



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:40 PM UTC

PDB ID : 9EWL / pdb_00009ewl
Title : The sTeLIC pentameric Ligand-Gated Ion Channel (wild-type) in complex with 4-bromoamphetamine
Authors : Fourati, Z.; Delarue, M.
Deposited on : 2024-04-04
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

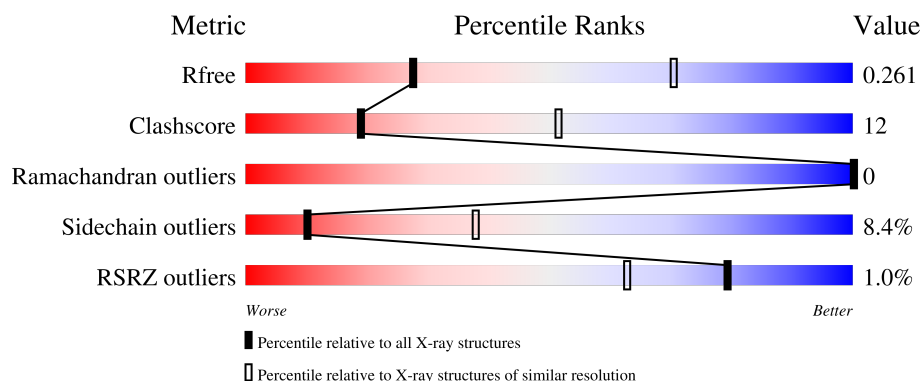
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

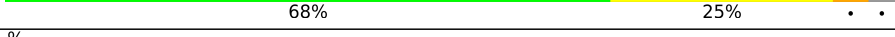
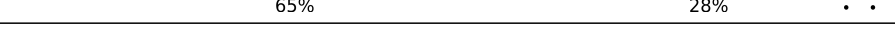
The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	AAA	320	
1	BBB	320	
1	CCC	320	
1	DDD	320	
1	EEE	320	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BNG	CCC	402	-	-	X	-

2 Entry composition [i](#)

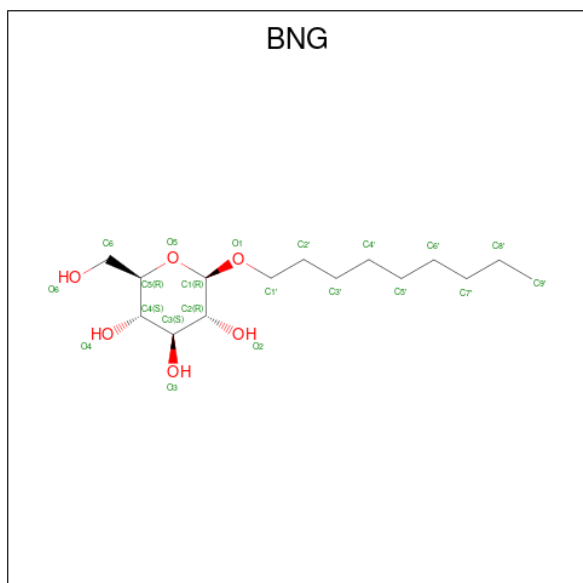
There are 4 unique types of molecules in this entry. The entry contains 13005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	310	Total	C	N	O	S	0	0	0
			2566	1690	423	448	5			
1	BBB	310	Total	C	N	O	S	0	0	0
			2566	1690	423	448	5			
1	CCC	310	Total	C	N	O	S	0	0	0
			2566	1690	423	448	5			
1	DDD	310	Total	C	N	O	S	0	0	0
			2566	1690	423	448	5			
1	EEE	310	Total	C	N	O	S	0	0	0
			2566	1690	423	448	5			

- Molecule 2 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



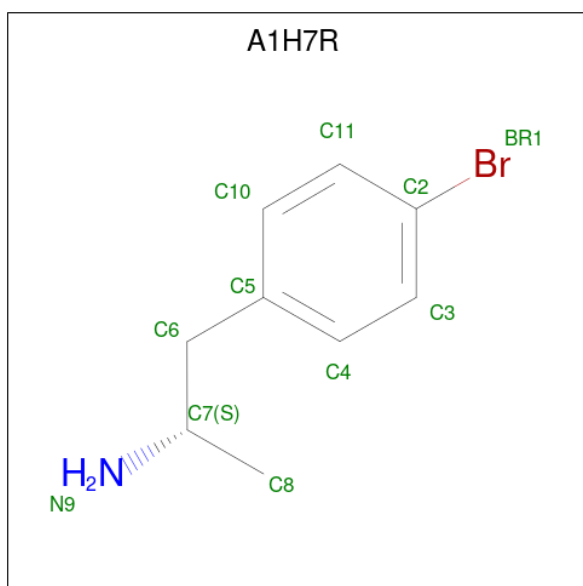
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			21	15	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	CCC	1	Total	C	O	0	0
			21	15	6		
2	DDD	1	Total	C	O	0	0
			21	15	6		
2	DDD	1	Total	C	O	0	0
			21	15	6		

- Molecule 3 is (2S)-1-(4-bromophenyl)propan-2-amine (CCD ID: A1H7R) (formula: C₉H₁₂BrN) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	Br	C	N	0	0
			11	1	9	1		
3	BBB	1	Total	Br	C	N	0	0
			11	1	9	1		
3	CCC	1	Total	Br	C	N	0	0
			11	1	9	1		
3	DDD	1	Total	Br	C	N	0	0
			11	1	9	1		
3	EEE	1	Total	Br	C	N	0	0
			11	1	9	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	7	Total	O	0	0
			7	7		

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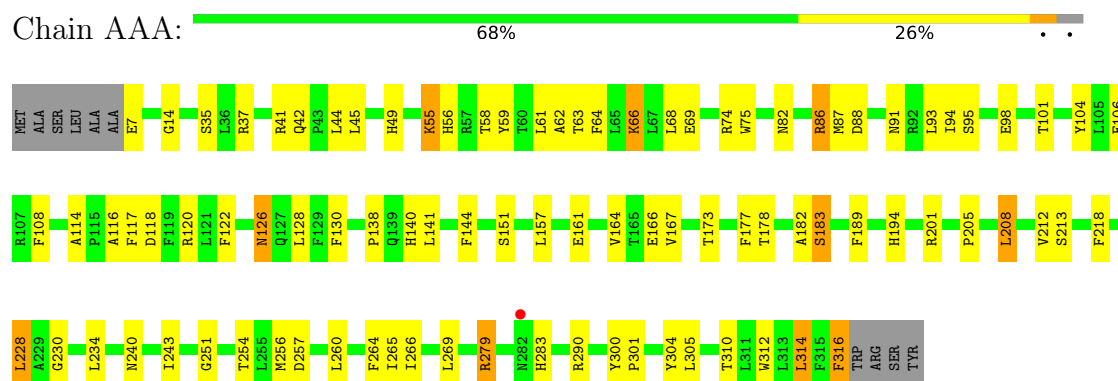
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	7	Total 7	O 7	0	0
4	CCC	7	Total 7	O 7	0	0
4	DDD	7	Total 7	O 7	0	0
4	EEE	8	Total 8	O 8	0	0

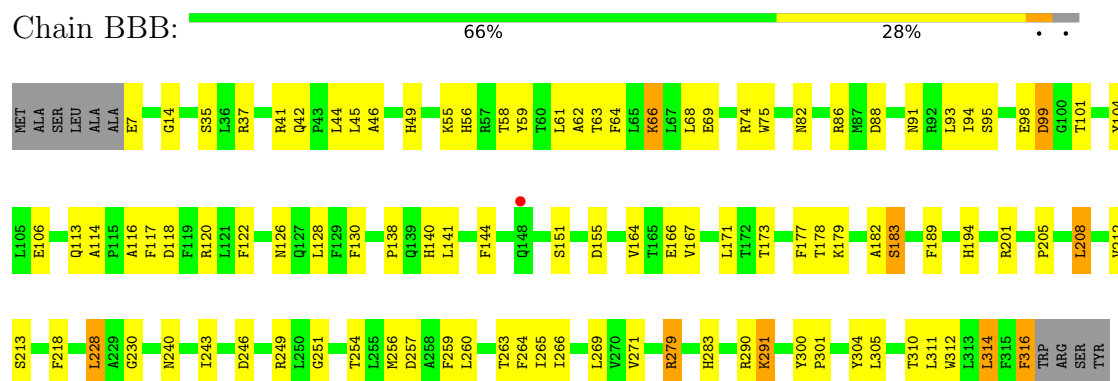
3 Residue-property plots

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

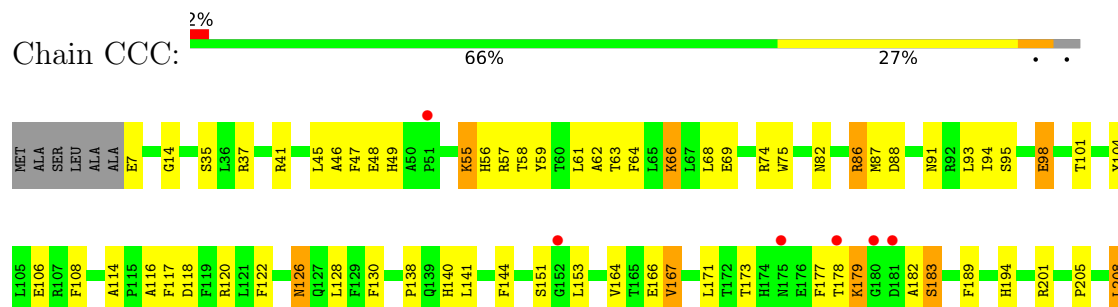
• Molecule 1: Cys-loop ligand-gated ion channel

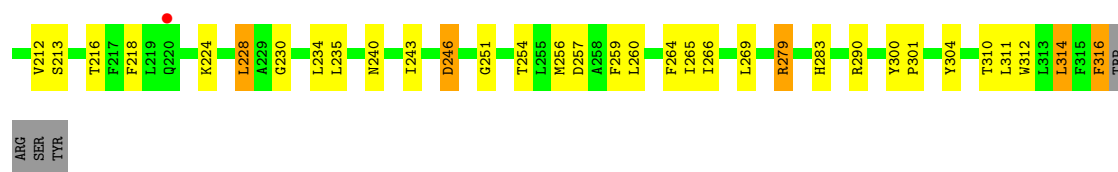


• Molecule 1: Cys-loop ligand-gated ion channel



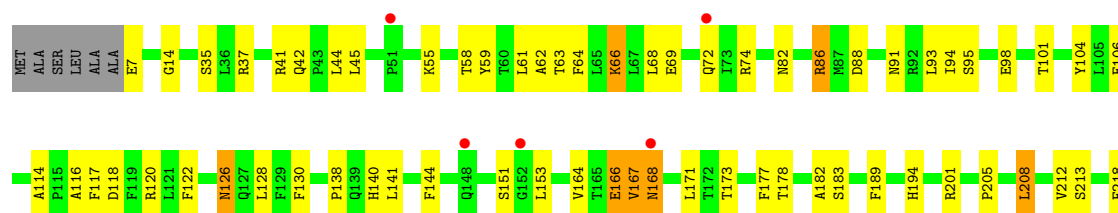
• Molecule 1: Cys-loop ligand-gated ion channel





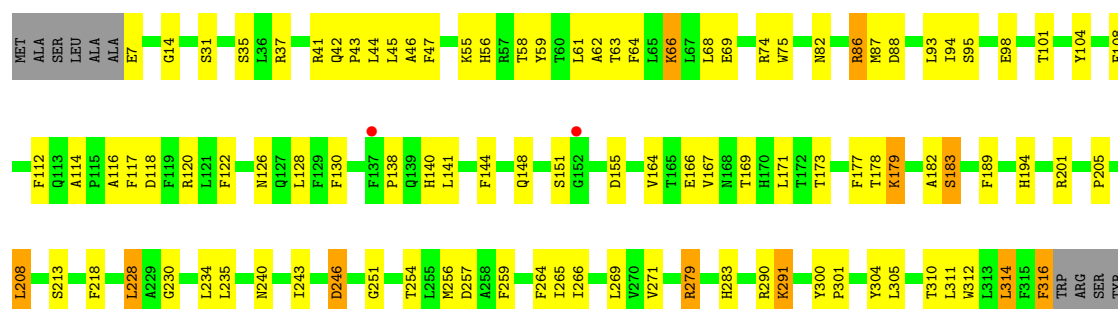
- Molecule 1: Cys-loop ligand-gated ion channel

Chain DDD: 68% 25%



- Molecule 1: Cys-loop ligand-gated ion channel

Chain EEE: 65% 28%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.38Å 114.32Å 142.44Å 90.00° 113.05° 90.00°	Depositor
Resolution (Å)	24.00 – 3.20 24.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	62.1 (24.00-3.20) 62.1 (24.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.260 0.223 , 0.261	Depositor DCC
R_{free} test set	1609 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13005	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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: BNG, A1H7R

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	AAA	0.95	0/2639	1.40	1/3583 (0.0%)
1	BBB	0.94	0/2639	1.41	4/3583 (0.1%)
1	CCC	0.95	0/2639	1.43	9/3583 (0.3%)
1	DDD	0.95	0/2639	1.41	4/3583 (0.1%)
1	EEE	0.95	0/2639	1.42	5/3583 (0.1%)
All	All	0.95	0/13195	1.42	23/17915 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	316	PHE	CA-CB-CG	6.17	119.97	113.80
1	AAA	316	PHE	CA-CB-CG	5.94	119.74	113.80
1	EEE	316	PHE	CA-CB-CG	5.93	119.73	113.80
1	BBB	316	PHE	CA-CB-CG	5.92	119.72	113.80
1	CCC	246	ASP	CA-CB-CG	5.73	118.33	112.60
1	CCC	316	PHE	CA-CB-CG	5.60	119.40	113.80
1	BBB	246	ASP	CA-CB-CG	5.54	118.14	112.60
1	CCC	48	GLU	CA-C-N	5.48	130.31	122.08
1	CCC	48	GLU	C-N-CA	5.48	130.31	122.08
1	CCC	179	LYS	CB-CA-C	5.28	118.41	109.55
1	EEE	246	ASP	CA-CB-CG	5.26	117.86	112.60
1	CCC	98	GLU	CA-C-N	5.24	128.03	120.38
1	CCC	98	GLU	C-N-CA	5.24	128.03	120.38
1	DDD	246	ASP	CA-CB-CG	5.22	117.82	112.60
1	BBB	230	GLY	CA-C-N	5.12	125.63	120.00
1	BBB	230	GLY	C-N-CA	5.12	125.63	120.00
1	DDD	230	GLY	CA-C-N	5.08	125.58	120.00
1	DDD	230	GLY	C-N-CA	5.08	125.58	120.00
1	EEE	179	LYS	CB-CA-C	5.03	118.00	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	230	GLY	CA-C-N	5.02	125.53	120.00
1	CCC	230	GLY	C-N-CA	5.02	125.53	120.00
1	EEE	230	GLY	CA-C-N	5.00	125.50	120.00
1	EEE	230	GLY	C-N-CA	5.00	125.50	120.00

There are no chirality outliers.

There are no planarity outliers.

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	AAA	2566	0	2539	66	7
1	BBB	2566	0	2539	72	0
1	CCC	2566	0	2539	78	7
1	DDD	2566	0	2539	64	0
1	EEE	2566	0	2539	69	0
2	AAA	21	0	30	5	0
2	CCC	21	0	30	9	0
2	DDD	42	0	60	5	0
3	AAA	11	0	0	0	0
3	BBB	11	0	0	0	0
3	CCC	11	0	0	1	0
3	DDD	11	0	0	0	0
3	EEE	11	0	0	0	0
4	AAA	7	0	0	1	0
4	BBB	7	0	0	1	0
4	CCC	7	0	0	4	0
4	DDD	7	0	0	1	0
4	EEE	8	0	0	2	0
All	All	13005	0	12815	305	7

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 12.

All (305) 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:BBB:49:HIS:CD2	1:BBB:98:GLU:OE2	2.00	1.15
1:BBB:49:HIS:NE2	1:BBB:98:GLU:OE2	1.98	0.95
2:CCC:402:BNG:H9'2	2:CCC:402:BNG:H3'1	1.53	0.91
1:CCC:57:ARG:NE	1:DDD:72:GLN:OE1	2.07	0.87
1:EEE:42:GLN:OE1	1:EEE:43:PRO:HD2	1.76	0.85
1:EEE:254:THR:N	1:EEE:257:ASP:OD2	2.09	0.85
1:CCC:49:HIS:HD2	1:CCC:98:GLU:HG3	1.45	0.82
1:CCC:208:LEU:HD21	1:DDD:264:PHE:HB3	1.62	0.82
1:AAA:194:HIS:ND1	1:BBB:251:GLY:HA3	1.96	0.81
1:DDD:42:GLN:OE1	1:DDD:44:LEU:HD13	1.81	0.80
1:EEE:254:THR:HB	1:EEE:257:ASP:OD2	1.82	0.79
2:CCC:402:BNG:H9'2	2:CCC:402:BNG:C3'	2.12	0.78
1:AAA:208:LEU:HD21	1:BBB:264:PHE:HB3	1.65	0.77
1:AAA:58:THR:HG21	1:BBB:74:ARG:HG3	1.66	0.76
1:EEE:47:PHE:O	1:EEE:98:GLU:HG3	1.87	0.75
1:AAA:42:GLN:OE1	1:AAA:44:LEU:HD13	1.87	0.74
1:BBB:208:LEU:HD21	1:CCC:264:PHE:HB3	1.71	0.73
1:BBB:55:LYS:HG3	1:BBB:98:GLU:CD	2.13	0.72
1:BBB:99:ASP:OD2	1:BBB:101:THR:OG1	2.07	0.72
1:EEE:112:PHE:HD2	4:EEE:501:HOH:O	1.73	0.71
1:CCC:234:LEU:HD11	2:CCC:402:BNG:H2'2	1.70	0.71
1:CCC:58:THR:HG21	1:DDD:74:ARG:HG3	1.73	0.70
1:DDD:208:LEU:HD21	1:EEE:264:PHE:HB3	1.73	0.70
1:EEE:55:LYS:HD3	1:EEE:98:GLU:OE1	1.90	0.70
1:AAA:114:ALA:HA	4:AAA:503:HOH:O	1.91	0.69
1:CCC:114:ALA:HA	4:CCC:505:HOH:O	1.92	0.69
1:EEE:254:THR:HB	1:EEE:257:ASP:CG	2.17	0.69
1:CCC:201:ARG:HA	1:DDD:240:ASN:HD21	1.59	0.68
1:AAA:264:PHE:HB3	1:EEE:208:LEU:HD21	1.76	0.68
1:BBB:49:HIS:HD2	1:BBB:98:GLU:OE2	1.69	0.67
1:AAA:56:HIS:HB2	1:BBB:74:ARG:HH22	1.59	0.66
1:CCC:234:LEU:HD11	2:CCC:402:BNG:C2'	2.25	0.66
1:AAA:254:THR:HG22	1:AAA:256:MET:N	2.12	0.64
1:BBB:114:ALA:HA	4:BBB:503:HOH:O	1.96	0.64
1:AAA:201:ARG:HA	1:BBB:240:ASN:HD21	1.63	0.64
1:EEE:173:THR:HA	1:EEE:182:ALA:O	1.98	0.64
1:DDD:254:THR:HG22	1:DDD:256:MET:N	2.12	0.64
1:EEE:254:THR:HG22	1:EEE:256:MET:N	2.12	0.64
1:CCC:254:THR:HG22	1:CCC:256:MET:N	2.12	0.64
1:BBB:254:THR:HG22	1:BBB:256:MET:N	2.13	0.63
1:EEE:254:THR:CB	1:EEE:257:ASP:OD2	2.46	0.63
1:CCC:47:PHE:O	1:CCC:98:GLU:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:49:HIS:CD2	1:CCC:98:GLU:HG3	2.32	0.63
2:CCC:402:BNG:H9'2	2:CCC:402:BNG:C4'	2.28	0.63
1:DDD:173:THR:HA	1:DDD:182:ALA:O	1.99	0.63
1:DDD:194:HIS:ND1	1:EEE:251:GLY:HA3	2.13	0.63
1:BBB:55:LYS:O	1:BBB:55:LYS:HG2	1.98	0.62
1:BBB:173:THR:HA	1:BBB:182:ALA:O	1.99	0.62
1:CCC:173:THR:HA	1:CCC:182:ALA:O	1.99	0.62
1:AAA:63:THR:HG21	1:BBB:69:GLU:OE1	1.99	0.62
1:AAA:173:THR:HA	1:AAA:182:ALA:O	1.99	0.62
1:AAA:69:GLU:OE1	1:EEE:63:THR:HG21	2.00	0.61
1:AAA:254:THR:HG22	1:AAA:256:MET:H	1.66	0.61
1:CCC:218:PHE:O	1:DDD:279:ARG:NH1	2.34	0.60
1:CCC:56:HIS:HB2	1:DDD:74:ARG:HH22	1.65	0.60
1:CCC:63:THR:HG21	1:DDD:69:GLU:OE1	2.02	0.60
1:CCC:254:THR:HG22	1:CCC:256:MET:H	1.67	0.60
1:EEE:254:THR:HG22	1:EEE:256:MET:H	1.67	0.59
1:DDD:55:LYS:HG3	1:DDD:98:GLU:HB2	1.84	0.59
1:BBB:254:THR:HG22	1:BBB:256:MET:H	1.68	0.59
1:DDD:254:THR:HG22	1:DDD:256:MET:H	1.67	0.59
1:BBB:201:ARG:HA	1:CCC:240:ASN:HD21	1.68	0.58
1:AAA:234:LEU:HD21	2:AAA:401:BNG:H9'1	1.86	0.58
1:AAA:74:ARG:HG3	1:EEE:58:THR:HG21	1.85	0.58
1:AAA:240:ASN:HD21	1:EEE:201:ARG:HA	1.69	0.58
1:BBB:243:ILE:HG21	1:BBB:256:MET:HG2	1.86	0.58
1:DDD:218:PHE:O	1:EEE:279:ARG:NH1	2.37	0.58
1:AAA:55:LYS:HG3	1:AAA:55:LYS:O	2.03	0.58
1:AAA:74:ARG:HH22	1:EEE:56:HIS:HB2	1.69	0.58
1:EEE:291:LYS:HA	1:EEE:291:LYS:HE2	1.86	0.57
1:CCC:55:LYS:O	1:CCC:55:LYS:HG3	2.04	0.57
1:CCC:208:LEU:CD2	1:DDD:264:PHE:HB3	2.33	0.57
2:CCC:402:BNG:H3'1	2:CCC:402:BNG:C9'	2.32	0.57
1:DDD:63:THR:HG21	1:EEE:69:GLU:OE1	2.05	0.57
1:CCC:194:HIS:ND1	1:DDD:251:GLY:HA3	2.20	0.57
1:AAA:208:LEU:CD2	1:BBB:264:PHE:HB3	2.33	0.56
1:AAA:251:GLY:HA3	1:EEE:194:HIS:ND1	2.22	0.55
1:BBB:201:ARG:O	1:BBB:205:PRO:HG2	2.06	0.55
1:CCC:201:ARG:O	1:CCC:205:PRO:HG2	2.07	0.55
1:EEE:14:GLY:HA2	1:EEE:151:SER:OG	2.07	0.55
1:AAA:243:ILE:HG21	1:AAA:256:MET:HG2	1.89	0.55
1:CCC:310:THR:O	1:CCC:314:LEU:HB2	2.06	0.55
1:DDD:201:ARG:O	1:DDD:205:PRO:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:310:THR:O	1:BBB:314:LEU:HB2	2.08	0.54
1:AAA:310:THR:O	1:AAA:314:LEU:HB2	2.07	0.54
1:EEE:213:SER:HA	1:EEE:228:LEU:HD21	1.89	0.54
1:EEE:310:THR:O	1:EEE:314:LEU:HB2	2.08	0.54
1:BBB:208:LEU:CD2	1:CCC:264:PHE:HB3	2.38	0.54
1:EEE:201:ARG:O	1:EEE:205:PRO:HG2	2.07	0.54
1:AAA:213:SER:HA	1:AAA:228:LEU:HD21	1.89	0.54
1:DDD:310:THR:O	1:DDD:314:LEU:HB2	2.08	0.54
1:AAA:201:ARG:O	1:AAA:205:PRO:HG2	2.07	0.54
1:EEE:62:ALA:O	1:EEE:66:LYS:HD2	2.08	0.54
1:AAA:62:ALA:O	1:AAA:66:LYS:HD2	2.09	0.53
1:AAA:218:PHE:O	1:BBB:279:ARG:NH1	2.41	0.53
1:BBB:62:ALA:O	1:BBB:66:LYS:HD2	2.08	0.53
1:AAA:279:ARG:NH1	1:EEE:218:PHE:O	2.41	0.53
1:CCC:213:SER:HA	1:CCC:228:LEU:HD21	1.91	0.53
1:DDD:213:SER:HA	1:DDD:228:LEU:HD21	1.89	0.53
1:CCC:62:ALA:O	1:CCC:66:LYS:HD2	2.08	0.53
1:AAA:14:GLY:HA2	1:AAA:151:SER:OG	2.08	0.53
1:BBB:56:HIS:HB2	1:CCC:74:ARG:HH22	1.74	0.53
1:DDD:243:ILE:HG21	1:DDD:256:MET:HG2	1.90	0.53
1:CCC:14:GLY:HA2	1:CCC:151:SER:OG	2.09	0.53
1:DDD:62:ALA:O	1:DDD:66:LYS:HD2	2.08	0.53
1:BBB:14:GLY:HA2	1:BBB:151:SER:OG	2.09	0.53
1:AAA:264:PHE:HB3	1:EEE:208:LEU:CD2	2.39	0.52
1:BBB:55:LYS:HG3	1:BBB:98:GLU:OE1	2.09	0.52
1:DDD:14:GLY:HA2	1:DDD:151:SER:OG	2.09	0.52
1:EEE:243:ILE:HG21	1:EEE:256:MET:HG2	1.91	0.52
1:BBB:213:SER:HA	1:BBB:228:LEU:HD21	1.91	0.52
1:BBB:266:ILE:HG21	1:BBB:304:TYR:CE2	2.45	0.52
1:CCC:266:ILE:HG21	1:CCC:304:TYR:CE2	2.45	0.52
1:DDD:114:ALA:HA	4:DDD:503:HOH:O	2.10	0.51
1:AAA:266:ILE:HG21	1:AAA:304:TYR:CE2	2.45	0.51
2:DDD:401:BNG:H9'2	1:EEE:234:LEU:HD21	1.92	0.51
1:EEE:266:ILE:HG21	1:EEE:304:TYR:CE2	2.46	0.51
1:EEE:44:LEU:HD12	1:EEE:44:LEU:H	1.75	0.51
1:AAA:230:GLY:HA3	2:AAA:401:BNG:C4'	2.41	0.51
1:BBB:45:LEU:HD11	1:BBB:68:LEU:HD21	1.93	0.51
1:AAA:45:LEU:HD11	1:AAA:68:LEU:HD21	1.93	0.51
1:EEE:46:ALA:HA	1:EEE:98:GLU:O	2.11	0.51
1:EEE:31:SER:HA	4:EEE:501:HOH:O	2.10	0.51
1:DDD:82:ASN:ND2	1:DDD:130:PHE:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:243:ILE:HG21	1:CCC:256:MET:HG2	1.94	0.50
1:CCC:82:ASN:ND2	1:CCC:130:PHE:O	2.44	0.50
1:EEE:47:PHE:O	1:EEE:98:GLU:CG	2.57	0.50
1:AAA:312:TRP:O	1:AAA:316:PHE:HB2	2.12	0.50
1:BBB:212:VAL:CG1	2:CCC:402:BNG:H8'1	2.41	0.50
1:DDD:122:PHE:HB3	1:DDD:254:THR:HG23	1.94	0.50
1:AAA:82:ASN:ND2	1:AAA:130:PHE:O	2.45	0.50
1:DDD:201:ARG:HA	1:EEE:240:ASN:HD21	1.77	0.50
1:CCC:46:ALA:HA	1:CCC:98:GLU:O	2.12	0.50
1:CCC:122:PHE:HB3	1:CCC:254:THR:HG23	1.94	0.50
1:EEE:122:PHE:HB3	1:EEE:254:THR:HG23	1.94	0.50
1:BBB:58:THR:HG21	1:CCC:74:ARG:HG3	1.94	0.50
1:BBB:138:PRO:HG3	1:BBB:178:THR:HG21	1.93	0.50
1:EEE:138:PRO:HG3	1:EEE:178:THR:HG21	1.94	0.50
1:BBB:63:THR:HG21	1:CCC:69:GLU:OE1	2.11	0.50
1:BBB:82:ASN:ND2	1:BBB:130:PHE:O	2.45	0.49
1:BBB:312:TRP:O	1:BBB:316:PHE:HB2	2.12	0.49
1:CCC:312:TRP:O	1:CCC:316:PHE:HB2	2.12	0.49
1:DDD:138:PRO:HG3	1:DDD:178:THR:HG21	1.94	0.49
1:BBB:218:PHE:O	1:CCC:279:ARG:NH1	2.45	0.49
1:AAA:116:ALA:HB3	1:AAA:128:LEU:O	2.12	0.49
1:DDD:266:ILE:HG21	1:DDD:304:TYR:CE2	2.47	0.49
1:EEE:148:GLN:OE1	1:EEE:148:GLN:HA	2.12	0.49
1:DDD:230:GLY:HA3	2:DDD:402:BNG:H5'2	1.95	0.49
1:AAA:138:PRO:HG3	1:AAA:178:THR:HG21	1.95	0.49
1:DDD:116:ALA:HB3	1:DDD:128:LEU:O	2.13	0.49
1:DDD:312:TRP:O	1:DDD:316:PHE:HB2	2.11	0.49
1:EEE:312:TRP:O	1:EEE:316:PHE:HB2	2.12	0.49
1:BBB:116:ALA:HB3	1:BBB:128:LEU:O	2.12	0.49
1:CCC:116:ALA:HB3	1:CCC:128:LEU:O	2.13	0.49
1:EEE:116:ALA:HB3	1:EEE:128:LEU:O	2.13	0.49
1:AAA:122:PHE:HB3	1:AAA:254:THR:HG23	1.95	0.49
1:CCC:45:LEU:HD11	1:CCC:68:LEU:HD21	1.94	0.48
1:DDD:254:THR:HB	1:DDD:257:ASP:CG	2.39	0.48
1:EEE:45:LEU:HD11	1:EEE:68:LEU:HD21	1.96	0.48
1:DDD:7:GLU:HA	1:DDD:7:GLU:OE1	2.13	0.48
1:DDD:41:ARG:HA	1:DDD:101:THR:HA	1.95	0.48
1:BBB:291:LYS:HE2	1:BBB:291:LYS:HA	1.95	0.48
1:BBB:7:GLU:OE1	1:BBB:7:GLU:HA	2.13	0.48
1:CCC:61:LEU:HD11	3:CCC:401:A1H7R:C4	2.44	0.48
1:CCC:86:ARG:NH1	1:CCC:88:ASP:OD1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:254:THR:HB	1:CCC:257:ASP:CG	2.38	0.48
1:CCC:240:ASN:HA	1:CCC:260:LEU:HD13	1.96	0.48
1:EEE:82:ASN:ND2	1:EEE:130:PHE:O	2.45	0.48
1:CCC:138:PRO:HG3	1:CCC:178:THR:HG21	1.95	0.48
1:BBB:212:VAL:HG12	2:CCC:402:BNG:H8'1	1.94	0.48
1:BBB:254:THR:HB	1:BBB:257:ASP:CG	2.39	0.48
1:EEE:7:GLU:OE1	1:EEE:7:GLU:HA	2.14	0.48
1:BBB:122:PHE:HB3	1:BBB:254:THR:HG23	1.95	0.47
1:CCC:7:GLU:HA	1:CCC:7:GLU:OE1	2.14	0.47
1:CCC:153:LEU:HD13	1:CCC:167:VAL:CG1	2.44	0.47
2:DDD:402:BNG:H3'2	2:DDD:402:BNG:O5	2.13	0.47
1:BBB:243:ILE:HG21	1:BBB:256:MET:CG	2.44	0.47
1:CCC:300:TYR:OH	4:CCC:501:HOH:O	2.20	0.47
1:DDD:45:LEU:HD11	1:DDD:68:LEU:HD21	1.95	0.47
1:AAA:41:ARG:HA	1:AAA:101:THR:HA	1.96	0.47
1:AAA:254:THR:HB	1:AAA:257:ASP:CG	2.39	0.47
1:EEE:144:PHE:O	1:EEE:171:LEU:HD13	2.15	0.47
1:EEE:41:ARG:HA	1:EEE:101:THR:HA	1.97	0.47
1:BBB:41:ARG:HA	1:BBB:101:THR:HA	1.97	0.47
1:AAA:230:GLY:HA3	2:AAA:401:BNG:H4'2	1.96	0.46
1:BBB:58:THR:CG2	1:CCC:74:ARG:NH1	2.79	0.46
1:DDD:212:VAL:HG13	1:EEE:271:VAL:HG11	1.97	0.46
1:AAA:7:GLU:HA	1:AAA:7:GLU:OE1	2.16	0.46
1:AAA:86:ARG:NH1	1:AAA:88:ASP:OD1	2.40	0.46
1:CCC:216:THR:O	4:CCC:502:HOH:O	2.20	0.46
1:BBB:194:HIS:ND1	1:CCC:251:GLY:HA3	2.31	0.46
2:AAA:401:BNG:O2	2:AAA:401:BNG:H1'2	2.16	0.46
1:EEE:59:TYR:HB2	1:EEE:94:ILE:HB	1.99	0.45
1:DDD:86:ARG:NH1	1:DDD:88:ASP:OD1	2.40	0.45
1:CCC:61:LEU:HD13	1:CCC:104:TYR:CE1	2.51	0.45
1:EEE:55:LYS:O	1:EEE:55:LYS:HG3	2.16	0.45
1:BBB:144:PHE:O	1:BBB:171:LEU:HD13	2.17	0.45
1:EEE:243:ILE:HG21	1:EEE:256:MET:CG	2.47	0.45
1:CCC:57:ARG:CZ	1:DDD:72:GLN:OE1	2.64	0.45
1:DDD:59:TYR:HB2	1:DDD:94:ILE:HB	1.98	0.45
1:EEE:265:ILE:O	1:EEE:269:LEU:HG	2.17	0.45
1:CCC:41:ARG:HA	1:CCC:101:THR:HA	1.99	0.44
1:AAA:208:LEU:HD12	1:AAA:208:LEU:HA	1.85	0.44
1:AAA:243:ILE:HG21	1:AAA:256:MET:CG	2.47	0.44
1:BBB:42:GLN:OE1	1:BBB:44:LEU:HD13	2.18	0.44
1:BBB:265:ILE:O	1:BBB:269:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:61:LEU:HD13	1:DDD:104:TYR:CE1	2.52	0.44
1:DDD:259:PHE:HA	1:DDD:311:LEU:HD11	2.00	0.44
1:AAA:61:LEU:HD13	1:AAA:104:TYR:CE1	2.51	0.44
1:AAA:265:ILE:O	1:AAA:269:LEU:HG	2.17	0.44
1:BBB:86:ARG:NH1	1:BBB:88:ASP:OD1	2.41	0.44
1:CCC:178:THR:OG1	4:CCC:503:HOH:O	2.21	0.44
1:BBB:68:LEU:HD13	1:BBB:75:TRP:HB3	2.00	0.44
1:DDD:114:ALA:C	1:DDD:116:ALA:H	2.25	0.44
1:EEE:61:LEU:HD13	1:EEE:104:TYR:CE1	2.52	0.44
1:EEE:68:LEU:HD13	1:EEE:75:TRP:HB3	2.00	0.44
1:DDD:58:THR:HG21	1:EEE:74:ARG:HG3	1.99	0.44
1:CCC:59:TYR:HB2	1:CCC:94:ILE:HB	2.00	0.44
1:EEE:64:PHE:CE2	1:EEE:68:LEU:HD11	2.53	0.44
1:CCC:64:PHE:CE2	1:CCC:68:LEU:HD11	2.53	0.43
1:CCC:68:LEU:HD13	1:CCC:75:TRP:HB3	2.00	0.43
1:AAA:114:ALA:C	1:AAA:116:ALA:H	2.26	0.43
1:BBB:118:ASP:OD2	1:BBB:120:ARG:NH1	2.51	0.43
1:CCC:265:ILE:O	1:CCC:269:LEU:HG	2.17	0.43
1:DDD:265:ILE:O	1:DDD:269:LEU:HG	2.18	0.43
1:EEE:300:TYR:HB3	1:EEE:301:PRO:HD3	2.00	0.43
1:CCC:114:ALA:C	1:CCC:116:ALA:H	2.26	0.43
1:CCC:164:VAL:HG13	1:CCC:189:PHE:HD2	1.83	0.43
1:DDD:243:ILE:HG21	1:DDD:256:MET:CG	2.48	0.43
1:EEE:259:PHE:HA	1:EEE:311:LEU:HD11	2.00	0.43
1:AAA:157:LEU:O	1:BBB:113:GLN:NE2	2.51	0.43
1:CCC:240:ASN:HA	1:CCC:260:LEU:CD1	2.49	0.43
1:DDD:164:VAL:HG13	1:DDD:189:PHE:HD2	1.84	0.43
1:EEE:44:LEU:HD12	1:EEE:44:LEU:N	2.33	0.43
1:AAA:212:VAL:HG13	1:BBB:271:VAL:HG11	2.00	0.43
1:DDD:144:PHE:O	1:DDD:171:LEU:HD13	2.19	0.43
1:AAA:118:ASP:OD2	1:AAA:120:ARG:NH1	2.51	0.43
1:BBB:61:LEU:HD13	1:BBB:104:TYR:CE1	2.53	0.43
1:BBB:300:TYR:HB3	1:BBB:301:PRO:HD3	1.99	0.43
1:CCC:47:PHE:O	1:CCC:98:GLU:CG	2.66	0.43
1:AAA:300:TYR:HB3	1:AAA:301:PRO:HD3	2.00	0.43
1:CCC:243:ILE:HG21	1:CCC:256:MET:CG	2.49	0.43
1:DDD:64:PHE:CE2	1:DDD:68:LEU:HD11	2.54	0.43
1:EEE:118:ASP:OD2	1:EEE:120:ARG:NH1	2.52	0.43
1:BBB:46:ALA:HA	1:BBB:98:GLU:O	2.18	0.43
1:CCC:259:PHE:HA	1:CCC:311:LEU:HD11	2.01	0.43
1:EEE:164:VAL:HG13	1:EEE:189:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:402:BNG:C4'	2:CCC:402:BNG:C9'	2.97	0.43
1:AAA:64:PHE:CE2	1:AAA:68:LEU:HD11	2.54	0.42
1:AAA:68:LEU:HD13	1:AAA:75:TRP:HB3	2.00	0.42
1:BBB:59:TYR:HB2	1:BBB:94:ILE:HB	2.01	0.42
1:BBB:240:ASN:HA	1:BBB:260:LEU:CD1	2.49	0.42
1:EEE:55:LYS:O	1:EEE:55:LYS:CG	2.67	0.42
1:EEE:86:ARG:NH1	1:EEE:88:ASP:OD1	2.40	0.42
1:BBB:164:VAL:HG13	1:BBB:189:PHE:HD2	1.84	0.42
1:CCC:300:TYR:HB3	1:CCC:301:PRO:HD3	2.00	0.42
1:DDD:300:TYR:HB3	1:DDD:301:PRO:HD3	2.01	0.42
1:BBB:114:ALA:C	1:BBB:116:ALA:H	2.26	0.42
1:CCC:144:PHE:O	1:CCC:171:LEU:HD13	2.19	0.42
1:DDD:58:THR:CG2	1:EEE:74:ARG:NH1	2.83	0.42
1:AAA:161:GLU:HG3	1:BBB:249:ARG:HB2	2.00	0.42
1:CCC:49:HIS:CD2	1:CCC:49:HIS:H	2.38	0.42
1:CCC:86:ARG:NH1	1:DDD:86:ARG:NH2	2.68	0.42
1:DDD:240:ASN:HA	1:DDD:260:LEU:CD1	2.50	0.42
2:AAA:401:BNG:H62	2:DDD:401:BNG:O3	2.20	0.42
1:AAA:59:TYR:HB2	1:AAA:94:ILE:HB	2.01	0.42
1:AAA:144:PHE:HB2	1:AAA:183:SER:HB3	2.02	0.42
1:DDD:230:GLY:HA3	2:DDD:402:BNG:H7'2	2.01	0.42
1:AAA:240:ASN:HA	1:AAA:260:LEU:CD1	2.50	0.42
1:DDD:118:ASP:OD2	1:DDD:120:ARG:NH1	2.53	0.42
1:EEE:114:ALA:C	1:EEE:116:ALA:H	2.26	0.42
1:AAA:164:VAL:HG13	1:AAA:189:PHE:HD2	1.84	0.41
1:DDD:166:GLU:OE2	1:DDD:168:ASN:OD1	2.38	0.41
1:DDD:55:LYS:O	1:DDD:55:LYS:CG	2.68	0.41
1:BBB:64:PHE:CE2	1:BBB:68:LEU:HD11	2.54	0.41
1:CCC:144:PHE:HB2	1:CCC:183:SER:HB3	2.02	0.41
1:AAA:305:LEU:HD23	1:AAA:305:LEU:HA	1.94	0.41
1:BBB:91:ASN:O	1:BBB:106:GLU:HA	2.21	0.41
1:BBB:305:LEU:HD23	1:BBB:305:LEU:HA	1.93	0.41
1:AAA:86:ARG:NH1	1:BBB:86:ARG:HH21	2.18	0.41
1:AAA:201:ARG:HA	1:BBB:240:ASN:ND2	2.33	0.41
1:CCC:55:LYS:O	1:CCC:55:LYS:CG	2.66	0.41
1:AAA:74:ARG:NH1	1:EEE:58:THR:CG2	2.84	0.41
1:BBB:259:PHE:HA	1:BBB:311:LEU:HD11	2.03	0.41
1:CCC:87:MET:HE2	1:CCC:108:PHE:CD1	2.56	0.41
1:DDD:153:LEU:HD13	1:DDD:167:VAL:CG1	2.50	0.41
1:EEE:144:PHE:HB2	1:EEE:183:SER:HB3	2.03	0.41
1:AAA:87:MET:HE2	1:AAA:108:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:305:LEU:HD23	1:EEE:305:LEU:HA	1.93	0.41
1:AAA:55:LYS:O	1:AAA:55:LYS:CG	2.68	0.40
1:AAA:91:ASN:O	1:AAA:106:GLU:HA	2.21	0.40
1:CCC:212:VAL:HG13	1:DDD:271:VAL:HG11	2.02	0.40
1:CCC:224:LYS:O	1:CCC:228:LEU:HB2	2.21	0.40
1:BBB:144:PHE:HB2	1:BBB:183:SER:HB3	2.03	0.40
1:BBB:259:PHE:O	1:BBB:263:THR:HG23	2.22	0.40
1:CCC:118:ASP:OD2	1:CCC:120:ARG:NH1	2.53	0.40
1:CCC:126:ASN:ND2	1:CCC:126:ASN:C	2.79	0.40
1:DDD:237:ILE:O	1:DDD:240:ASN:HB3	2.21	0.40
1:CCC:86:ARG:NH1	1:DDD:86:ARG:HH21	2.18	0.40
1:CCC:91:ASN:O	1:CCC:106:GLU:HA	2.22	0.40
1:AAA:126:ASN:ND2	1:AAA:126:ASN:C	2.79	0.40
1:CCC:45:LEU:HD21	1:CCC:68:LEU:HD23	2.04	0.40
1:DDD:91:ASN:O	1:DDD:106:GLU:HA	2.21	0.40
1:DDD:126:ASN:ND2	1:DDD:126:ASN:C	2.79	0.40
1:EEE:87:MET:HE2	1:EEE:108:PHE:CD1	2.57	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:98:GLU:OE2	1:CCC:49:HIS:NE2[4_456]	1.22	0.98
1:AAA:49:HIS:NE2	1:CCC:49:HIS:ND1[4_456]	1.51	0.69
1:AAA:49:HIS:NE2	1:CCC:49:HIS:CE1[4_456]	1.67	0.53
1:AAA:98:GLU:CD	1:CCC:49:HIS:NE2[4_456]	1.73	0.47
1:AAA:49:HIS:CE1	1:CCC:49:HIS:ND1[4_456]	1.97	0.23
1:AAA:98:GLU:OE1	1:CCC:49:HIS:NE2[4_456]	2.13	0.07
1:AAA:98:GLU:OE2	1:CCC:49:HIS:CE1[4_456]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AAA	308/320 (96%)	290 (94%)	18 (6%)	0	100	100
1	BBB	308/320 (96%)	290 (94%)	18 (6%)	0	100	100
1	CCC	308/320 (96%)	290 (94%)	18 (6%)	0	100	100
1	DDD	308/320 (96%)	289 (94%)	19 (6%)	0	100	100
1	EEE	308/320 (96%)	291 (94%)	17 (6%)	0	100	100
All	All	1540/1600 (96%)	1450 (94%)	90 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	275/282 (98%)	254 (92%)	21 (8%)	12	42
1	BBB	275/282 (98%)	252 (92%)	23 (8%)	10	38
1	CCC	275/282 (98%)	251 (91%)	24 (9%)	9	36
1	DDD	275/282 (98%)	253 (92%)	22 (8%)	11	40
1	EEE	275/282 (98%)	249 (90%)	26 (10%)	8	32
All	All	1375/1410 (98%)	1259 (92%)	116 (8%)	10	38

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	35	SER
1	AAA	37	ARG
1	AAA	55	LYS
1	AAA	66	LYS
1	AAA	86	ARG
1	AAA	93	LEU
1	AAA	95	SER
1	AAA	117	PHE
1	AAA	126	ASN
1	AAA	140	HIS

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Mol	Chain	Res	Type
1	AAA	141	LEU
1	AAA	166	GLU
1	AAA	167	VAL
1	AAA	177	PHE
1	AAA	183	SER
1	AAA	208	LEU
1	AAA	228	LEU
1	AAA	279	ARG
1	AAA	283	HIS
1	AAA	290	ARG
1	AAA	314	LEU
1	BBB	35	SER
1	BBB	37	ARG
1	BBB	66	LYS
1	BBB	93	LEU
1	BBB	95	SER
1	BBB	99	ASP
1	BBB	117	PHE
1	BBB	126	ASN
1	BBB	140	HIS
1	BBB	141	LEU
1	BBB	155	ASP
1	BBB	166	GLU
1	BBB	167	VAL
1	BBB	177	PHE
1	BBB	179	LYS
1	BBB	183	SER
1	BBB	208	LEU
1	BBB	228	LEU
1	BBB	279	ARG
1	BBB	283	HIS
1	BBB	290	ARG
1	BBB	291	LYS
1	BBB	314	LEU
1	CCC	35	SER
1	CCC	37	ARG
1	CCC	55	LYS
1	CCC	66	LYS
1	CCC	86	ARG
1	CCC	93	LEU
1	CCC	95	SER
1	CCC	117	PHE

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Mol	Chain	Res	Type
1	CCC	126	ASN
1	CCC	140	HIS
1	CCC	141	LEU
1	CCC	166	GLU
1	CCC	167	VAL
1	CCC	177	PHE
1	CCC	179	LYS
1	CCC	183	SER
1	CCC	208	LEU
1	CCC	228	LEU
1	CCC	235	LEU
1	CCC	246	ASP
1	CCC	279	ARG
1	CCC	283	HIS
1	CCC	290	ARG
1	CCC	314	LEU
1	DDD	35	SER
1	DDD	37	ARG
1	DDD	66	LYS
1	DDD	86	ARG
1	DDD	93	LEU
1	DDD	95	SER
1	DDD	117	PHE
1	DDD	126	ASN
1	DDD	140	HIS
1	DDD	141	LEU
1	DDD	166	GLU
1	DDD	167	VAL
1	DDD	168	ASN
1	DDD	177	PHE
1	DDD	183	SER
1	DDD	208	LEU
1	DDD	228	LEU
1	DDD	246	ASP
1	DDD	279	ARG
1	DDD	283	HIS
1	DDD	290	ARG
1	DDD	314	LEU
1	EEE	35	SER
1	EEE	37	ARG
1	EEE	66	LYS
1	EEE	86	ARG

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Mol	Chain	Res	Type
1	EEE	93	LEU
1	EEE	95	SER
1	EEE	117	PHE
1	EEE	126	ASN
1	EEE	140	HIS
1	EEE	141	LEU
1	EEE	155	ASP
1	EEE	166	GLU
1	EEE	167	VAL
1	EEE	169	THR
1	EEE	177	PHE
1	EEE	179	LYS
1	EEE	183	SER
1	EEE	208	LEU
1	EEE	228	LEU
1	EEE	235	LEU
1	EEE	246	ASP
1	EEE	279	ARG
1	EEE	283	HIS
1	EEE	290	ARG
1	EEE	291	LYS
1	EEE	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

9 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	A1H7R	AAA	402	-	11,11,11	0.27	0	14,14,14	0.47	0
3	A1H7R	BBB	401	-	11,11,11	0.33	0	14,14,14	0.35	0
2	BNG	CCC	402	-	21,21,21	0.84	1 (4%)	26,26,26	1.66	3 (11%)
3	A1H7R	EEE	401	-	11,11,11	0.29	0	14,14,14	0.80	1 (7%)
3	A1H7R	CCC	401	-	11,11,11	0.23	0	14,14,14	0.44	0
2	BNG	AAA	401	-	21,21,21	0.81	1 (4%)	26,26,26	1.01	2 (7%)
2	BNG	DDD	401	-	21,21,21	0.84	1 (4%)	26,26,26	1.54	7 (26%)
2	BNG	DDD	402	-	21,21,21	1.06	1 (4%)	26,26,26	1.43	4 (15%)
3	A1H7R	DDD	403	-	11,11,11	0.27	0	14,14,14	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1H7R	AAA	402	-	-	2/4/4/4	0/1/1/1
3	A1H7R	BBB	401	-	-	2/4/4/4	0/1/1/1
2	BNG	CCC	402	-	-	8/12/32/32	0/1/1/1
3	A1H7R	EEE	401	-	-	2/4/4/4	0/1/1/1
3	A1H7R	CCC	401	-	-	4/4/4/4	0/1/1/1
2	BNG	AAA	401	-	-	11/12/32/32	0/1/1/1
2	BNG	DDD	401	-	-	7/12/32/32	0/1/1/1
2	BNG	DDD	402	-	-	8/12/32/32	0/1/1/1
3	A1H7R	DDD	403	-	-	3/4/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	402	BNG	O1-C1	3.74	1.46	1.40
2	DDD	401	BNG	O1-C1	3.11	1.45	1.40
2	CCC	402	BNG	O1-C1	2.45	1.44	1.40
2	AAA	401	BNG	O1-C1	2.24	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	402	BNG	C1-O5-C5	4.75	122.99	113.72
2	DDD	402	BNG	O1-C1-C2	4.08	114.47	108.27
2	CCC	402	BNG	O5-C5-C4	4.03	116.96	109.70
2	DDD	401	BNG	C1-O5-C5	3.68	120.90	113.72
2	CCC	402	BNG	C4-C3-C2	-3.12	105.36	110.83
2	DDD	401	BNG	C1-C2-C3	3.03	116.39	110.01
2	DDD	402	BNG	C1'-O1-C1	2.97	118.75	113.68
2	DDD	401	BNG	O3-C3-C4	-2.88	103.58	110.38
2	AAA	401	BNG	C1-O5-C5	2.86	119.31	113.72
2	DDD	401	BNG	C1'-O1-C1	2.81	118.48	113.68
2	DDD	401	BNG	C6-C5-C4	-2.42	107.07	113.02
2	DDD	401	BNG	O5-C5-C4	2.34	113.91	109.70
2	AAA	401	BNG	O5-C5-C6	2.31	112.15	106.44
2	DDD	402	BNG	C1-C2-C3	2.24	114.73	110.01
2	DDD	402	BNG	O2-C2-C3	-2.16	105.30	110.38
2	DDD	401	BNG	O2-C2-C1	-2.14	104.96	110.08
3	EEE	401	A1H7R	C8-C7-C6	2.02	114.18	111.72

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	401	BNG	O5-C1-O1-C1'
2	DDD	401	BNG	O5-C1-O1-C1'
3	AAA	402	A1H7R	C5-C6-C7-C8
3	BBB	401	A1H7R	C5-C6-C7-C8
3	BBB	401	A1H7R	C5-C6-C7-N9
3	CCC	401	A1H7R	C5-C6-C7-C8
3	CCC	401	A1H7R	C5-C6-C7-N9
3	DDD	403	A1H7R	C5-C6-C7-C8
2	CCC	402	BNG	O5-C1-O1-C1'
2	AAA	401	BNG	O5-C5-C6-O6
2	CCC	402	BNG	C2-C1-O1-C1'
2	DDD	401	BNG	C2-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
2	AAA	401	BNG	C4-C5-C6-O6
2	CCC	402	BNG	C1'-C2'-C3'-C4'
2	DDD	402	BNG	O5-C5-C6-O6
2	CCC	402	BNG	C2'-C3'-C4'-C5'
2	CCC	402	BNG	O1-C1'-C2'-C3'
2	CCC	402	BNG	C5'-C6'-C7'-C8'
3	EEE	401	A1H7R	C10-C5-C6-C7
2	AAA	401	BNG	C2-C1-O1-C1'
2	AAA	401	BNG	O1-C1'-C2'-C3'
2	DDD	401	BNG	C4'-C5'-C6'-C7'
2	AAA	401	BNG	C3'-C4'-C5'-C6'
2	DDD	402	BNG	C6'-C7'-C8'-C9'
2	DDD	402	BNG	C4'-C5'-C6'-C7'
3	EEE	401	A1H7R	C4-C5-C6-C7
2	DDD	402	BNG	C3'-C4'-C5'-C6'
2	AAA	401	BNG	C5'-C6'-C7'-C8'
2	DDD	401	BNG	C2'-C3'-C4'-C5'
2	AAA	401	BNG	C1'-C2'-C3'-C4'
2	AAA	401	BNG	C2'-C1'-O1-C1
2	CCC	402	BNG	C2'-C1'-O1-C1
2	DDD	402	BNG	C2'-C3'-C4'-C5'
2	DDD	401	BNG	C6'-C7'-C8'-C9'
2	AAA	401	BNG	C2'-C3'-C4'-C5'
2	DDD	401	BNG	O1-C1'-C2'-C3'
2	DDD	402	BNG	C4-C5-C6-O6
2	DDD	402	BNG	C1'-C2'-C3'-C4'
3	AAA	402	A1H7R	C5-C6-C7-N9
3	DDD	403	A1H7R	C5-C6-C7-N9
2	DDD	402	BNG	C2'-C1'-O1-C1
2	CCC	402	BNG	C3'-C4'-C5'-C6'
2	DDD	401	BNG	C2'-C1'-O1-C1
3	CCC	401	A1H7R	C10-C5-C6-C7
3	CCC	401	A1H7R	C4-C5-C6-C7
3	DDD	403	A1H7R	C4-C5-C6-C7
2	AAA	401	BNG	C6'-C7'-C8'-C9'

There are no ring outliers.

5 monomers are involved in 19 short contacts:

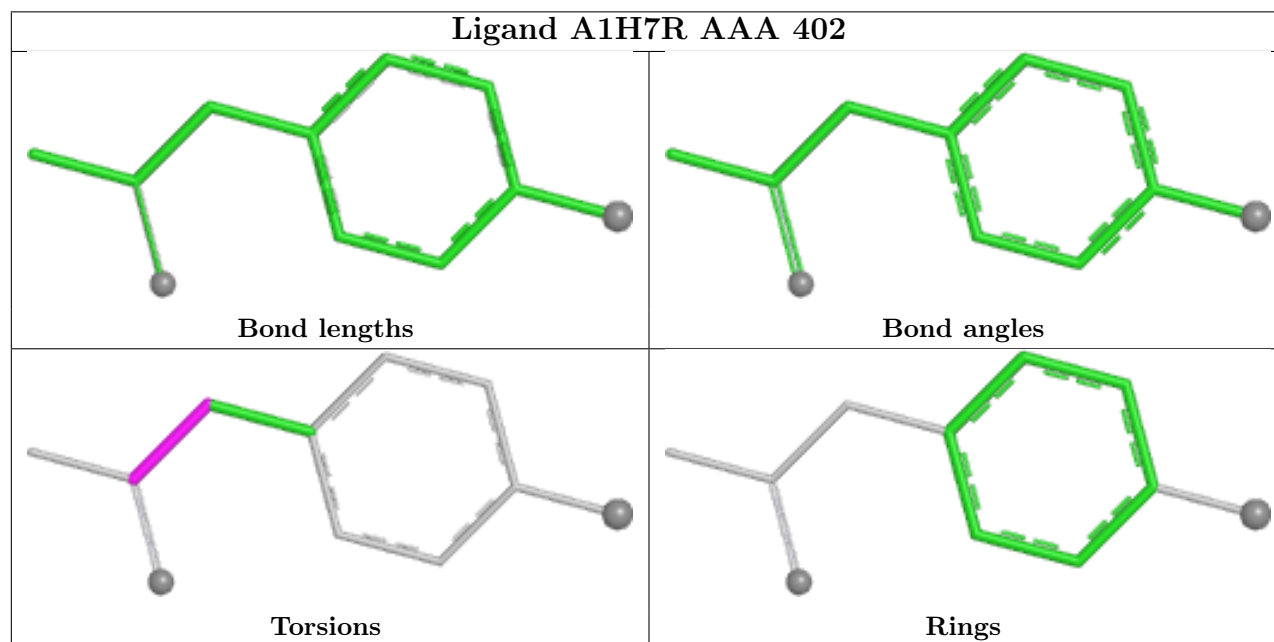
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	402	BNG	9	0
3	CCC	401	A1H7R	1	0

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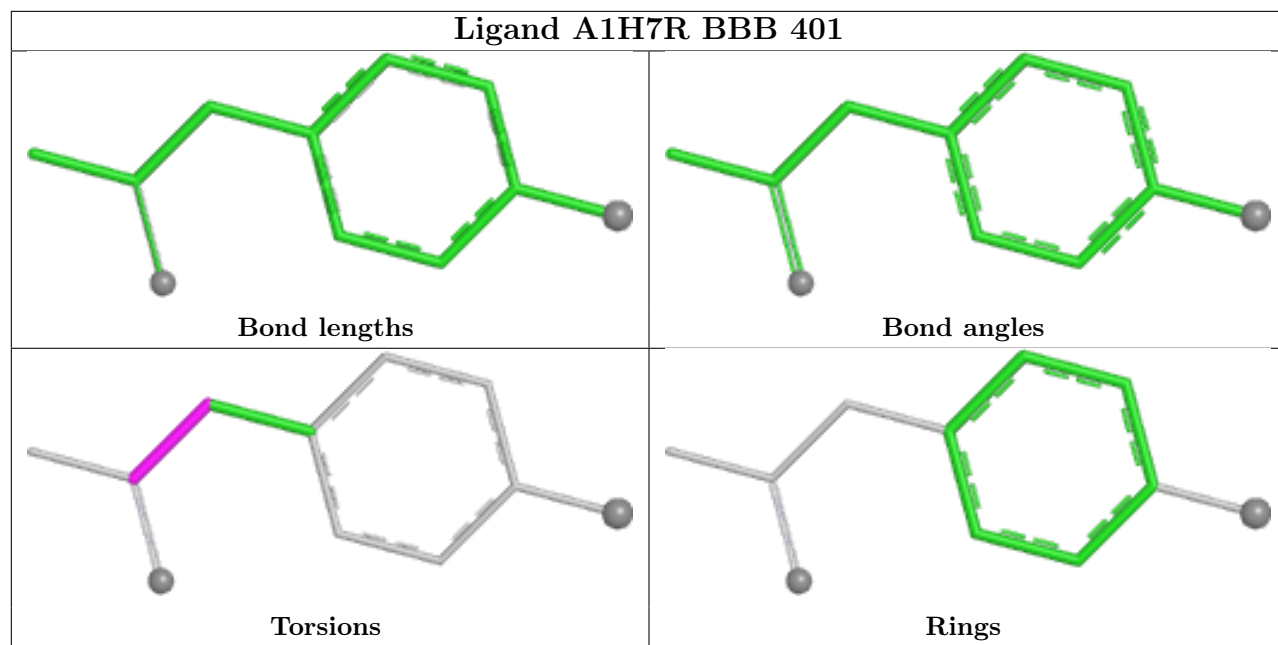
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	401	BNG	5	0
2	DDD	401	BNG	2	0
2	DDD	402	BNG	3	0

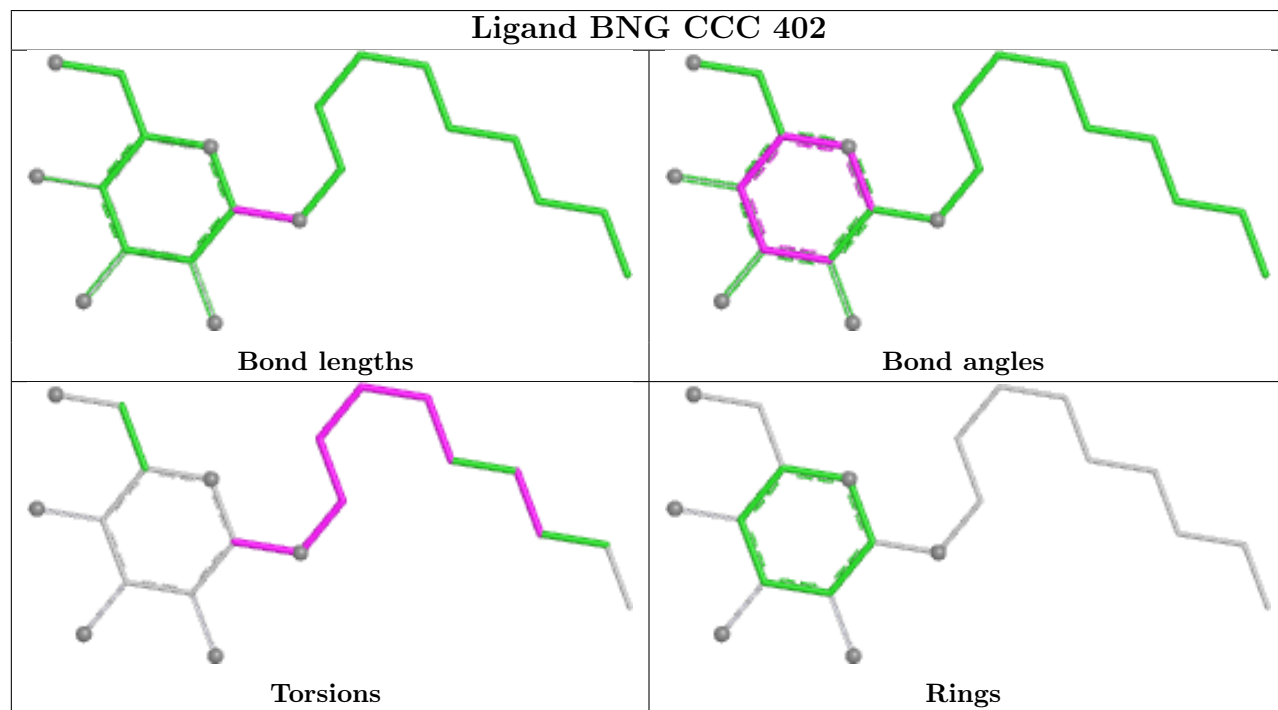
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



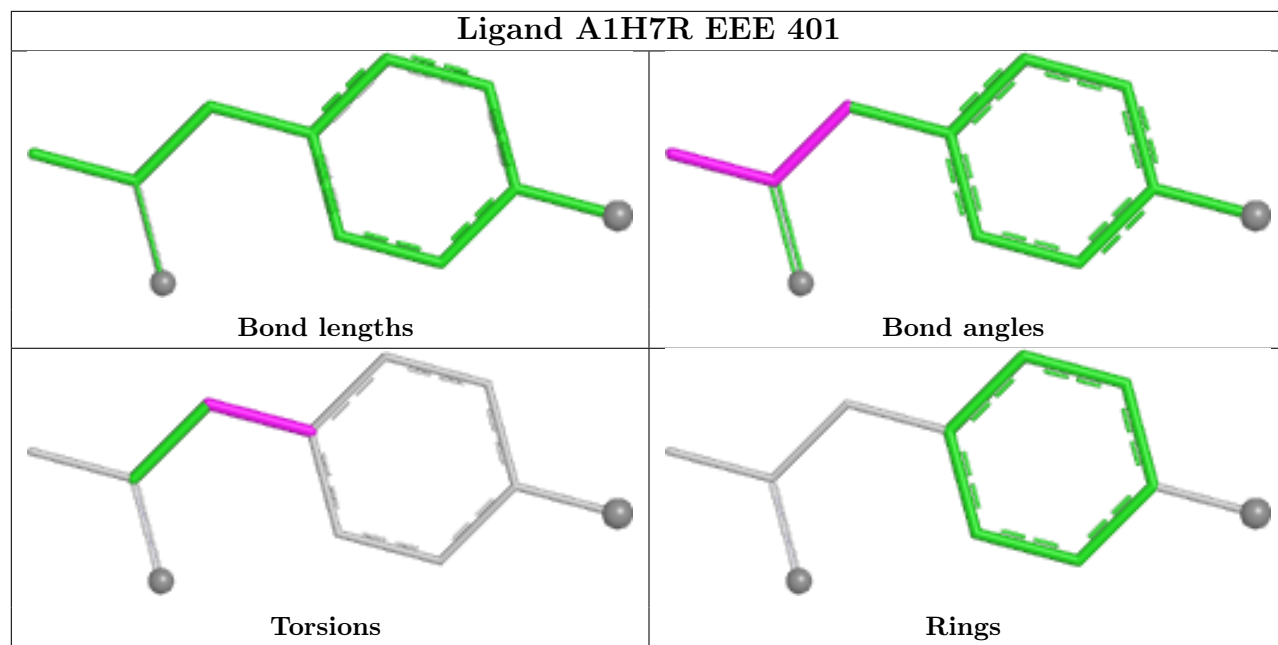
Ligand A1H7R BBB 401



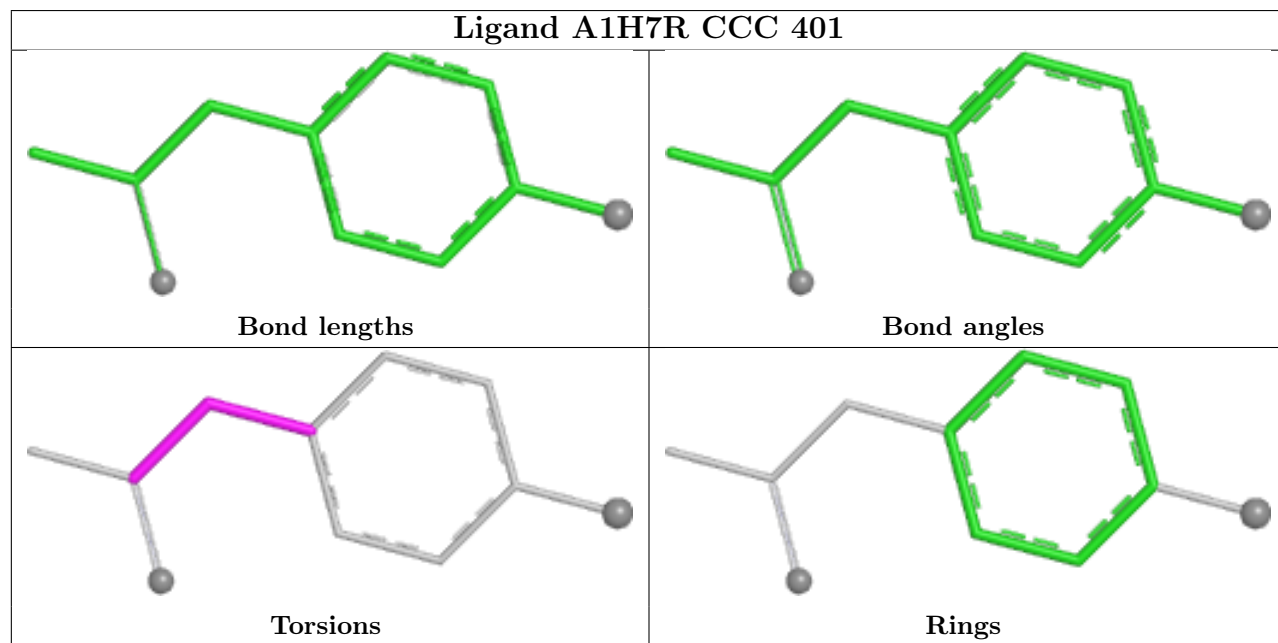
Ligand BNG CCC 402

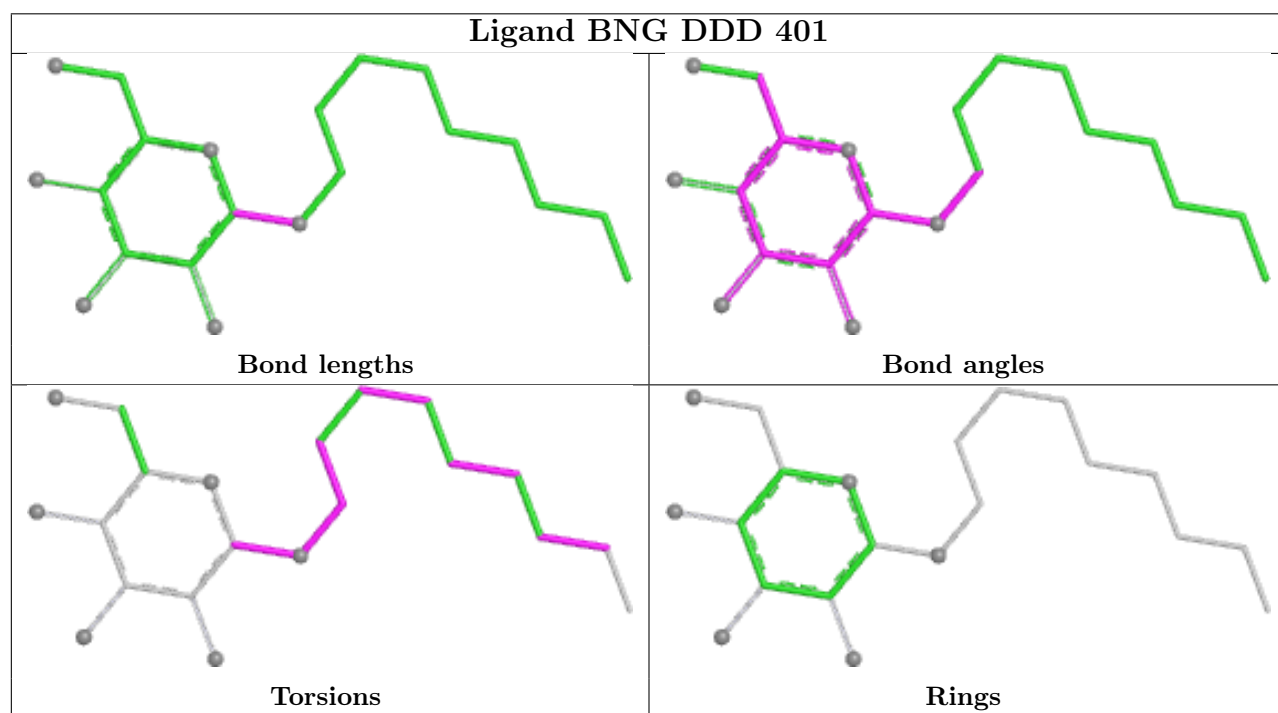
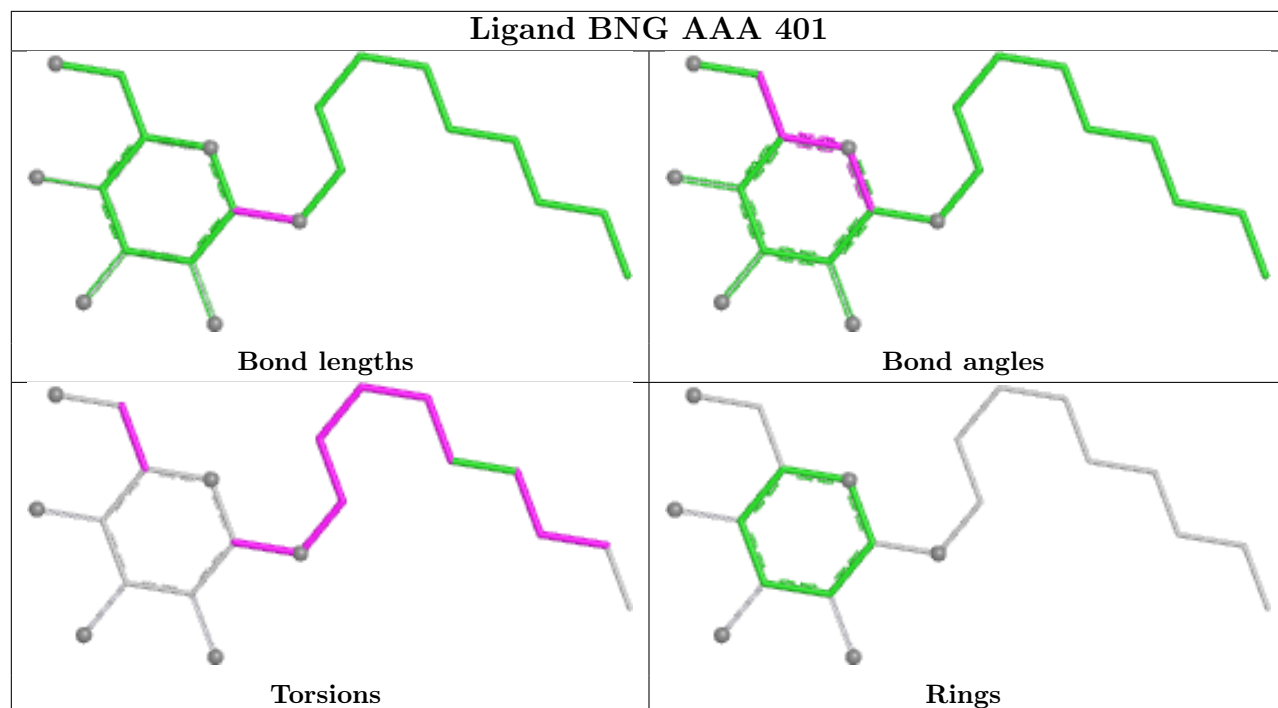


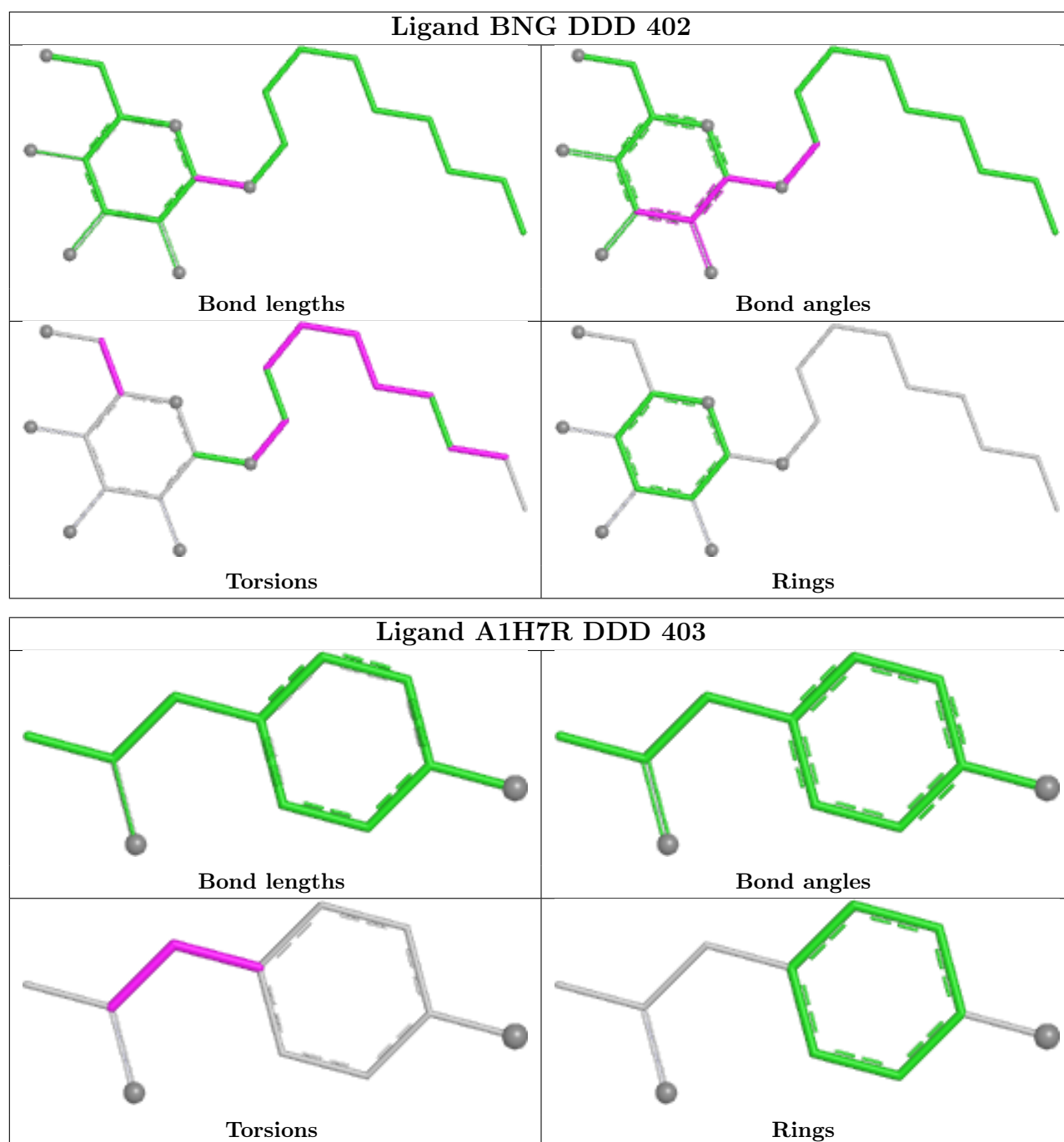
Ligand A1H7R EEE 401



Ligand A1H7R CCC 401







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	AAA	310/320 (96%)	-0.13	1 (0%) 90 81	45, 76, 112, 145	0
1	BBB	310/320 (96%)	-0.24	1 (0%) 90 81	43, 71, 108, 177	0
1	CCC	310/320 (96%)	-0.13	7 (2%) 61 41	39, 74, 105, 140	0
1	DDD	310/320 (96%)	0.01	5 (1%) 70 51	42, 79, 121, 172	0
1	EEE	310/320 (96%)	0.04	2 (0%) 85 73	50, 87, 132, 167	0
All	All	1550/1600 (96%)	-0.09	16 (1%) 79 63	39, 77, 120, 177	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	152	GLY	3.5
1	CCC	175	ASN	3.5
1	DDD	148	GLN	3.4
1	CCC	220	GLN	3.3
1	EEE	152	GLY	3.1
1	DDD	152	GLY	2.9
1	CCC	178	THR	2.7
1	BBB	148	GLN	2.6
1	CCC	181	ASP	2.4
1	DDD	168	ASN	2.3
1	EEE	137	PHE	2.3
1	CCC	180	GLY	2.2
1	AAA	282	ASN	2.2
1	DDD	51	PRO	2.1
1	CCC	51	PRO	2.1
1	DDD	72	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

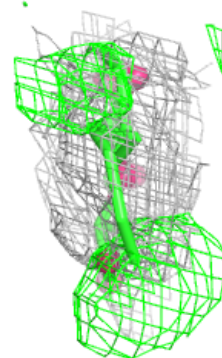
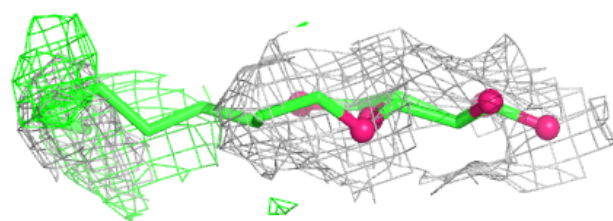
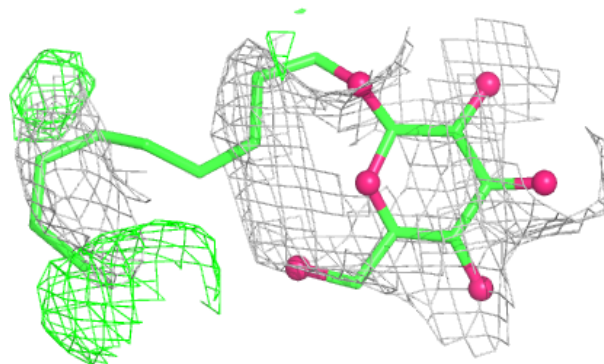
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BNG	DDD	402	21/21	0.80	0.19	67,128,149,154	0
2	BNG	CCC	402	21/21	0.82	0.18	74,117,137,141	0
3	A1H7R	DDD	403	11/11	0.83	0.28	112,133,144,147	0
3	A1H7R	AAA	402	11/11	0.86	0.20	97,121,133,139	0
2	BNG	AAA	401	21/21	0.88	0.18	64,140,156,169	0
2	BNG	DDD	401	21/21	0.89	0.17	52,128,155,169	0
3	A1H7R	CCC	401	11/11	0.91	0.19	99,105,115,120	0
3	A1H7R	EEE	401	11/11	0.94	0.16	116,136,144,146	0
3	A1H7R	BBB	401	11/11	0.95	0.14	85,105,114,116	0

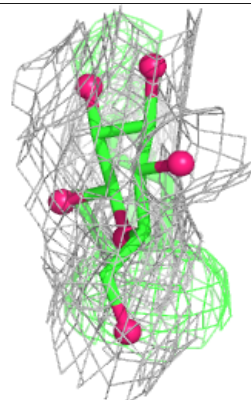
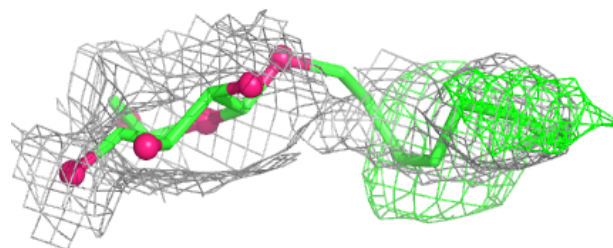
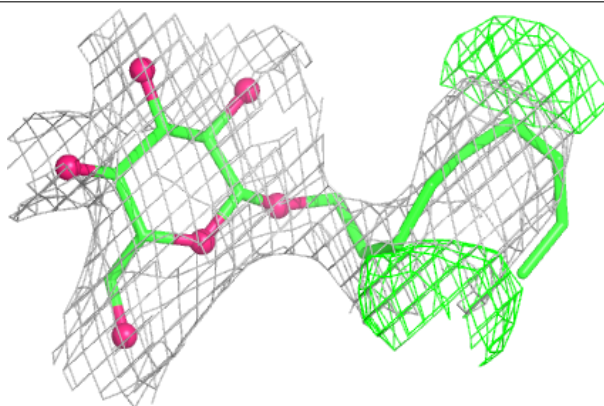
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNG DDD 402:

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

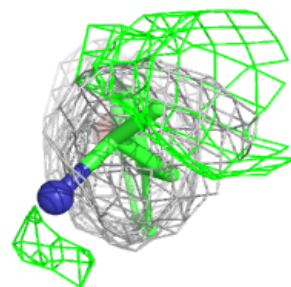
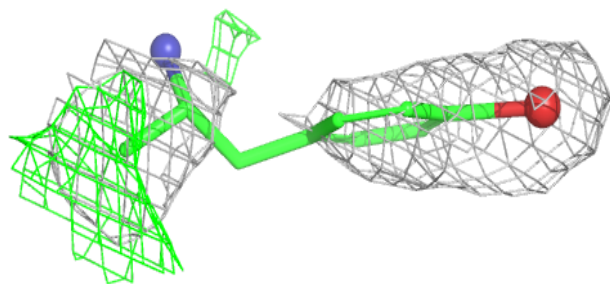
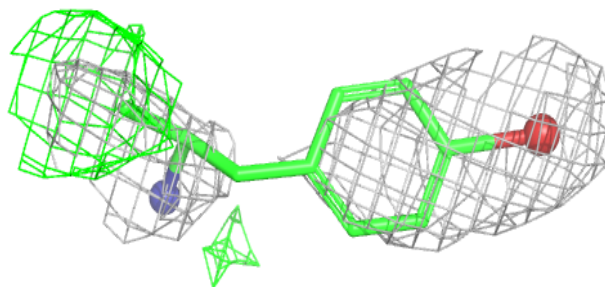
**Electron density around BNG CCC 402:**

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

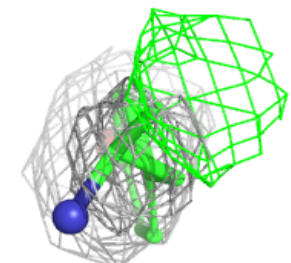
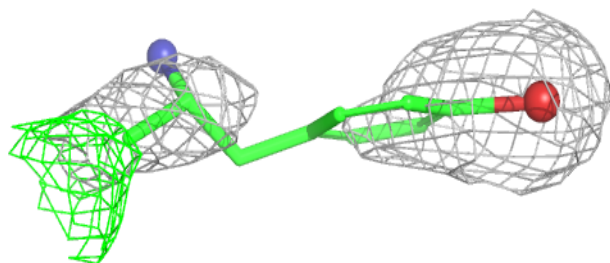
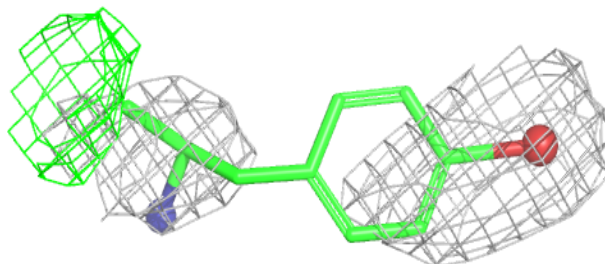


Electron density around A1H7R DDD 403:

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

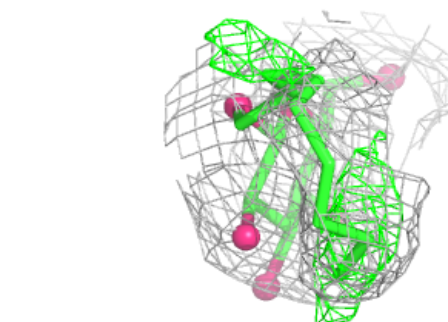
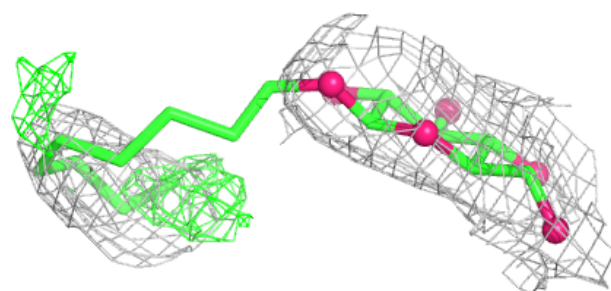
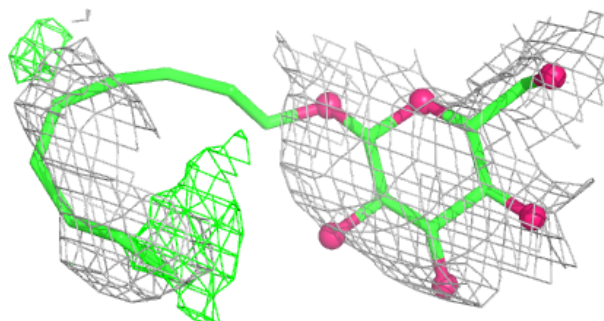
**Electron density around A1H7R AAA 402:**

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

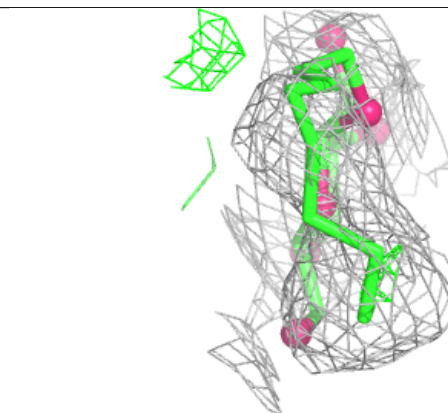
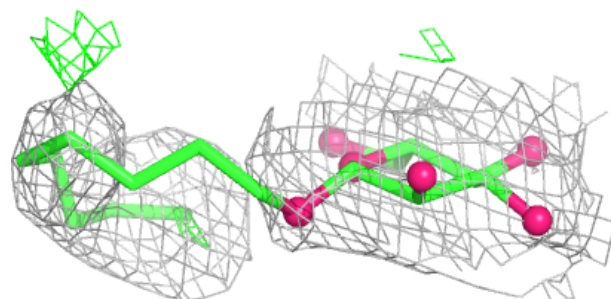
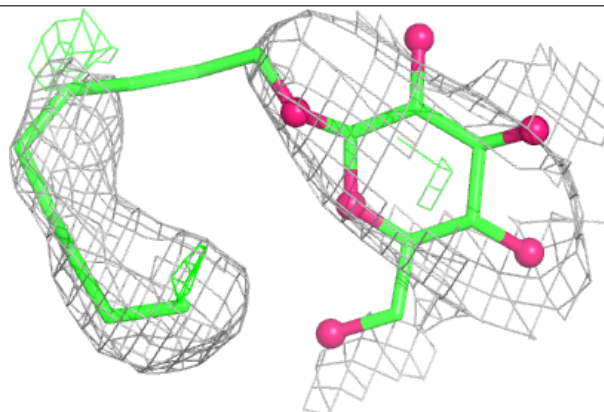


Electron density around BNG AAA 401:

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

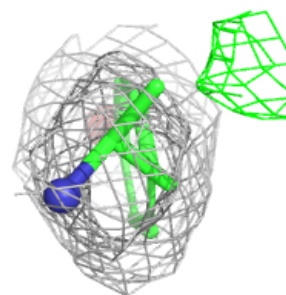
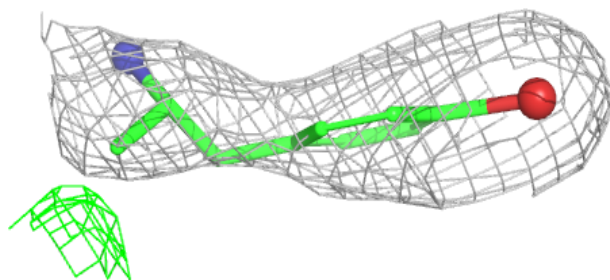
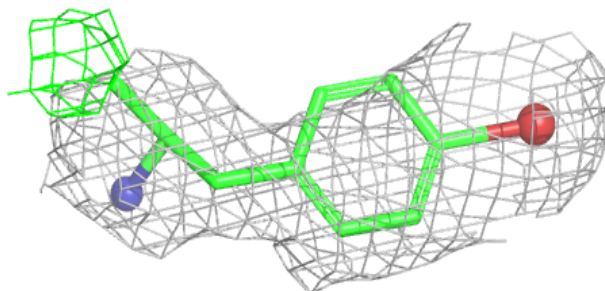
**Electron density around BNG DDD 401:**

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

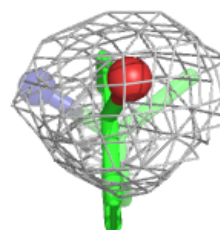
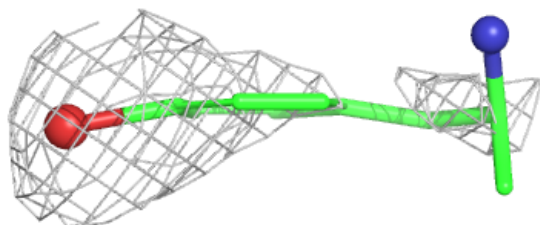
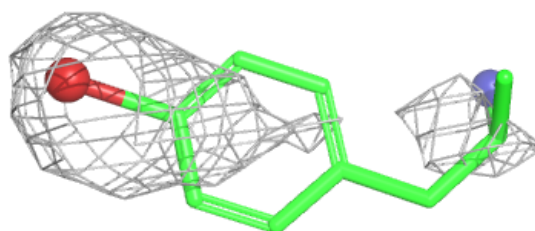


Electron density around A1H7R CCC 401:

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

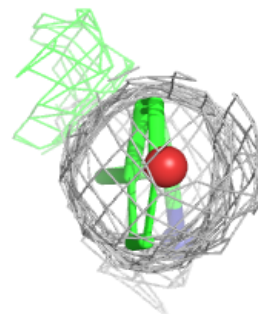
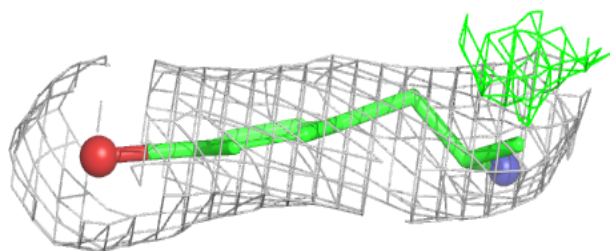
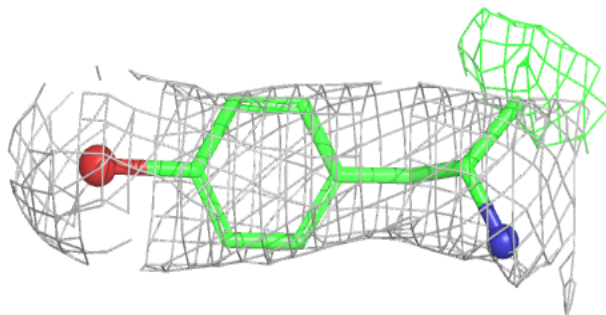
**Electron density around A1H7R EEE 401:**

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



Electron density around A1H7R BBB 401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.