A:276:LYS:HA	1.91	0.52
1:D:288:GLU:HA	1:D:288:GLU:OE1	2.10	0.52
1:F:284:GLU:C	1:F:286:CYS:N	2.60	0.52
1:D:192:GLY:O	1:D:193:ALA:O	2.27	0.52
1:D:197:LYS:CG	1:D:198:PRO:CD	2.88	0.52
1:E:319:PHE:N	1:E:319:PHE:CD1	2.74	0.52
1:F:187:ARG:HA	1:F:190:ALA:CB	2.37	0.52
1:F:299:VAL:O	1:F:303:ARG:CB	2.58	0.52
1:D:275:ALA:HB1	1:D:287:ILE:HD12	1.92	0.52
1:E:189:GLN:HG2	1:E:272:ALA:HB1	1.91	0.52
1:F:316:VAL:HG13	1:F:317:GLU:N	2.24	0.52
1:C:187:ARG:NH1	1:C:187:ARG:CG	2.73	0.52
1:D:204:ALA:HA	1:D:207:ARG:CZ	2.40	0.52
1:D:180:GLU:OE2	1:D:199:MET:HA	2.10	0.51
1:A:224:HIS:CE1	3:A:402:PGE:C1	2.88	0.51
1:F:239:ASN:O	1:F:241:ASP:N	2.44	0.51
1:B:203:GLY:O	1:B:207:ARG:CG	2.45	0.51
1:C:197:LYS:N	1:C:198:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ARG:HG2	1:D:216:VAL:N	2.26	0.51
1:E:199:MET:SD	1:E:206:SER:CB	2.98	0.51
1:F:215:ARG:HH22	1:F:319:PHE:HB3	1.76	0.51
1:C:210:LEU:O	1:C:214:ARG:HG3	2.11	0.51
1:D:299:VAL:O	1:D:303:ARG:HB2	2.11	0.51
1:E:216:VAL:HG12	1:E:265:VAL:HG11	1.92	0.51
1:E:229:GLN:NE2	1:E:229:GLN:CA	2.71	0.51
1:F:212:THR:CG2	1:F:319:PHE:HB2	2.41	0.50
1:F:278:LEU:HD13	1:F:286:CYS:HB2	1.93	0.50
1:B:213:LEU:O	1:B:217:GLY:N	2.41	0.50
1:B:197:LYS:HG2	1:B:198:PRO:CD	2.38	0.50
1:D:189:GLN:HG3	1:D:276:LYS:HZ3	1.75	0.50
1:E:221:GLN:HE22	1:E:276:LYS:NZ	2.10	0.50
1:A:224:HIS:CD2	3:A:402:PGE:H1	2.47	0.50
1:F:258:VAL:CG2	1:F:259:THR:H	2.12	0.50
1:F:215:ARG:NH2	1:F:319:PHE:O	2.45	0.50
1:C:267:LEU:HD12	2:C:400:19H:H10	1.92	0.50
1:F:284:GLU:O	1:F:285:SER:C	2.45	0.50
1:E:185:TYR:HE2	1:E:272:ALA:HB2	1.77	0.49
1:B:259:THR:HG23	1:B:302:LYS:HE3	1.95	0.49
1:C:216:VAL:O	1:C:220:VAL:HG23	2.13	0.49
1:E:278:LEU:HD21	1:E:286:CYS:CB	2.43	0.49
1:C:185:TYR:O	1:C:189:GLN:HG2	2.13	0.49
1:C:253:VAL:HG13	2:C:400:19H:H11	1.94	0.49
1:A:191:THR:HG23	1:A:192:GLY:O	2.12	0.49
1:C:180:GLU:O	1:C:184:ARG:HB2	2.13	0.49
1:B:176:ARG:HH12	1:B:201:ARG:H	1.61	0.49
1:B:272:ALA:O	1:B:276:LYS:HG3	2.13	0.49
1:E:259:THR:CG2	1:E:302:LYS:NZ	2.75	0.49
1:A:256:ASP:O	1:A:263:ARG:NH2	2.46	0.48
1:C:238:LYS:HE2	1:C:239:ASN:OD1	2.12	0.48
1:C:242:ASP:OD1	1:C:242:ASP:N	2.46	0.48
1:A:248:ARG:CG	1:A:248:ARG:NH1	2.73	0.48
1:C:286:CYS:C	1:C:289:PRO:HD2	2.33	0.48
1:E:259:THR:CG2	1:E:302:LYS:HZ3	2.26	0.48
1:F:211:GLU:OE1	1:F:214:ARG:NH1	2.40	0.48
1:B:191:THR:O	1:B:193:ALA:N	2.46	0.48
1:F:279:LYS:HA	1:F:284:GLU:OE2	2.14	0.48
1:A:240:GLU:O	1:A:244:LYS:HD2	2.11	0.48
1:A:299:VAL:O	1:A:303:ARG:HB2	2.13	0.48
1:B:299:VAL:O	1:B:303:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LEU:HD21	1:E:286:CYS:HB2	1.91	0.48
1:E:203:GLY:HA2	1:E:206:SER:HB2	1.96	0.48
1:C:171:GLY:HA2	1:C:303:ARG:CZ	2.33	0.48
1:E:221:GLN:HE22	1:E:276:LYS:HZ1	1.61	0.48
1:B:189:GLN:HG2	1:B:272:ALA:CB	2.41	0.48
1:C:203:GLY:HA2	1:C:206:SER:HB2	1.96	0.48
1:D:189:GLN:CG	1:D:276:LYS:NZ	2.77	0.48
1:E:261:TRP:CZ3	1:E:315:PHE:HB2	2.48	0.47
1:F:299:VAL:O	1:F:303:ARG:HB3	2.14	0.47
1:A:187:ARG:O	1:A:191:THR:CG2	2.56	0.47
1:C:215:ARG:NH1	1:C:319:PHE:HB3	2.29	0.47
1:E:284:GLU:O	1:E:287:ILE:HG13	2.13	0.47
1:F:212:THR:O	1:F:216:VAL:HG13	2.13	0.47
1:C:253:VAL:HG11	2:C:400:19H:H12	1.96	0.47
1:A:184:ARG:O	1:A:188:GLU:HB2	2.15	0.47
1:E:216:VAL:HG11	1:E:319:PHE:CE2	2.49	0.47
1:A:265:VAL:O	1:A:269:SER:OG	2.25	0.46
1:D:190:ALA:O	1:D:192:GLY:N	2.44	0.46
1:E:275:ALA:HB1	1:E:287:ILE:HD13	1.97	0.46
1:B:275:ALA:HB1	1:B:287:ILE:HD13	1.97	0.46
1:D:189:GLN:HG3	1:D:276:LYS:HZ1	1.79	0.46
1:D:180:GLU:CD	1:D:199:MET:HG2	2.36	0.46
1:F:186:LEU:O	1:F:190:ALA:CB	2.62	0.46
1:F:199:MET:CE	1:F:207:ARG:HD2	2.43	0.46
1:F:258:VAL:HG22	1:F:259:THR:H	1.70	0.46
1:D:189:GLN:CG	1:D:276:LYS:HZ1	2.29	0.46
1:F:238:LYS:HB3	1:F:238:LYS:HE2	1.63	0.46
1:C:253:VAL:CG1	2:C:400:19H:H11	2.45	0.46
1:F:259:THR:HG22	1:F:305:TRP:NE1	2.31	0.46
1:B:243:VAL:HG21	1:B:286:CYS:HB3	1.98	0.46
1:C:239:ASN:ND2	1:C:241:ASP:HB2	2.31	0.46
1:B:184:ARG:HB2	1:B:210:LEU:HD11	1.98	0.45
1:E:197:LYS:HG3	1:E:198:PRO:HD2	1.98	0.45
1:E:215:ARG:CG	1:E:216:VAL:N	2.79	0.45
1:E:185:TYR:CE2	1:E:272:ALA:HB2	2.51	0.45
1:B:173:GLU:OE2	1:B:176:ARG:CZ	2.63	0.45
1:F:250:MET:HE3	1:F:294:ILE:HG12	1.99	0.45
1:B:231:MET:O	1:B:235:LEU:HG	2.16	0.45
1:E:261:TRP:O	1:E:265:VAL:HG23	2.16	0.45
1:B:192:GLY:O	1:B:193:ALA:HB3	2.16	0.45
1:F:248:ARG:NH1	1:F:248:ARG:CG	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:TRP:CE3	1:F:315:PHE:HD1	2.34	0.45
1:C:204:ALA:O	1:C:207:ARG:HB2	2.17	0.45
1:C:216:VAL:CG1	1:C:265:VAL:HG11	2.42	0.45
1:D:210:LEU:HD13	1:D:210:LEU:HA	1.49	0.45
1:F:259:THR:HG21	1:F:305:TRP:CG	2.50	0.45
1:E:187:ARG:O	1:E:190:ALA:O	2.35	0.45
1:C:191:THR:CG2	1:C:193:ALA:CB	2.83	0.45
1:D:199:MET:O	1:D:200:GLY:O	2.35	0.45
1:D:232:LEU:HD23	1:D:273:PHE:HE1	1.82	0.45
1:B:207:ARG:HB2	1:B:207:ARG:NH1	2.30	0.45
1:C:244:LYS:NZ	1:C:244:LYS:HB2	2.32	0.45
1:C:199:MET:O	1:C:200:GLY:O	2.36	0.44
1:E:221:GLN:CD	1:E:276:LYS:HZ3	2.20	0.44
1:E:319:PHE:HD1	1:E:319:PHE:N	2.11	0.44
1:A:171:GLY:HA2	1:A:303:ARG:NH2	2.32	0.44
1:D:321:VAL:CG1	1:D:321:VAL:O	2.62	0.44
1:E:211:GLU:HA	1:E:211:GLU:OE1	2.17	0.44
1:B:201:ARG:CG	1:B:202:SER:N	2.80	0.44
1:D:309:GLN:O	1:D:314:GLY:HA3	2.17	0.44
1:E:207:ARG:NH2	2:F:400:19H:OAD	2.51	0.44
1:F:318:PHE:CD2	1:F:319:PHE:CE2	3.05	0.44
1:B:191:THR:HG22	1:B:279:LYS:HD2	2.00	0.43
1:E:210:LEU:O	1:E:214:ARG:HB2	2.18	0.43
1:F:189:GLN:NE2	1:F:189:GLN:CA	2.54	0.43
1:F:235:LEU:HA	1:F:235:LEU:HD23	1.79	0.43
1:C:235:LEU:HD22	1:C:246:LEU:HD21	1.99	0.43
1:F:184:ARG:O	1:F:188:GLU:HB2	2.18	0.43
1:A:190:ALA:CB	1:A:276:LYS:HA	2.48	0.43
1:D:232:LEU:HD21	1:D:277:HIS:HB2	1.99	0.43
1:F:226:THR:HG22	1:F:227:ALA:N	2.31	0.43
1:B:191:THR:O	1:B:191:THR:OG1	2.26	0.43
1:F:299:VAL:O	1:F:303:ARG:HB2	2.19	0.43
1:B:224:HIS:NE2	3:B:403:PGE:H12	2.29	0.43
1:B:189:GLN:HG3	1:B:276:LYS:HE3	2.01	0.43
1:B:288:GLU:HA	1:B:288:GLU:OE1	2.18	0.43
1:F:187:ARG:CA	1:F:190:ALA:HB3	2.43	0.43
1:F:208:LYS:H	1:F:208:LYS:HG2	1.63	0.43
1:B:191:THR:HG22	1:B:284:GLU:OE2	2.19	0.43
1:D:230:GLY:O	1:D:234:LYS:HG3	2.19	0.43
1:C:244:LYS:NZ	1:C:244:LYS:CB	2.81	0.43
1:D:197:LYS:HG3	1:D:198:PRO:CD	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:GLU:O	1:F:320:HIS:CD2	2.72	0.42
1:A:318:PHE:CD2	1:A:318:PHE:O	2.72	0.42
1:A:240:GLU:O	1:A:244:LYS:CD	2.68	0.42
1:E:185:TYR:CE1	1:E:214:ARG:HA	2.49	0.42
1:F:316:VAL:CG1	1:F:317:GLU:N	2.82	0.42
1:A:221:GLN:HE21	1:A:276:LYS:HE3	1.85	0.42
1:F:279:LYS:CA	1:F:284:GLU:OE2	2.67	0.42
1:B:239:ASN:O	1:B:242:ASP:HB2	2.19	0.42
1:C:254:PHE:CD2	2:C:400:19H:H8	2.54	0.42
1:F:222:ARG:HH11	1:F:222:ARG:CG	2.32	0.42
1:F:232:LEU:HD21	1:F:277:HIS:CB	2.50	0.42
1:A:299:VAL:HG11	1:A:303:ARG:NH2	2.34	0.42
1:A:312:TRP:O	1:A:315:PHE:HB3	2.20	0.42
1:C:202:SER:OG	1:C:205:THR:CG2	2.68	0.42
1:E:320:HIS:N	1:E:320:HIS:ND1	2.68	0.42
1:E:188:GLU:HG2	1:E:193:ALA:O	2.19	0.42
1:F:251:ILE:O	1:F:255:SER:HB2	2.20	0.42
1:D:171:GLY:N	1:D:303:ARG:NH2	2.68	0.42
1:F:171:GLY:HA3	1:F:175:TYR:HB2	2.01	0.42
1:A:179:LEU:O	1:A:183:SER:HB3	2.20	0.42
1:B:188:GLU:HG2	1:B:194:LYS:HA	2.02	0.42
1:D:193:ALA:HB1	1:D:194:LYS:C	2.33	0.42
1:C:259:THR:HG23	1:C:302:LYS:HE3	2.02	0.42
1:E:246:LEU:HD13	2:E:400:19H:CL1	2.57	0.42
1:F:199:MET:CE	1:F:207:ARG:CD	2.98	0.42
1:A:309:GLN:O	1:A:314:GLY:HA3	2.19	0.41
1:D:171:GLY:HA3	1:D:303:ARG:CZ	2.46	0.41
1:E:174:LEU:HA	1:E:174:LEU:HD12	1.89	0.41
1:E:176:ARG:HE	1:E:176:ARG:HB3	1.60	0.41
1:E:310:ARG:O	1:E:313:ASP:HB2	2.21	0.41
1:F:201:ARG:O	1:F:202:SER:CB	2.67	0.41
1:A:231:MET:O	1:A:235:LEU:HG	2.21	0.41
1:F:186:LEU:O	1:F:190:ALA:N	2.53	0.41
1:A:300:ARG:HD3	1:A:300:ARG:HH11	1.71	0.41
1:B:176:ARG:HB3	1:B:176:ARG:HE	1.59	0.41
1:E:318:PHE:C	1:E:319:PHE:CD1	2.86	0.41
1:F:214:ARG:O	1:F:218:ASP:OD2	2.38	0.41
1:A:190:ALA:O	1:A:191:THR:CB	2.69	0.41
1:C:254:PHE:CG	1:C:254:PHE:O	2.73	0.41
1:E:300:ARG:NH1	1:E:300:ARG:HG2	2.35	0.41
1:C:224:HIS:N	1:C:224:HIS:ND1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:VAL:O	1:C:303:ARG:HB2	2.21	0.41
1:E:318:PHE:CD2	1:E:319:PHE:CD1	3.00	0.41
1:D:176:ARG:NH1	1:D:201:ARG:CB	2.84	0.40
1:E:199:MET:SD	1:E:206:SER:HB2	2.60	0.40
1:F:236:ASP:OD1	1:F:236:ASP:C	2.56	0.40
1:C:299:VAL:CG1	1:C:303:ARG:HH21	2.34	0.40
1:E:221:GLN:HE21	1:E:221:GLN:HB3	1.54	0.40
1:A:256:ASP:O	1:A:263:ARG:NH1	2.54	0.40
1:A:288:GLU:CB	1:A:289:PRO:HD3	2.51	0.40
1:C:215:ARG:CZ	1:C:319:PHE:O	2.69	0.40
1:E:180:GLU:O	1:E:184:ARG:HB2	2.20	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	145/153 (95%)	142 (98%)	2 (1%)	1 (1%)	22	53
1	B	149/153 (97%)	144 (97%)	4 (3%)	1 (1%)	22	53
1	C	148/153 (97%)	140 (95%)	5 (3%)	3 (2%)	7	24
1	D	149/153 (97%)	139 (93%)	6 (4%)	4 (3%)	5	17
1	E	149/153 (97%)	140 (94%)	9 (6%)	0	100	100
1	F	148/153 (97%)	135 (91%)	7 (5%)	6 (4%)	3	9
All	All	888/918 (97%)	840 (95%)	33 (4%)	15 (2%)	9	29

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	GLY

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Mol	Chain	Res	Type
1	C	197	LYS
1	C	200	GLY
1	D	193	ALA
1	F	197	LYS
1	F	202	SER
1	F	240	GLU
1	F	259	THR
1	D	200	GLY
1	D	318	PHE
1	A	191	THR
1	C	201	ARG
1	D	172	ASP
1	F	258	VAL
1	F	192	GLY

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	127/133 (96%)	110 (87%)	17 (13%)	4	12
1	B	131/133 (98%)	103 (79%)	28 (21%)	1	3
1	C	125/133 (94%)	92 (74%)	33 (26%)	0	1
1	D	129/133 (97%)	114 (88%)	15 (12%)	5	17
1	E	130/133 (98%)	109 (84%)	21 (16%)	2	7
1	F	127/133 (96%)	106 (84%)	21 (16%)	2	7
All	All	769/798 (96%)	634 (82%)	135 (18%)	2	5

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	210	LEU
1	A	215	ARG
1	A	221	GLN

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Mol	Chain	Res	Type
1	A	225	GLU
1	A	233	ARG
1	A	244	LYS
1	A	248	ARG
1	A	249	VAL
1	A	269	SER
1	A	278	LEU
1	A	279	LYS
1	A	289	PRO
1	A	296	ASP
1	A	302	LYS
1	A	303	ARG
1	A	321	VAL
1	B	172	ASP
1	B	176	ARG
1	B	184	ARG
1	B	189	GLN
1	B	199	MET
1	B	201	ARG
1	B	205	THR
1	B	206	SER
1	B	207	ARG
1	B	213	LEU
1	B	226	THR
1	B	231	MET
1	B	234	LYS
1	B	236	ASP
1	B	244	LYS
1	B	245	SER
1	B	247	SER
1	B	248	ARG
1	B	250	MET
1	B	256	ASP
1	B	259	THR
1	B	263	ARG
1	B	267	LEU
1	B	269	SER
1	B	278	LEU
1	B	285	SER
1	B	287	ILE
1	B	296	ASP
1	C	172	ASP

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Mol	Chain	Res	Type
1	C	176	ARG
1	C	184	ARG
1	C	187	ARG
1	C	196	THR
1	C	210	LEU
1	C	211	GLU
1	C	212	THR
1	C	213	LEU
1	C	224	HIS
1	C	225	GLU
1	C	231	MET
1	C	232	LEU
1	C	233	ARG
1	C	234	LYS
1	C	238	LYS
1	C	239	ASN
1	C	240	GLU
1	C	247	SER
1	C	248	ARG
1	C	249	VAL
1	C	250	MET
1	C	258	VAL
1	C	259	THR
1	C	267	LEU
1	C	269	SER
1	C	279	LYS
1	C	282	ASN
1	C	285	SER
1	C	293	SER
1	C	296	ASP
1	C	307	VAL
1	C	308	LYS
1	D	176	ARG
1	D	189	GLN
1	D	191	THR
1	D	194	LYS
1	D	196	THR
1	D	202	SER
1	D	206	SER
1	D	207	ARG
1	D	208	LYS
1	D	210	LEU

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Mol	Chain	Res	Type
1	D	233	ARG
1	D	259	THR
1	D	278	LEU
1	D	307	VAL
1	D	317	GLU
1	E	172	ASP
1	E	176	ARG
1	E	184	ARG
1	E	194	LYS
1	E	202	SER
1	E	207	ARG
1	E	210	LEU
1	E	211	GLU
1	E	215	ARG
1	E	221	GLN
1	E	229	GLN
1	E	232	LEU
1	E	241	ASP
1	E	248	ARG
1	E	256	ASP
1	E	278	LEU
1	E	284	GLU
1	E	288	GLU
1	E	309	GLN
1	E	320	HIS
1	E	321	VAL
1	F	172	ASP
1	F	176	ARG
1	F	183	SER
1	F	187	ARG
1	F	189	GLN
1	F	195	ASP
1	F	199	MET
1	F	207	ARG
1	F	210	LEU
1	F	215	ARG
1	F	222	ARG
1	F	226	THR
1	F	238	LYS
1	F	247	SER
1	F	248	ARG
1	F	259	THR

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Mol	Chain	Res	Type
1	F	279	LYS
1	F	284	GLU
1	F	287	ILE
1	F	303	ARG
1	F	320	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	B	177	GLN
1	D	277	HIS
1	E	189	GLN
1	E	229	GLN
1	F	189	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	19H	C	400	-	23,28,28	3.86	10 (43%)	32,40,40	2.55	11 (34%)
2	19H	D	400	-	23,28,28	3.72	11 (47%)	32,40,40	2.69	9 (28%)
2	19H	F	400	-	23,28,28	3.81	9 (39%)	32,40,40	2.52	10 (31%)
2	19H	A	401	-	23,28,28	3.78	11 (47%)	32,40,40	2.41	7 (21%)
3	PGE	A	402	-	9,9,9	0.68	0	8,8,8	0.74	0
3	PGE	B	403	-	9,9,9	0.69	0	8,8,8	0.98	0
4	EDO	B	404	-	3,3,3	0.62	0	2,2,2	0.43	0
2	19H	B	401	-	23,28,28	3.85	10 (43%)	32,40,40	2.60	10 (31%)
3	PGE	B	402	-	9,9,9	0.71	0	8,8,8	0.67	0
2	19H	E	400	-	23,28,28	3.78	11 (47%)	32,40,40	2.49	10 (31%)

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	19H	C	400	-	-	4/7/11/11	0/3/3/3
2	19H	D	400	-	-	0/7/11/11	0/3/3/3
2	19H	F	400	-	-	2/7/11/11	0/3/3/3
2	19H	A	401	-	-	2/7/11/11	0/3/3/3
3	PGE	A	402	-	-	4/7/7/7	-
3	PGE	B	403	-	-	4/7/7/7	-
4	EDO	B	404	-	-	0/1/1/1	-
2	19H	B	401	-	-	1/7/11/11	0/3/3/3
3	PGE	B	402	-	-	3/7/7/7	-
2	19H	E	400	-	-	0/7/11/11	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	19H	CAB-CAS	-10.07	1.30	1.51
2	B	401	19H	CAB-CAS	-9.89	1.31	1.51
2	B	401	19H	CAA-CAR	-9.86	1.31	1.51
2	F	400	19H	CAB-CAS	-9.85	1.31	1.51
2	A	401	19H	CAB-CAS	-9.67	1.31	1.51
2	F	400	19H	CAA-CAR	-9.67	1.31	1.51
2	C	400	19H	CAA-CAR	-9.63	1.31	1.51
2	E	400	19H	CAB-CAS	-9.62	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	19H	CAA-CAR	-9.53	1.31	1.51
2	E	400	19H	CAA-CAR	-9.46	1.32	1.51
2	D	400	19H	CAA-CAR	-9.46	1.32	1.51
2	D	400	19H	CAB-CAS	-9.41	1.32	1.51
2	A	401	19H	CAK-CAY	-7.09	1.30	1.41
2	B	401	19H	CAK-CAY	-7.08	1.30	1.41
2	C	400	19H	CAK-CAY	-7.07	1.30	1.41
2	F	400	19H	CAK-CAY	-6.94	1.31	1.41
2	E	400	19H	CAK-CAY	-6.82	1.31	1.41
2	D	400	19H	CAK-CAY	-6.66	1.31	1.41
2	E	400	19H	CAN-CAX	5.43	1.61	1.52
2	D	400	19H	CAN-CAX	5.20	1.61	1.52
2	C	400	19H	CAH-CAZ	-5.11	1.31	1.42
2	F	400	19H	CAN-CAX	5.09	1.61	1.52
2	B	401	19H	CAH-CAZ	-5.06	1.31	1.42
2	C	400	19H	CAN-CAX	4.99	1.61	1.52
2	E	400	19H	CAH-CAZ	-4.95	1.32	1.42
2	F	400	19H	CAH-CAZ	-4.91	1.32	1.42
2	B	401	19H	CAN-CAX	4.88	1.60	1.52
2	A	401	19H	CAH-CAZ	-4.87	1.32	1.42
2	A	401	19H	CAN-CAX	4.85	1.60	1.52
2	D	400	19H	CAH-CAZ	-4.80	1.32	1.42
2	A	401	19H	CAZ-CAY	-3.29	1.33	1.42
2	E	400	19H	CAZ-CAY	-3.11	1.34	1.42
2	F	400	19H	CAZ-CAY	-3.07	1.34	1.42
2	C	400	19H	CAZ-CAY	-3.06	1.34	1.42
2	B	401	19H	CAH-CAG	3.03	1.43	1.36
2	D	400	19H	CAZ-CAY	-2.98	1.34	1.42
2	B	401	19H	CAZ-CAY	-2.96	1.34	1.42
2	C	400	19H	CAH-CAG	2.95	1.42	1.36
2	A	401	19H	CAH-CAG	2.91	1.42	1.36
2	F	400	19H	CAH-CAG	2.89	1.42	1.36
2	E	400	19H	CAH-CAG	2.85	1.42	1.36
2	D	400	19H	CAH-CAG	2.85	1.42	1.36
2	B	401	19H	CAI-CAR	2.54	1.43	1.39
2	A	401	19H	CAI-CAR	2.52	1.43	1.39
2	E	400	19H	CAK-CAT	2.46	1.41	1.36
2	F	400	19H	CAK-CAT	2.42	1.41	1.36
2	D	400	19H	CAJ-CAS	2.39	1.43	1.39
2	A	401	19H	CAK-CAT	2.39	1.41	1.36
2	D	400	19H	CAK-CAT	2.25	1.41	1.36
2	C	400	19H	CAK-CAT	2.25	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	19H	CAI-CAR	2.21	1.42	1.39
2	C	400	19H	CAJ-CAS	2.20	1.42	1.39
2	A	401	19H	CAJ-CAS	2.19	1.42	1.39
2	C	400	19H	OAP-CAU	-2.17	1.32	1.37
2	E	400	19H	CAJ-CAS	2.15	1.42	1.39
2	B	401	19H	CAJ-CAS	2.13	1.42	1.39
2	B	401	19H	CAK-CAT	2.11	1.40	1.36
2	F	400	19H	CAJ-CAS	2.09	1.42	1.39
2	E	400	19H	OAP-CAU	-2.08	1.32	1.37
2	A	401	19H	OAP-CAU	-2.08	1.32	1.37
2	D	400	19H	OAP-CAU	-2.07	1.32	1.37
2	E	400	19H	CAI-CAR	2.06	1.42	1.39

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	19H	CAX-CAW-NAO	-8.53	98.12	110.32
2	B	401	19H	CAX-CAW-NAO	-8.38	98.34	110.32
2	E	400	19H	CAX-CAW-NAO	-8.24	98.54	110.32
2	C	400	19H	CAX-CAW-NAO	-7.92	98.99	110.32
2	F	400	19H	CAX-CAW-NAO	-7.92	99.00	110.32
2	A	401	19H	CAX-CAW-NAO	-7.64	99.39	110.32
2	A	401	19H	CAN-CAX-CAW	-7.21	119.65	127.48
2	B	401	19H	CAN-CAX-CAW	-6.88	120.00	127.48
2	C	400	19H	CAN-CAX-CAW	-6.36	120.57	127.48
2	E	400	19H	CAN-CAX-CAW	-6.33	120.60	127.48
2	F	400	19H	CAN-CAX-CAW	-6.22	120.73	127.48
2	D	400	19H	CAN-CAX-CAW	-5.60	121.40	127.48
2	D	400	19H	CAG-CAT-CAK	-4.91	116.18	121.99
2	F	400	19H	CAG-CAT-CAK	-4.72	116.40	121.99
2	B	401	19H	CAG-CAT-CAK	-4.63	116.51	121.99
2	D	400	19H	CAW-NAO-CAY	4.50	113.14	103.90
2	C	400	19H	CAG-CAT-CAK	-4.41	116.77	121.99
2	D	400	19H	CAK-CAT-CL2	4.30	125.02	119.64
2	B	401	19H	CAW-NAO-CAY	4.24	112.61	103.90
2	A	401	19H	CAG-CAT-CAK	-4.16	117.06	121.99
2	E	400	19H	CAW-NAO-CAY	4.05	112.21	103.90
2	F	400	19H	CAW-NAO-CAY	3.98	112.08	103.90
2	D	400	19H	CAT-CAK-CAY	3.92	122.81	119.50
2	C	400	19H	CAW-NAO-CAY	3.88	111.86	103.90
2	A	401	19H	CAW-NAO-CAY	3.73	111.55	103.90
2	E	400	19H	CAG-CAT-CAK	-3.70	117.61	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	19H	CAA-CAR-CAI	3.44	125.85	119.49
2	B	401	19H	CAB-CAS-CAJ	3.27	125.54	119.49
2	C	400	19H	CAT-CAK-CAY	3.27	122.25	119.50
2	E	400	19H	CAK-CAT-CL2	3.18	123.61	119.64
2	B	401	19H	CAT-CAK-CAY	3.11	122.11	119.50
2	E	400	19H	CAU-CAJ-CAS	2.85	123.66	120.59
2	D	400	19H	CAA-CAR-CAI	2.80	124.67	119.49
2	C	400	19H	CAU-CAI-CAR	2.73	123.53	120.59
2	E	400	19H	CAB-CAS-CAJ	2.71	124.51	119.49
2	C	400	19H	CAK-CAT-CL2	2.70	123.03	119.64
2	F	400	19H	CAT-CAK-CAY	2.64	121.72	119.50
2	B	401	19H	CAK-CAT-CL2	2.63	122.93	119.64
2	D	400	19H	CAU-CAJ-CAS	2.59	123.38	120.59
2	C	400	19H	CAM-OAP-CAU	-2.54	111.28	117.93
2	C	400	19H	CAU-CAJ-CAS	2.37	123.14	120.59
2	B	401	19H	CAH-CAZ-CAX	2.36	138.25	134.17
2	F	400	19H	CAU-CAI-CAR	2.34	123.11	120.59
2	C	400	19H	CAH-CAG-CAT	-2.26	116.59	119.21
2	E	400	19H	CAH-CAG-CAT	-2.24	116.61	119.21
2	C	400	19H	OAP-CAM-CAL	2.23	116.61	108.33
2	F	400	19H	CAH-CAZ-CAX	2.18	137.94	134.17
2	D	400	19H	CAU-CAI-CAR	2.16	122.92	120.59
2	A	401	19H	CAK-CAY-CAZ	2.15	123.93	121.16
2	E	400	19H	CAT-CAK-CAY	2.14	121.30	119.50
2	F	400	19H	CAK-CAT-CL2	2.11	122.28	119.64
2	A	401	19H	CAH-CAZ-CAX	2.10	137.81	134.17
2	B	401	19H	CAH-CAG-CAT	-2.06	116.82	119.21
2	A	401	19H	CAT-CAK-CAY	2.06	121.23	119.50
2	B	401	19H	CAG-CAH-CAZ	2.06	123.99	121.13
2	F	400	19H	CAB-CAS-CAJ	2.02	123.22	119.49
2	E	400	19H	CAA-CAR-CAI	2.01	123.20	119.49

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	PGE	O2-C3-C4-O3
3	A	402	PGE	O1-C1-C2-O2
3	A	402	PGE	O3-C5-C6-O4
3	B	403	PGE	O1-C1-C2-O2
2	C	400	19H	CAN-CAL-CAM-OAP
3	B	402	PGE	C4-C3-O2-C2

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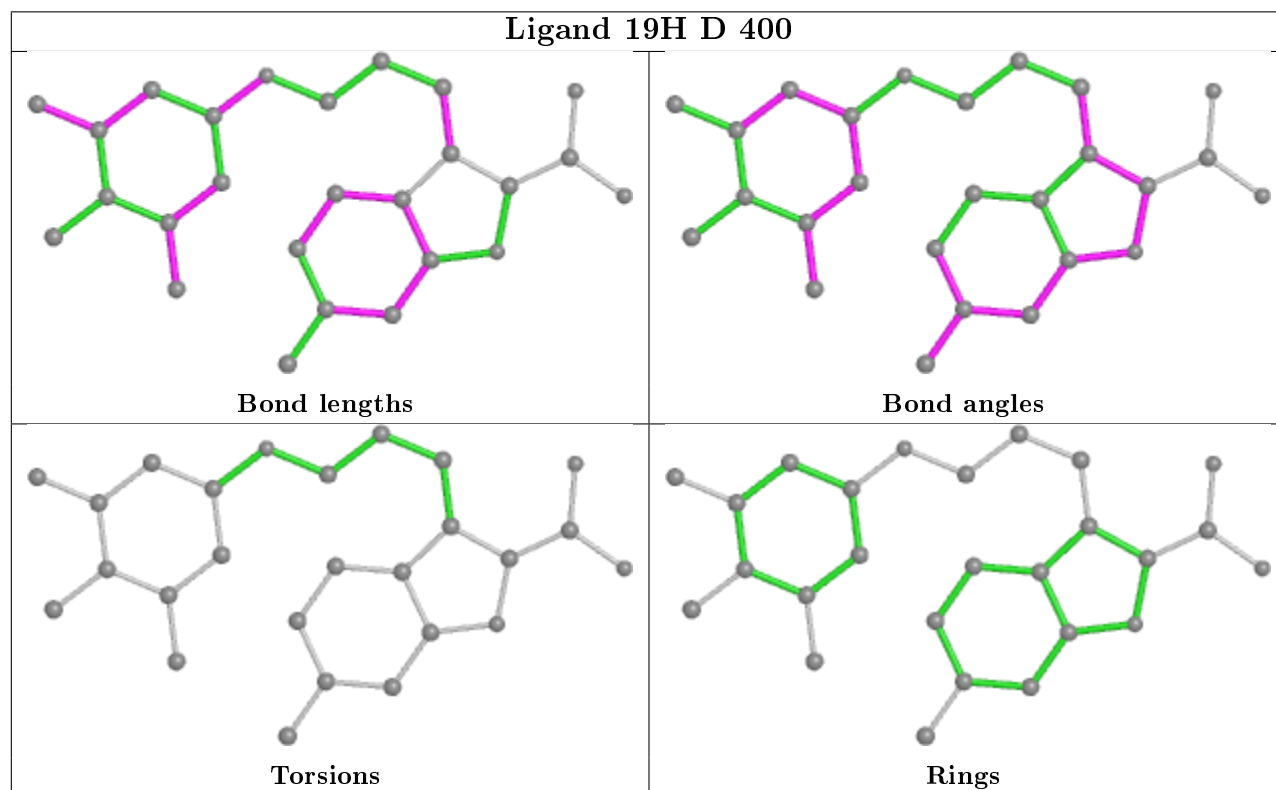
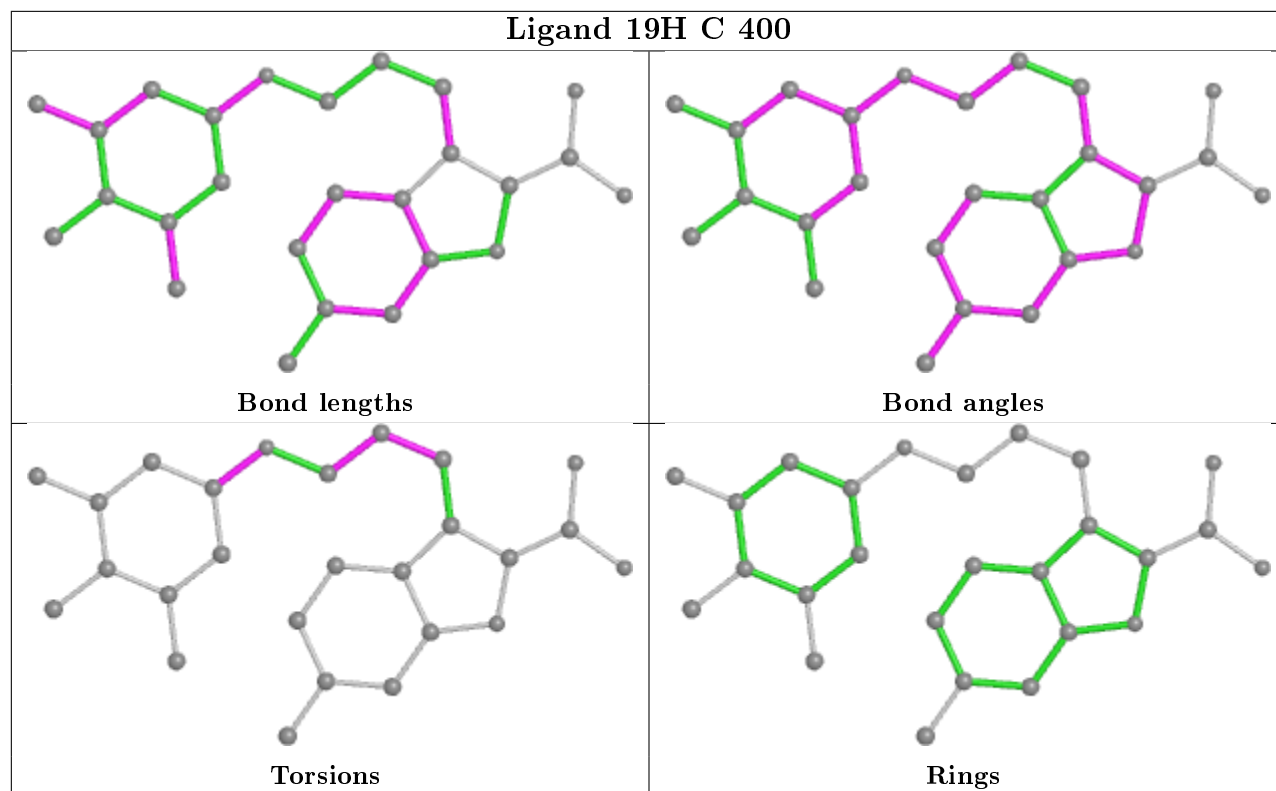
Mol	Chain	Res	Type	Atoms
2	C	400	19H	CAI-CAU-OAP-CAM
2	C	400	19H	CAJ-CAU-OAP-CAM
3	B	403	PGE	C3-C4-O3-C5
3	B	402	PGE	O2-C3-C4-O3
3	B	402	PGE	C1-C2-O2-C3
2	F	400	19H	CAI-CAU-OAP-CAM
2	C	400	19H	CAM-CAL-CAN-CAX
3	B	403	PGE	C6-C5-O3-C4
3	A	402	PGE	C4-C3-O2-C2
2	A	401	19H	CAI-CAU-OAP-CAM
3	A	402	PGE	C1-C2-O2-C3
2	B	401	19H	CAI-CAU-OAP-CAM
2	F	400	19H	CAJ-CAU-OAP-CAM
2	A	401	19H	CAM-CAL-CAN-CAX

There are no ring outliers.

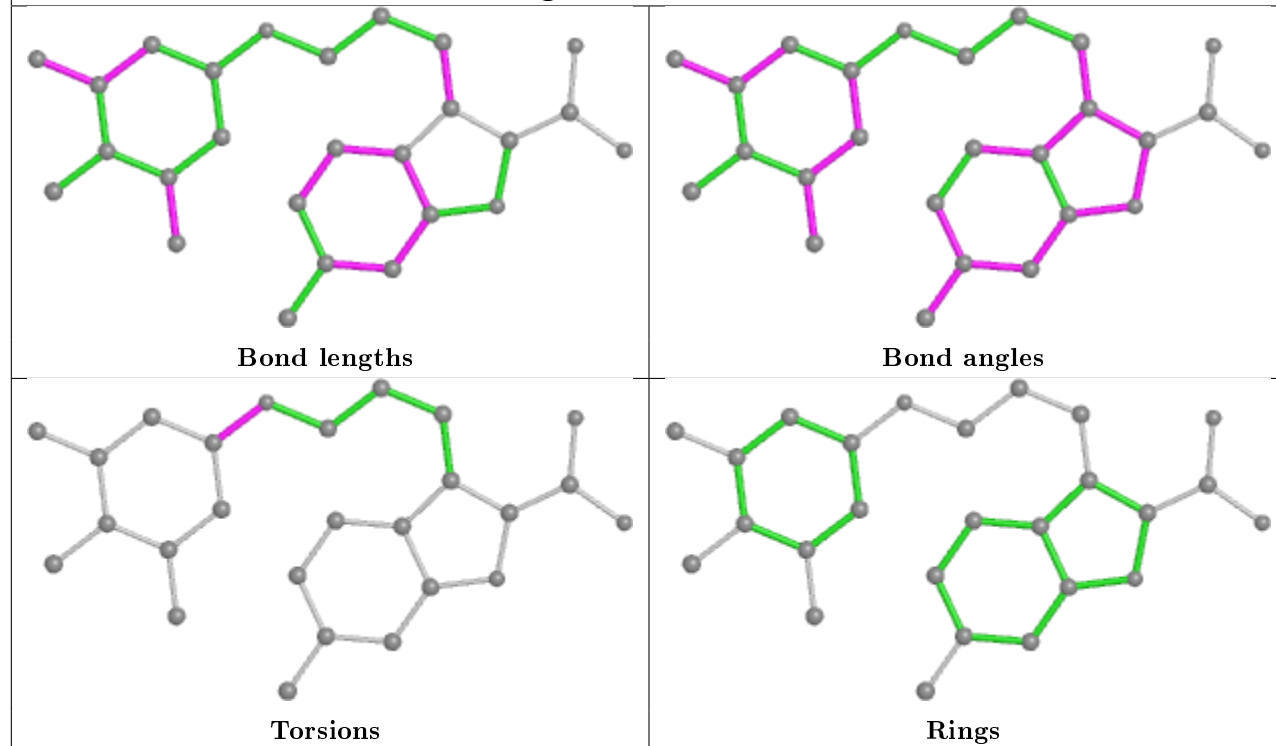
8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	19H	5	0
2	D	400	19H	1	0
2	F	400	19H	1	0
2	A	401	19H	1	0
3	A	402	PGE	4	0
3	B	403	PGE	2	0
4	B	404	EDO	1	0
2	E	400	19H	1	0

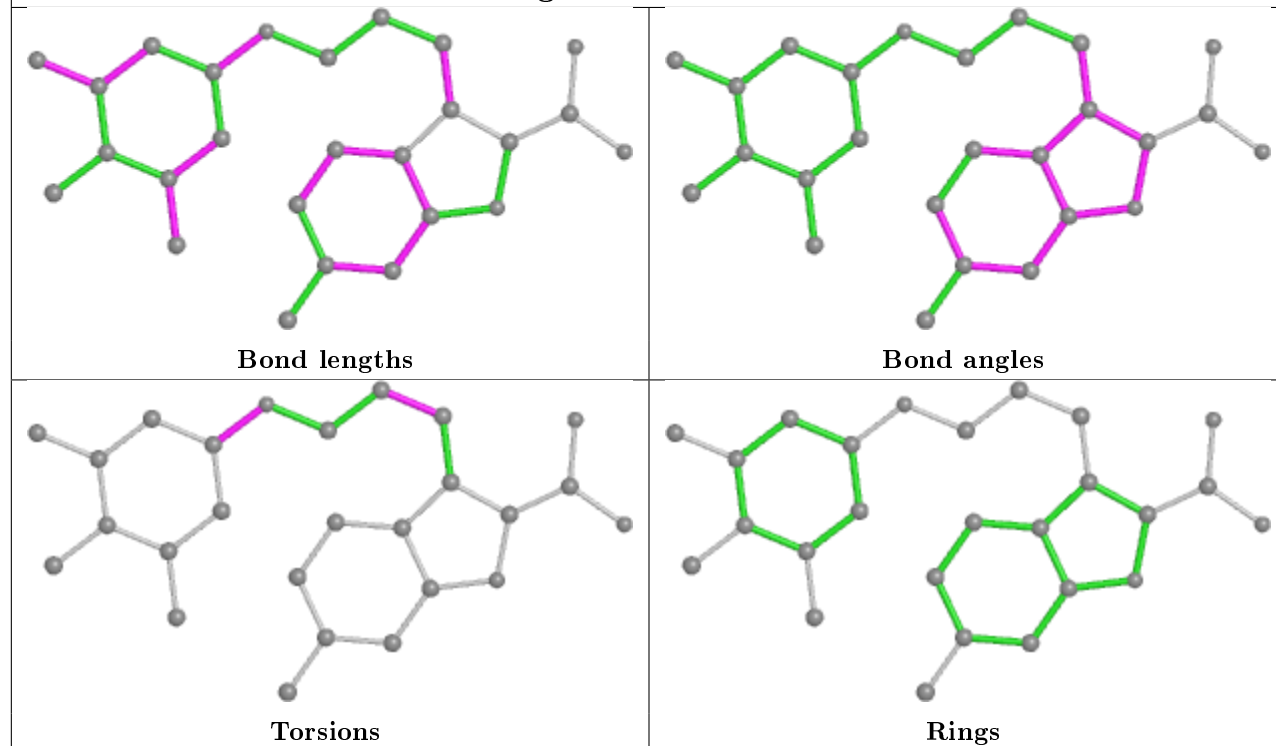
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

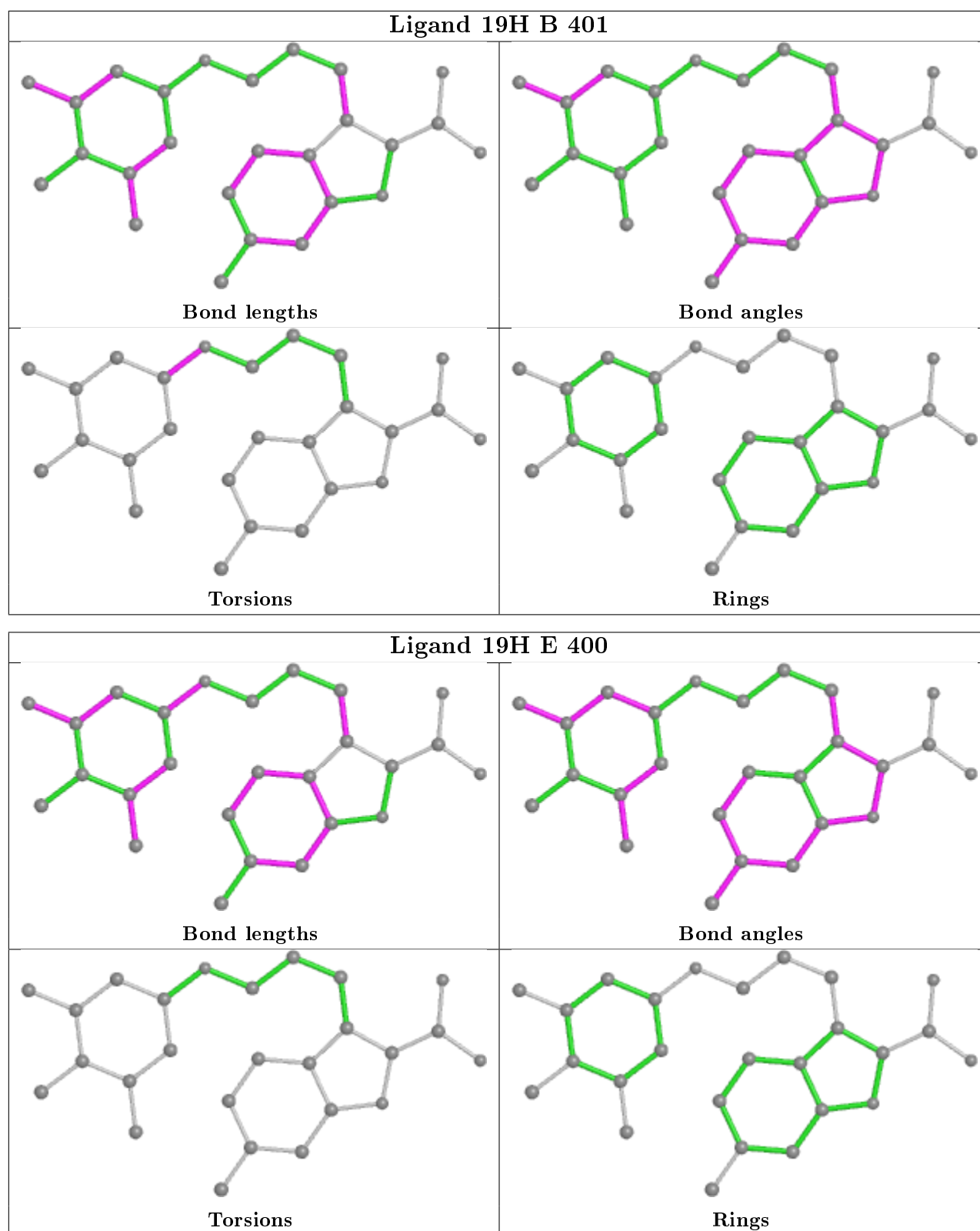


Ligand 19H F 400



Ligand 19H A 401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	149/153 (97%)	-0.16	3 (2%) 65 56	26, 46, 70, 85	0
1	B	151/153 (98%)	-0.16	0 100 100	7, 44, 65, 73	0
1	C	150/153 (98%)	-0.27	1 (0%) 87 84	27, 50, 72, 78	0
1	D	151/153 (98%)	-0.19	3 (1%) 65 56	28, 48, 69, 81	0
1	E	151/153 (98%)	-0.16	3 (1%) 65 56	28, 49, 71, 87	0
1	F	150/153 (98%)	-0.01	4 (2%) 54 44	24, 49, 77, 87	0
All	All	902/918 (98%)	-0.16	14 (1%) 72 66	7, 48, 71, 87	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	196	THR	3.9
1	A	196	THR	3.5
1	A	202	SER	3.2
1	F	194	LYS	2.9
1	D	202	SER	2.8
1	F	193	ALA	2.8
1	E	223	ASN	2.6
1	D	320	HIS	2.3
1	E	256	ASP	2.3
1	C	198	PRO	2.3
1	A	203	GLY	2.2
1	D	191	THR	2.1
1	E	226	THR	2.1
1	F	222	ARG	2.0

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

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](#)

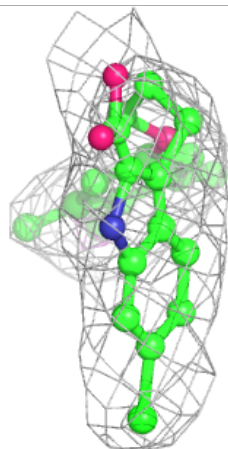
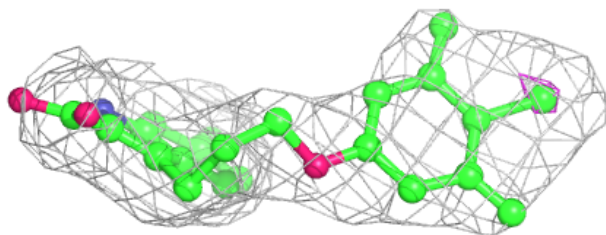
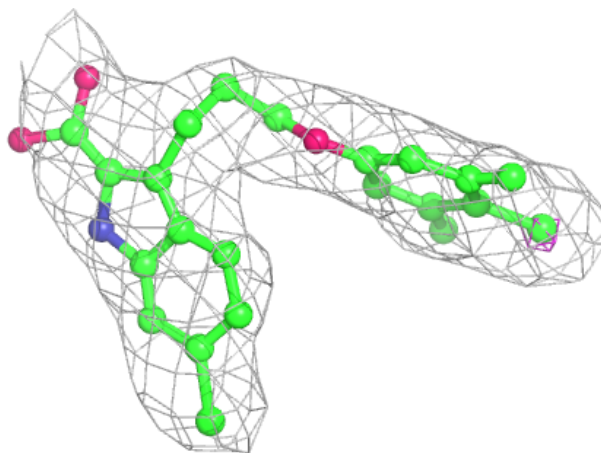
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PGE	A	402	10/10	0.83	0.26	36,56,76,79	0
4	EDO	B	404	4/4	0.85	0.24	33,41,62,77	0
3	PGE	B	403	10/10	0.86	0.23	32,48,61,65	0
3	PGE	B	402	10/10	0.93	0.19	26,60,74,80	0
2	19H	F	400	26/26	0.95	0.15	10,42,61,87	0
2	19H	A	401	26/26	0.95	0.17	1,40,57,66	0
2	19H	B	401	26/26	0.95	0.14	1,23,37,47	0
2	19H	C	400	26/26	0.95	0.14	29,55,73,89	0
2	19H	D	400	26/26	0.96	0.14	17,37,59,79	0
2	19H	E	400	26/26	0.97	0.14	1,43,62,70	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.

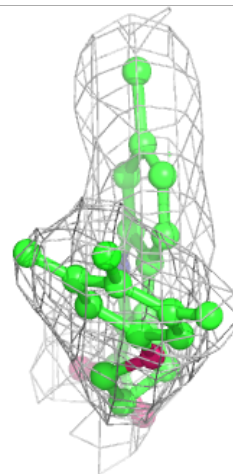
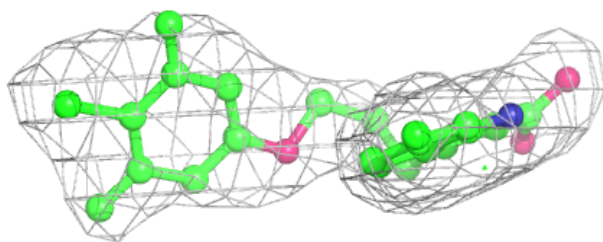
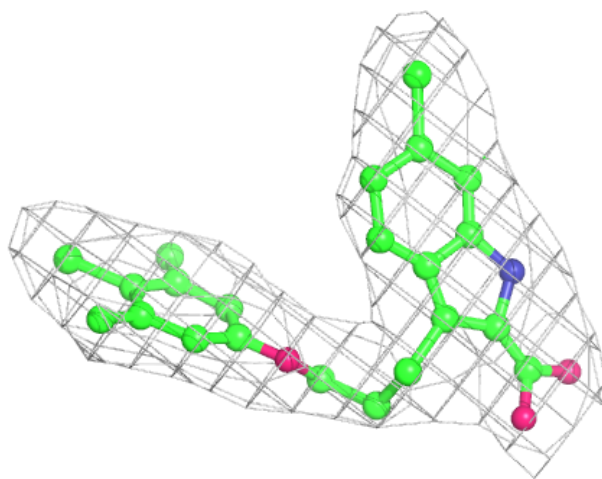
Electron density around 19H F 400:

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



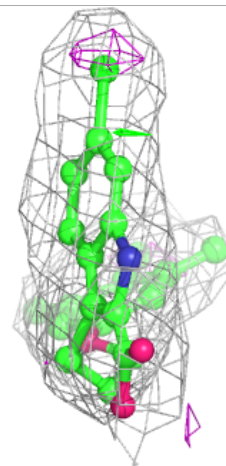
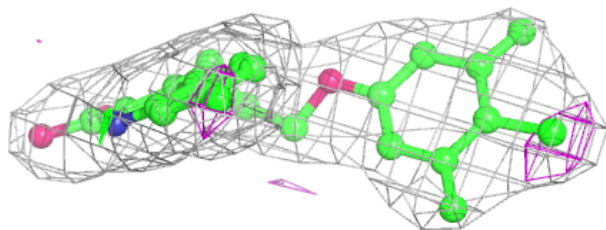
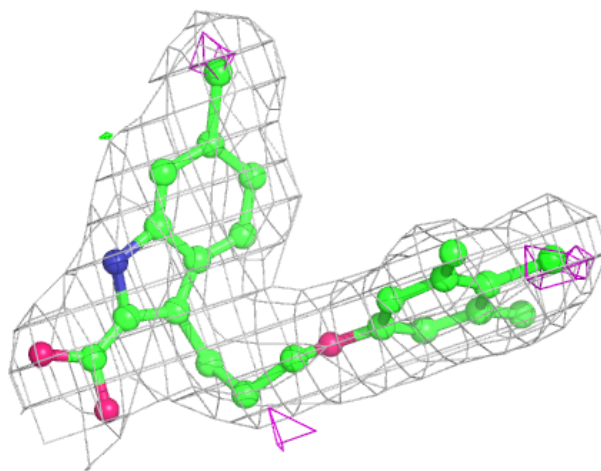
Electron density around 19H A 401:

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



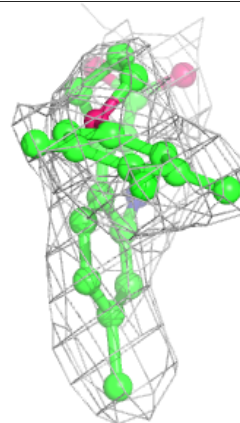
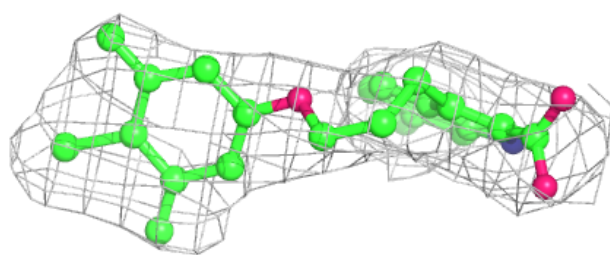
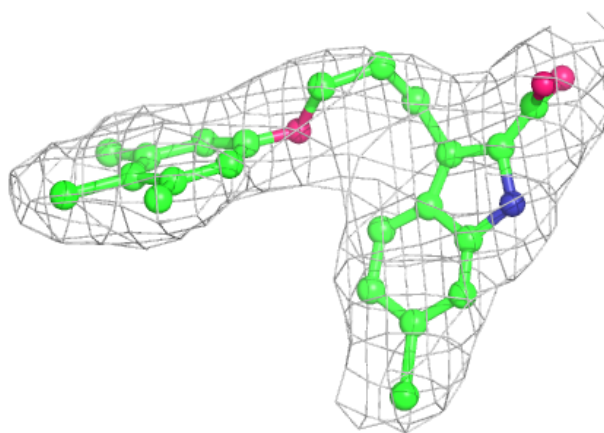
Electron density around 19H B 401:

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



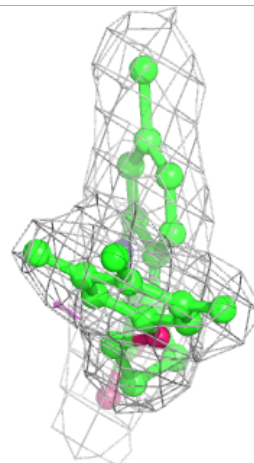
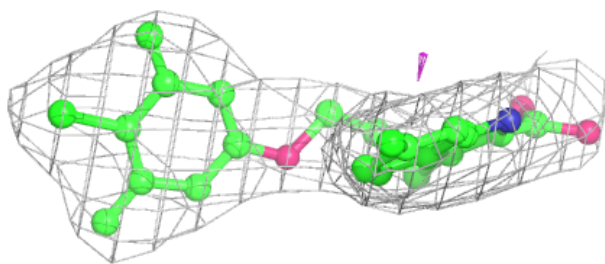
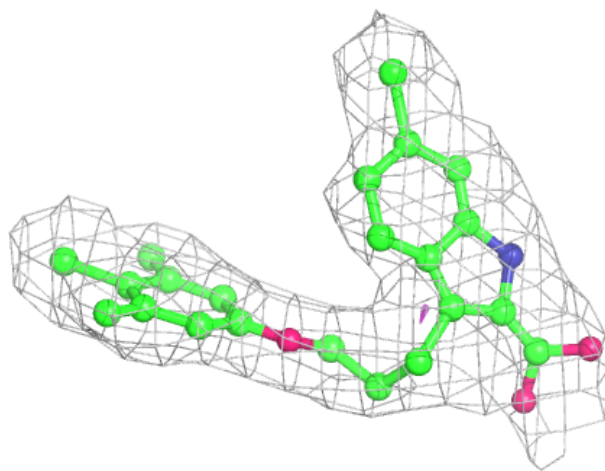
Electron density around 19H C 400:

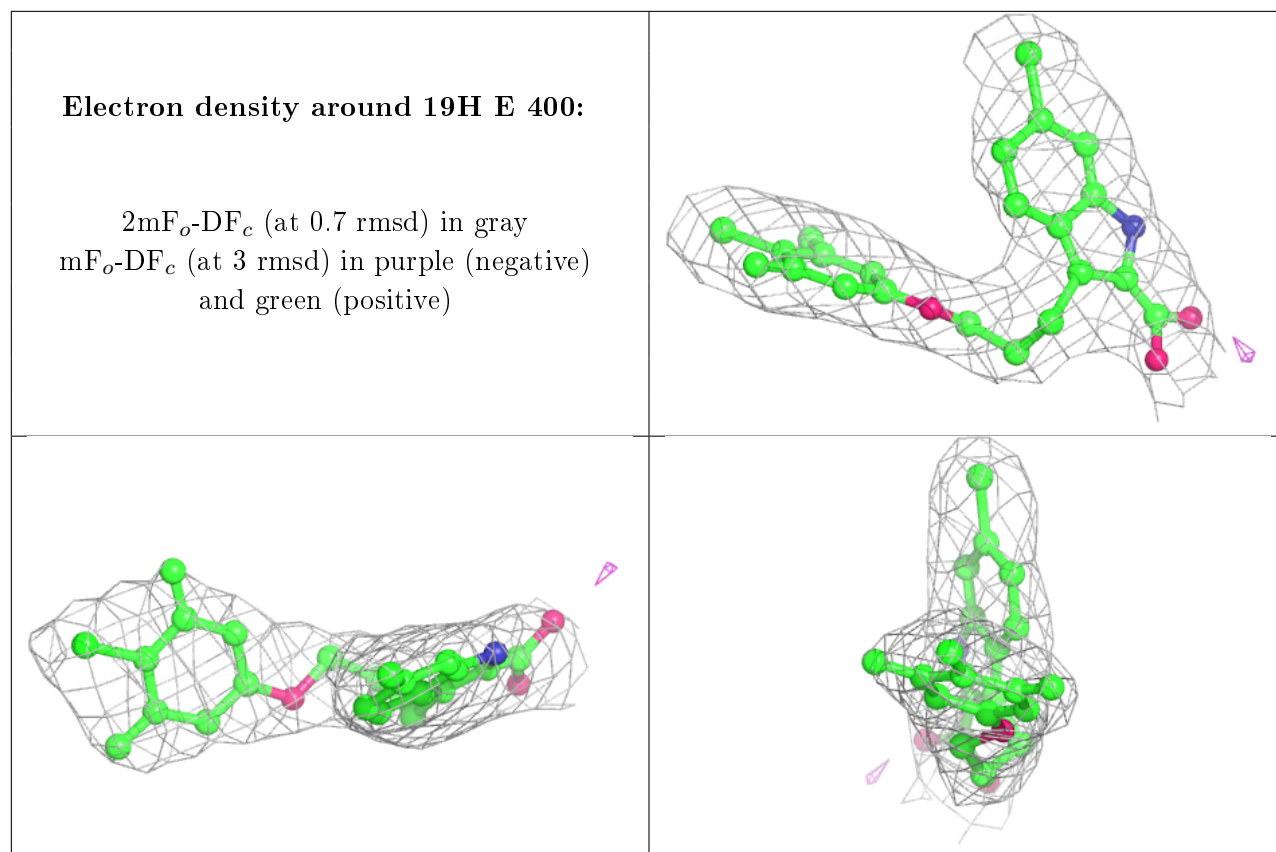
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 19H D 400:

$2mF_o-DF_c$ (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.