



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:14 PM UTC

PDB ID : 5LG3 / pdb_00005lg3
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with chlorpromazine
Authors : Nys, M.; Wijckmans, E.; Farinha, A.; Brams, M.; Spurny, R.; Ulens, C.
Deposited on : 2016-07-05
Resolution : 3.57 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:

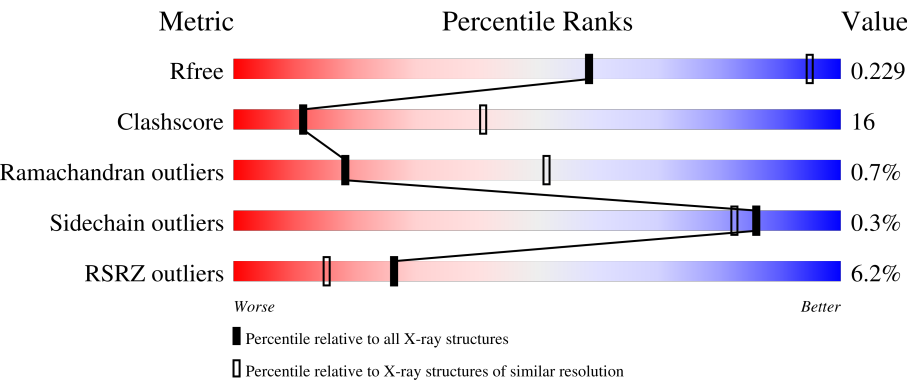
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	307	4% 68% 31% .
1	B	307	10% 67% 32% .
1	C	307	7% 67% 32% .
1	D	307	7% 64% 34% .
1	E	307	6% 69% 30% .

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Mol	Chain	Length	Quality of chain
1	F	307	 3% 67% 32%
1	G	307	 6% 64% 35%
1	H	307	 5% 67% 32%
1	I	307	 6% 69% 30%
1	J	307	 7% 67% 32%

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	Z80	G	401	-	-	X	-

2 Entry composition

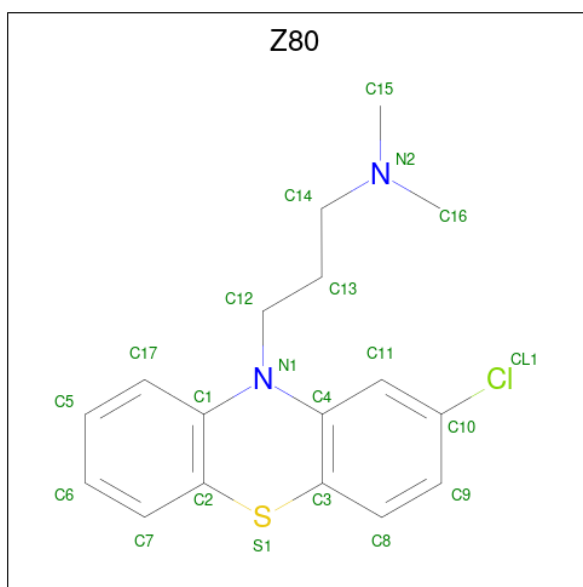
There are 2 unique types of molecules in this entry. The entry contains 25255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gamma-aminobutyric-acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2504	1633	415	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2501	1631	416	448	6			
1	J	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			

- Molecule 2 is 3-(2-chloro-10H-phenothiazin-10-yl)-N,N-dimethylpropan-1-amine (CCD ID: Z80) (formula: C₁₇H₁₉ClN₂S).

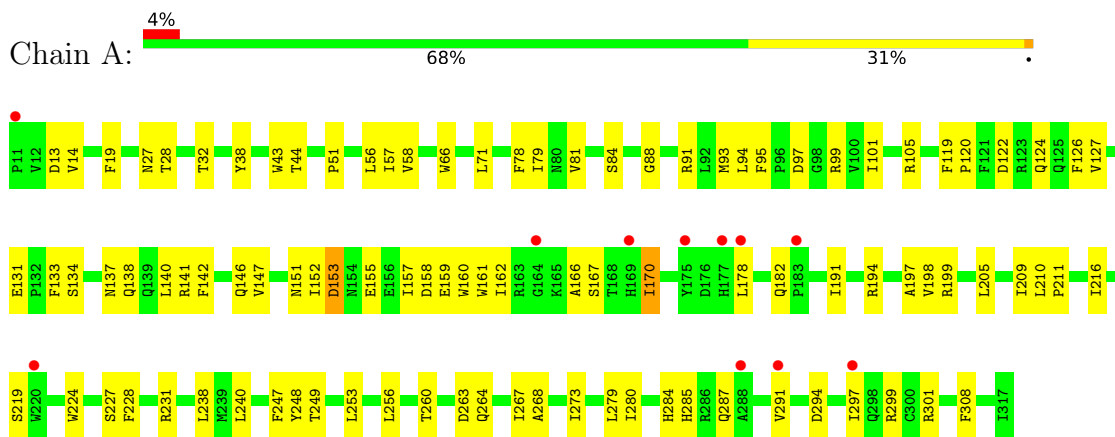


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	B	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	C	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	D	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	E	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	F	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	G	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	H	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	I	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		
2	J	1	Total	C	Cl	N	S	0	0
			21	17	1	2	1		

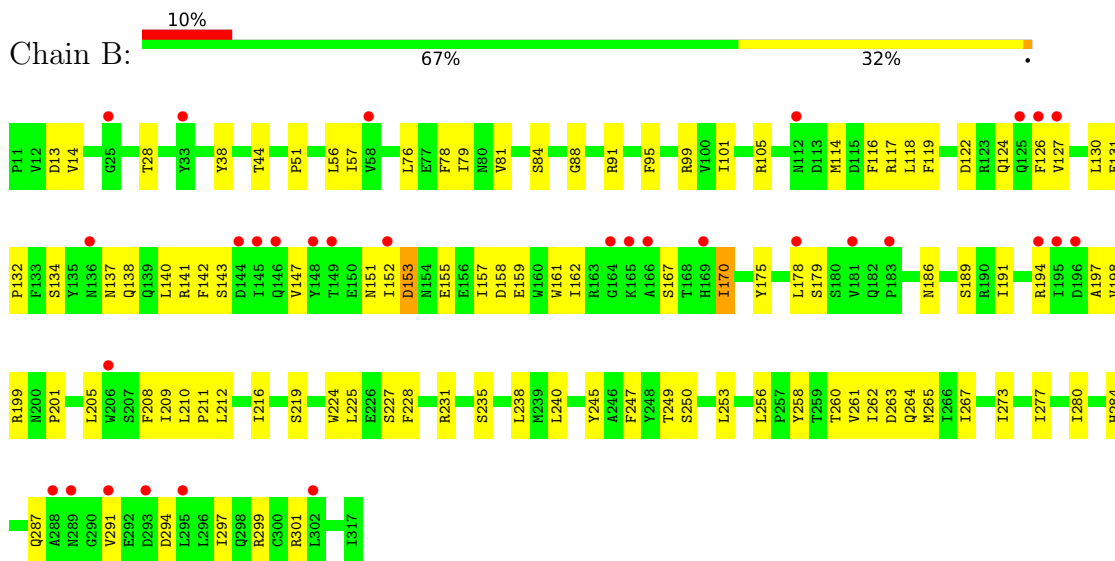
3 Residue-property plots

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: Gamma-aminobutyric-acid receptor subunit beta-1

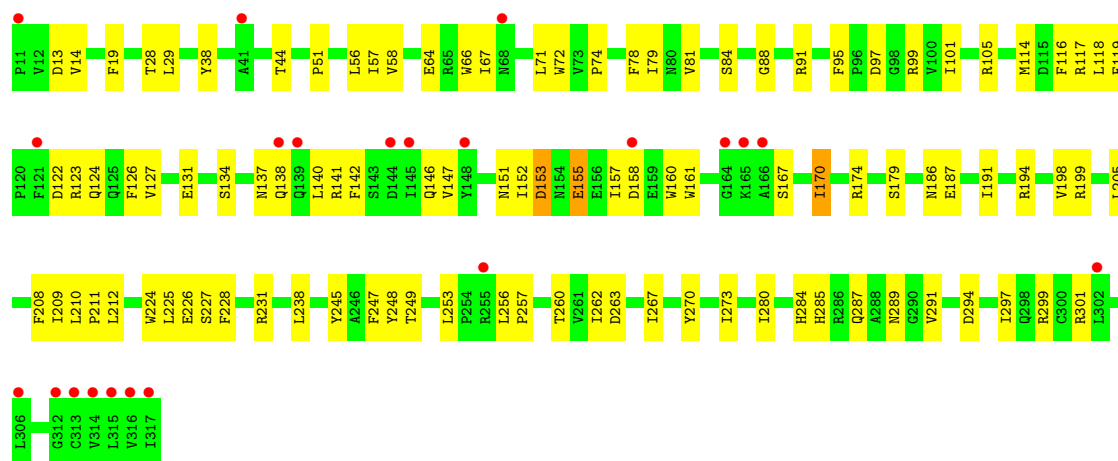


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

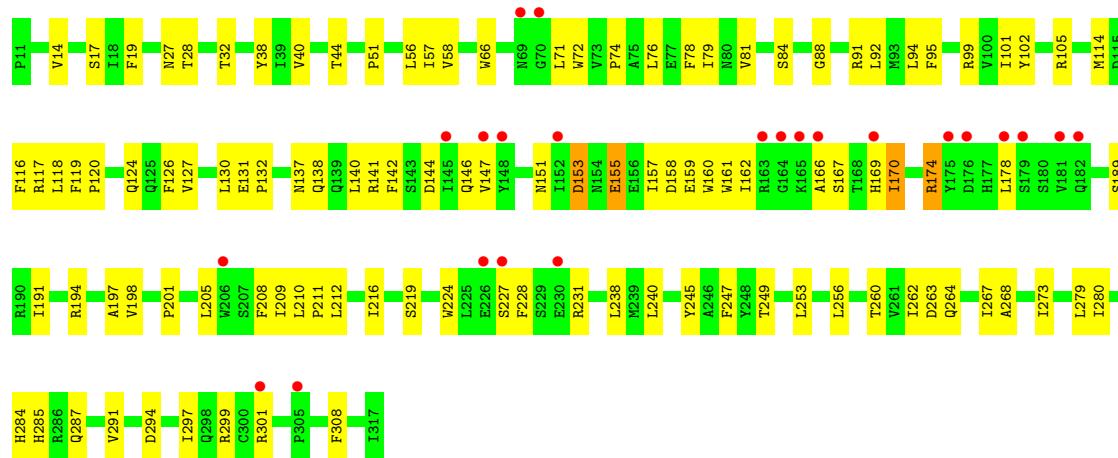


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

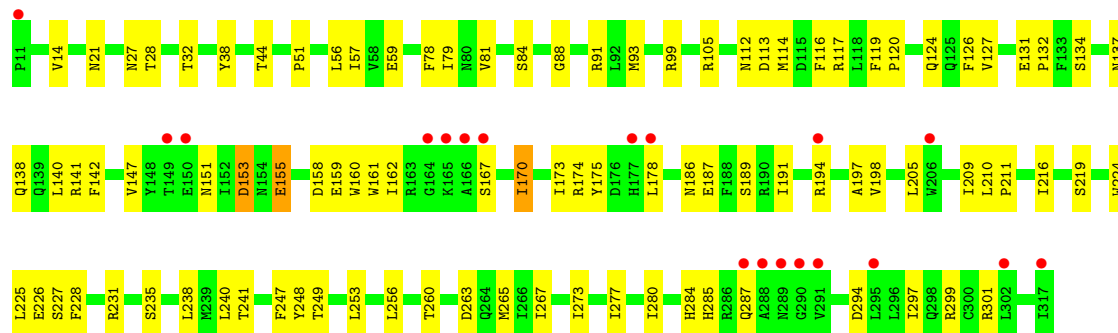




• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

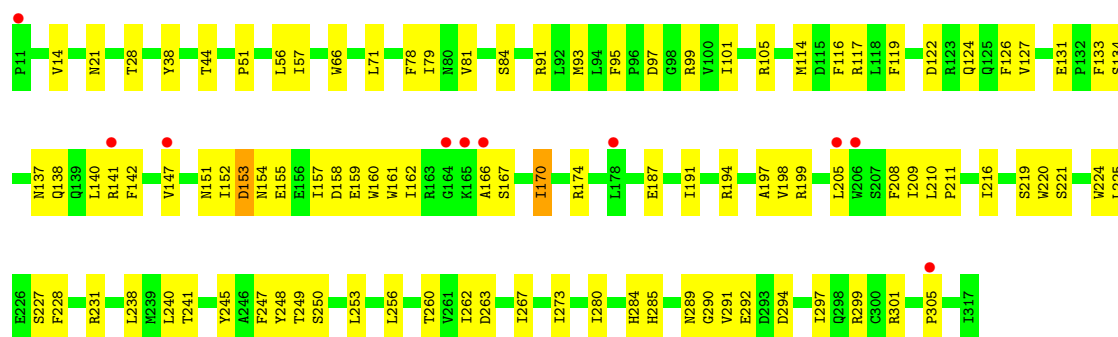


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

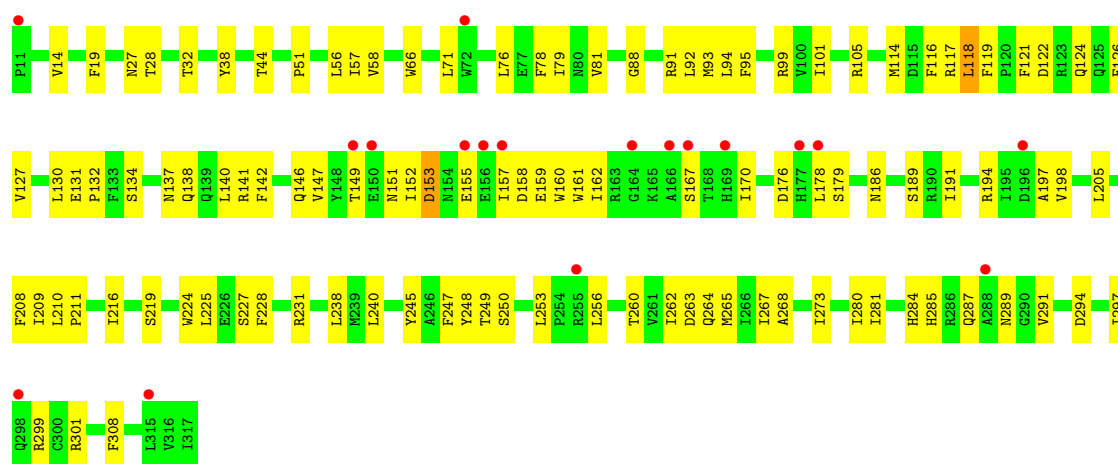


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

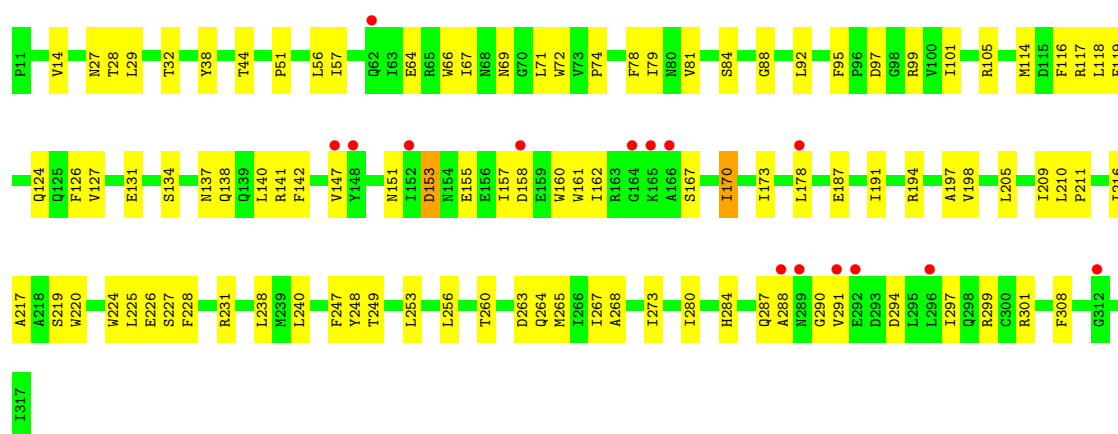




- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

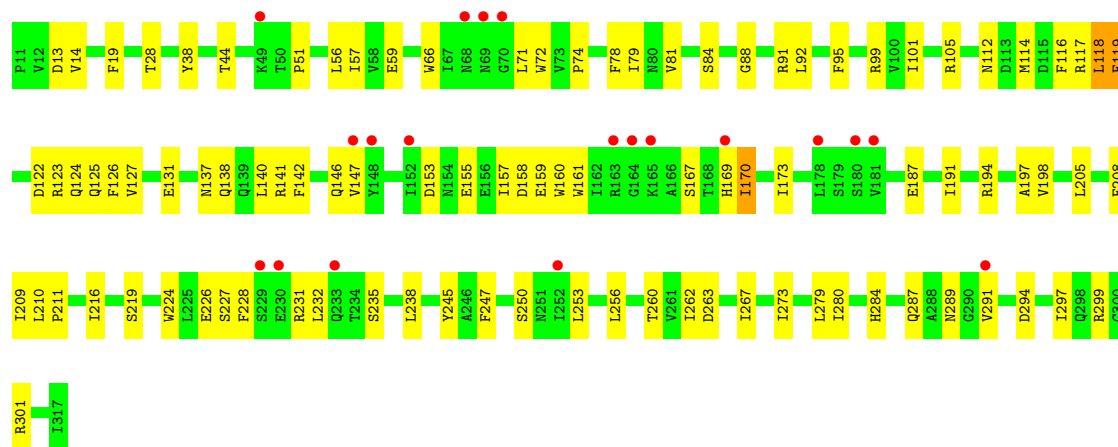


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

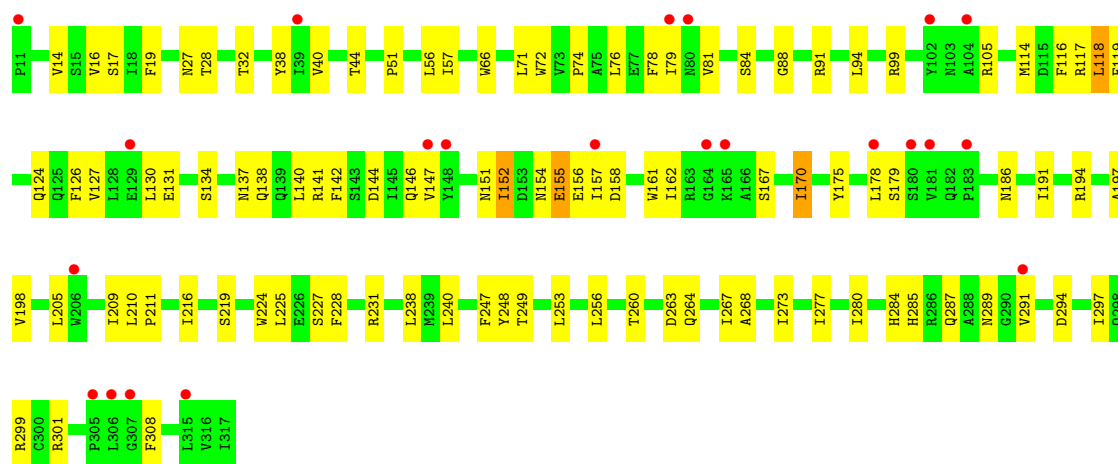


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1





- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.20Å 266.65Å 111.04Å 90.00° 107.71° 90.00°	Depositor
Resolution (Å)	44.75 – 3.57 44.75 – 3.57	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.75-3.57) 97.5 (44.75-3.57)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.220 , 0.253 (Not available) , 0.229	Depositor DCC
R_{free} test set	3417 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	92.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 70.3	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	0.89	EDS
Total number of atoms	25255	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: Z80

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/2571	0.53	0/3503
1	B	0.22	0/2573	0.54	0/3507
1	C	0.21	0/2573	0.56	1/3507 (0.0%)
1	D	0.27	0/2573	0.56	2/3507 (0.1%)
1	E	0.22	0/2573	0.54	1/3507 (0.0%)
1	F	0.24	0/2573	0.54	0/3507
1	G	0.24	0/2573	0.60	3/3507 (0.1%)
1	H	0.23	0/2573	0.54	0/3507
1	I	0.19	0/2569	0.54	4/3502 (0.1%)
1	J	0.26	0/2573	0.61	3/3507 (0.1%)
All	All	0.23	0/25724	0.56	14/35061 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
All	All	0	16

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	118	LEU	N-CA-C	8.74	122.69	112.72
1	J	118	LEU	N-CA-C	8.30	122.18	112.72
1	I	118	LEU	N-CA-C	7.61	121.40	112.72
1	D	155	GLU	CA-CB-CG	-6.10	101.89	114.10
1	J	118	LEU	CA-C-N	5.81	126.28	119.83
1	J	118	LEU	C-N-CA	5.81	126.28	119.83
1	D	174	ARG	CG-CD-NE	5.60	124.31	112.00
1	C	155	GLU	CA-CB-CG	-5.59	102.91	114.10
1	G	118	LEU	CA-C-N	5.49	125.93	119.83
1	G	118	LEU	C-N-CA	5.49	125.93	119.83
1	I	119	PHE	N-CA-C	-5.32	104.94	112.17
1	I	118	LEU	CA-C-N	5.20	125.60	119.83
1	I	118	LEU	C-N-CA	5.20	125.60	119.83
1	E	155	GLU	CA-CB-CG	-5.09	103.91	114.10

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASN	Peptide
1	B	137	ASN	Peptide
1	C	118	LEU	Peptide
1	C	137	ASN	Peptide
1	D	118	LEU	Peptide
1	D	137	ASN	Peptide
1	E	137	ASN	Peptide
1	F	137	ASN	Peptide
1	G	118	LEU	Peptide
1	G	137	ASN	Peptide
1	H	118	LEU	Peptide
1	H	137	ASN	Peptide
1	I	118	LEU	Peptide
1	I	137	ASN	Peptide
1	J	118	LEU	Peptide
1	J	137	ASN	Peptide

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	2504	0	2475	95	0
1	B	2505	0	2478	86	0
1	C	2505	0	2478	84	0
1	D	2505	0	2478	89	0
1	E	2505	0	2478	86	0
1	F	2505	0	2478	88	0
1	G	2505	0	2478	93	0
1	H	2505	0	2478	83	1
1	I	2501	0	2474	77	0
1	J	2505	0	2478	101	0
2	A	21	0	19	7	0
2	B	21	0	19	6	0
2	C	21	0	19	5	0
2	D	21	0	19	4	0
2	E	21	0	19	7	0
2	F	21	0	19	8	0
2	G	21	0	19	9	0
2	H	21	0	19	6	0
2	I	21	0	19	3	0
2	J	21	0	19	7	0
All	All	25255	0	24963	807	1

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 16.

All (807) 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:H:155:GLU:HG3	1:H:161:TRP:CD1	1.99	0.97
1:I:122:ASP:HB3	1:I:124:GLN:NE2	1.81	0.95
1:D:155:GLU:HG3	1:D:161:TRP:CD1	2.02	0.94
1:E:155:GLU:HG3	1:E:161:TRP:CD1	2.02	0.93
1:J:155:GLU:HG3	1:J:161:TRP:CD1	2.05	0.91
1:B:170:ILE:HG12	1:B:191:ILE:HG12	1.55	0.89
1:A:155:GLU:HG3	1:A:161:TRP:CD1	2.12	0.85
1:I:44:THR:HA	1:I:99:ARG:HA	1.59	0.85
1:D:170:ILE:HG12	1:D:191:ILE:HG12	1.60	0.84
1:C:155:GLU:HG3	1:C:161:TRP:CD1	2.13	0.84
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:ASP:HB3	1:I:124:GLN:HE22	1.40	0.83
1:F:231:ARG:HB3	1:F:280:ILE:HD13	1.61	0.83
1:G:155:GLU:HG3	1:G:161:TRP:CD1	2.14	0.83
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.60	0.83
1:A:44:THR:HA	1:A:99:ARG:HA	1.61	0.83
1:H:231:ARG:HB3	1:H:280:ILE:HD13	1.59	0.82
1:D:231:ARG:HB3	1:D:280:ILE:HD13	1.61	0.82
1:C:44:THR:HA	1:C:99:ARG:HA	1.62	0.82
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.63	0.80
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.62	0.80
1:H:44:THR:HA	1:H:99:ARG:HA	1.62	0.80
1:C:167:SER:HB2	1:C:194:ARG:HG3	1.63	0.80
1:J:154:ASN:O	1:J:156:GLU:N	2.15	0.80
1:E:155:GLU:HB3	2:E:401:Z80:H15	1.65	0.79
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.63	0.79
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.64	0.79
1:J:44:THR:HA	1:J:99:ARG:HA	1.65	0.78
1:G:44:THR:HA	1:G:99:ARG:HA	1.64	0.78
1:B:231:ARG:HB3	1:B:280:ILE:HD13	1.65	0.77
1:F:44:THR:HA	1:F:99:ARG:HA	1.66	0.76
1:H:287:GLN:NE2	1:H:290:GLY:O	2.18	0.76
1:H:155:GLU:HG3	1:H:161:TRP:HD1	1.48	0.76
1:G:231:ARG:HB3	1:G:280:ILE:HD13	1.66	0.76
1:G:287:GLN:OE1	1:G:289:ASN:O	2.03	0.76
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.68	0.75
1:G:299:ARG:HA	1:G:301:ARG:HG3	1.69	0.74
1:H:170:ILE:HG12	1:H:191:ILE:HG12	1.69	0.74
1:A:231:ARG:HB3	1:A:280:ILE:HD13	1.69	0.74
1:I:170:ILE:HG12	1:I:191:ILE:HG12	1.68	0.74
1:C:170:ILE:HG12	1:C:191:ILE:HG12	1.69	0.73
1:C:249:THR:HG23	1:C:253:LEU:HD22	1.71	0.73
1:E:44:THR:HA	1:E:99:ARG:HA	1.70	0.73
1:B:44:THR:HA	1:B:99:ARG:HA	1.69	0.73
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.70	0.73
1:C:147:VAL:HG13	2:C:401:Z80:H4	1.71	0.72
1:F:155:GLU:HB3	2:F:401:Z80:H12	1.71	0.72
1:H:167:SER:HB2	1:H:194:ARG:HG3	1.71	0.72
1:I:155:GLU:HA	1:I:158:ASP:HB2	1.71	0.72
1:E:167:SER:HB2	1:E:194:ARG:HG3	1.71	0.72
1:A:170:ILE:HG12	1:A:191:ILE:HG12	1.70	0.72
1:G:240:LEU:HD12	1:H:240:LEU:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:THR:HA	1:D:99:ARG:HA	1.72	0.72
1:E:170:ILE:HG12	1:E:191:ILE:HG12	1.72	0.71
1:J:170:ILE:HG12	1:J:191:ILE:HG12	1.72	0.71
1:E:299:ARG:HA	1:E:301:ARG:HG3	1.72	0.71
1:E:155:GLU:HG3	1:E:161:TRP:HD1	1.53	0.71
1:B:88:GLY:HA2	1:C:84:SER:HB3	1.71	0.71
1:A:240:LEU:HD12	1:B:240:LEU:HD11	1.73	0.70
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.71	0.70
1:I:126:PHE:CZ	2:I:401:Z80:H2	2.26	0.70
1:D:155:GLU:HG3	1:D:161:TRP:HD1	1.53	0.70
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.74	0.70
1:F:240:LEU:HD11	1:J:240:LEU:HD12	1.74	0.69
1:G:249:THR:HG23	1:G:253:LEU:HD22	1.75	0.69
1:D:126:PHE:CZ	2:D:401:Z80:H2	2.28	0.69
1:D:155:GLU:HA	1:D:158:ASP:HB2	1.74	0.68
1:G:155:GLU:HA	1:G:158:ASP:HB2	1.74	0.68
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.75	0.68
1:F:299:ARG:HA	1:F:301:ARG:HG3	1.74	0.68
1:G:147:VAL:HG13	2:G:401:Z80:H4	1.75	0.68
1:B:147:VAL:HG13	2:B:401:Z80:H4	1.74	0.68
1:A:127:VAL:HG22	1:A:194:ARG:HB3	1.74	0.68
1:C:155:GLU:HA	1:C:158:ASP:HB2	1.75	0.68
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.74	0.68
1:F:151:ASN:HD22	2:F:401:Z80:H15	1.57	0.68
1:C:126:PHE:CZ	2:C:401:Z80:H2	2.29	0.68
1:F:127:VAL:HG22	1:F:194:ARG:HB3	1.75	0.67
1:H:249:THR:HG23	1:H:253:LEU:HD22	1.74	0.67
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.77	0.67
1:D:51:PRO:HD2	1:D:56:LEU:HD23	1.76	0.67
1:J:155:GLU:HG3	1:J:161:TRP:HD1	1.58	0.67
1:A:155:GLU:HA	1:A:158:ASP:HB2	1.76	0.67
1:I:299:ARG:HA	1:I:301:ARG:HG3	1.76	0.67
1:F:79:ILE:HD11	1:F:131:GLU:HB3	1.77	0.67
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.77	0.67
1:G:105:ARG:NH2	1:H:81:VAL:O	2.27	0.67
1:D:240:LEU:HD12	1:E:240:LEU:HD11	1.76	0.67
1:J:287:GLN:OE1	1:J:287:GLN:N	2.27	0.67
1:A:51:PRO:HD2	1:A:56:LEU:HD23	1.77	0.67
1:F:170:ILE:HG12	1:F:191:ILE:HG12	1.75	0.66
1:B:51:PRO:HD2	1:B:56:LEU:HD23	1.77	0.66
1:C:174:ARG:HH11	1:C:187:GLU:HG3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:VAL:HG22	1:E:194:ARG:HB3	1.78	0.66
1:H:299:ARG:HA	1:H:301:ARG:HG3	1.78	0.66
1:J:51:PRO:HD2	1:J:56:LEU:HD23	1.78	0.66
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.78	0.66
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.61	0.66
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.78	0.65
1:J:155:GLU:HA	1:J:158:ASP:H	1.60	0.65
1:A:299:ARG:HA	1:A:301:ARG:HG3	1.79	0.65
1:H:127:VAL:HG22	1:H:194:ARG:HB3	1.79	0.65
1:J:151:ASN:HA	1:J:152:ILE:O	1.96	0.65
1:F:152:ILE:HA	1:F:155:GLU:OE2	1.97	0.64
1:A:205:LEU:HD23	1:A:209:ILE:HG13	1.78	0.64
1:G:51:PRO:HD2	1:G:56:LEU:HD23	1.79	0.64
1:D:249:THR:HG23	1:D:253:LEU:HD22	1.78	0.64
1:E:51:PRO:HD2	1:E:56:LEU:HD23	1.79	0.64
1:H:151:ASN:HD22	2:H:401:Z80:H15	1.62	0.64
1:A:249:THR:HG23	1:A:253:LEU:HD22	1.78	0.64
1:C:152:ILE:HA	1:C:155:GLU:OE2	1.97	0.64
1:F:155:GLU:HA	1:F:158:ASP:HB2	1.78	0.64
1:H:205:LEU:HD23	1:H:209:ILE:HG13	1.79	0.64
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.78	0.64
1:J:14:VAL:O	1:J:141:ARG:N	2.29	0.64
1:J:127:VAL:HG22	1:J:194:ARG:HB3	1.80	0.64
1:B:155:GLU:HA	1:B:158:ASP:HB2	1.79	0.63
1:C:153:ASP:H	1:C:155:GLU:CD	2.06	0.63
1:C:127:VAL:HG22	1:C:194:ARG:HB3	1.80	0.63
1:H:155:GLU:HA	1:H:158:ASP:HB2	1.81	0.63
1:G:88:GLY:HA2	1:H:84:SER:HB3	1.80	0.63
1:H:284:HIS:CE1	1:H:291:VAL:HG13	2.33	0.63
1:B:205:LEU:HD23	1:B:209:ILE:HG13	1.81	0.63
1:J:249:THR:HG23	1:J:253:LEU:HD22	1.79	0.63
1:C:155:GLU:HG3	1:C:161:TRP:NE1	2.14	0.63
1:J:224:TRP:NE1	1:J:301:ARG:HB3	2.14	0.63
1:F:133:PHE:CE2	1:J:91:ARG:HG2	2.34	0.62
1:B:151:ASN:HD22	2:B:401:Z80:H15	1.64	0.62
1:C:38:TYR:CZ	1:C:105:ARG:HD2	2.34	0.62
1:C:299:ARG:HA	1:C:301:ARG:HG3	1.81	0.62
1:E:224:TRP:NE1	1:E:301:ARG:HB3	2.14	0.62
1:B:284:HIS:CE1	1:B:291:VAL:HG13	2.35	0.62
1:G:127:VAL:HG22	1:G:194:ARG:HB3	1.79	0.62
1:F:249:THR:HG23	1:F:253:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:GLN:CD	1:G:289:ASN:O	2.43	0.62
1:F:133:PHE:HE2	1:J:91:ARG:HG2	1.65	0.62
1:J:238:LEU:HB3	1:J:273:ILE:HD13	1.81	0.62
1:D:151:ASN:ND2	1:D:155:GLU:OE2	2.33	0.62
1:G:155:GLU:HG3	1:G:161:TRP:HD1	1.64	0.61
1:H:161:TRP:O	1:H:198:VAL:N	2.33	0.61
1:G:151:ASN:HD22	2:G:401:Z80:H15	1.65	0.61
1:F:51:PRO:HD2	1:F:56:LEU:HD23	1.82	0.61
1:H:238:LEU:HB3	1:H:273:ILE:HD13	1.83	0.61
1:A:84:SER:HB3	1:E:88:GLY:HA2	1.82	0.61
1:A:153:ASP:H	1:A:155:GLU:CD	2.08	0.60
1:G:224:TRP:NE1	1:G:301:ARG:HB3	2.16	0.60
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.36	0.60
1:A:105:ARG:NH2	1:B:81:VAL:O	2.34	0.60
1:B:126:PHE:CZ	2:B:401:Z80:H2	2.36	0.60
1:D:155:GLU:H	1:D:155:GLU:CD	2.08	0.60
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.84	0.60
1:H:51:PRO:HD2	1:H:56:LEU:HD23	1.82	0.60
1:J:66:TRP:HE3	1:J:71:LEU:HD12	1.66	0.59
1:F:84:SER:HB3	1:J:88:GLY:HA2	1.83	0.59
1:G:161:TRP:O	1:G:198:VAL:N	2.32	0.59
1:I:284:HIS:CE1	1:I:291:VAL:HG13	2.37	0.59
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.82	0.59
1:E:227:SER:OG	1:E:228:PHE:N	2.35	0.59
1:G:155:GLU:HB3	2:G:401:Z80:H12	1.84	0.59
1:J:38:TYR:CZ	1:J:105:ARG:HD2	2.37	0.59
1:F:161:TRP:O	1:F:198:VAL:N	2.36	0.59
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.83	0.59
1:G:161:TRP:HB2	1:G:198:VAL:HB	1.84	0.59
1:H:38:TYR:CZ	1:H:105:ARG:HD2	2.37	0.59
1:J:284:HIS:CE1	1:J:291:VAL:HG13	2.37	0.59
1:I:227:SER:OG	1:I:228:PHE:N	2.36	0.59
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.85	0.59
1:A:155:GLU:OE1	2:A:401:Z80:H12	2.03	0.59
1:B:161:TRP:HB2	1:B:198:VAL:HB	1.83	0.59
1:E:155:GLU:HA	1:E:158:ASP:HB2	1.83	0.59
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.85	0.59
1:C:238:LEU:HB3	1:C:273:ILE:HD13	1.84	0.59
1:E:227:SER:O	1:E:231:ARG:HD3	2.03	0.59
1:B:127:VAL:HG22	1:B:194:ARG:HB3	1.85	0.58
1:C:227:SER:OG	1:C:228:PHE:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.85	0.58
1:A:224:TRP:NE1	1:A:301:ARG:HB3	2.18	0.58
1:A:227:SER:O	1:A:231:ARG:HD3	2.02	0.58
1:H:224:TRP:NE1	1:H:301:ARG:HB3	2.17	0.58
1:I:279:LEU:HD22	1:I:297:ILE:HD11	1.85	0.58
1:B:253:LEU:HD21	1:B:262:ILE:HD12	1.84	0.58
1:D:147:VAL:HG13	2:D:401:Z80:H4	1.85	0.58
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.84	0.58
1:A:227:SER:OG	1:A:228:PHE:N	2.37	0.58
1:B:299:ARG:HA	1:B:301:ARG:HG3	1.86	0.58
1:D:227:SER:O	1:D:231:ARG:HD3	2.02	0.58
1:B:284:HIS:HE1	1:B:291:VAL:HG13	1.68	0.58
1:C:284:HIS:CE1	1:C:291:VAL:HG13	2.39	0.58
1:D:227:SER:OG	1:D:228:PHE:N	2.37	0.58
1:G:284:HIS:CE1	1:G:291:VAL:HG13	2.38	0.58
1:H:79:ILE:HD11	1:H:131:GLU:HB3	1.85	0.58
1:J:227:SER:OG	1:J:228:PHE:N	2.36	0.58
1:B:224:TRP:NE1	1:B:301:ARG:HB3	2.18	0.58
1:B:227:SER:O	1:B:231:ARG:HD3	2.03	0.58
1:A:38:TYR:CZ	1:A:105:ARG:HD2	2.39	0.58
1:G:209:ILE:HG23	1:G:265:MET:HE1	1.84	0.58
1:J:155:GLU:HG3	1:J:161:TRP:NE1	2.19	0.57
1:D:224:TRP:NE1	1:D:301:ARG:HB3	2.19	0.57
1:D:287:GLN:N	1:D:287:GLN:OE1	2.37	0.57
1:D:210:LEU:HB3	1:D:211:PRO:HD3	1.87	0.57
1:E:147:VAL:HG13	2:E:401:Z80:H4	1.85	0.57
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.86	0.57
1:B:153:ASP:H	1:B:155:GLU:CD	2.13	0.57
1:E:126:PHE:CZ	2:E:401:Z80:H2	2.39	0.57
1:B:79:ILE:HD11	1:B:131:GLU:HB3	1.85	0.57
1:B:227:SER:OG	1:B:228:PHE:N	2.38	0.57
1:C:227:SER:O	1:C:231:ARG:HD3	2.04	0.57
1:F:14:VAL:O	1:F:141:ARG:N	2.34	0.57
1:F:28:THR:HB	1:F:256:LEU:HD21	1.87	0.57
1:I:284:HIS:HE1	1:I:291:VAL:HG13	1.69	0.57
1:J:79:ILE:HD11	1:J:131:GLU:HB3	1.87	0.57
1:A:79:ILE:HD11	1:A:131:GLU:HB3	1.87	0.57
1:E:14:VAL:O	1:E:141:ARG:N	2.32	0.57
1:G:38:TYR:CZ	1:G:105:ARG:HD2	2.40	0.57
1:A:210:LEU:HB3	1:A:211:PRO:HD3	1.86	0.57
1:D:151:ASN:CG	1:D:155:GLU:OE2	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:TRP:O	1:B:198:VAL:N	2.36	0.56
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.86	0.56
1:F:227:SER:OG	1:F:228:PHE:N	2.38	0.56
1:F:38:TYR:CZ	1:F:105:ARG:HD2	2.40	0.56
1:H:227:SER:OG	1:H:228:PHE:N	2.38	0.56
1:J:227:SER:O	1:J:231:ARG:HD3	2.04	0.56
1:B:210:LEU:HB3	1:B:211:PRO:HD3	1.86	0.56
1:J:66:TRP:CE3	1:J:71:LEU:HD12	2.40	0.56
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.87	0.56
1:D:14:VAL:O	1:D:141:ARG:N	2.34	0.56
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.86	0.56
1:H:14:VAL:O	1:H:141:ARG:N	2.36	0.56
1:A:126:PHE:CZ	2:A:401:Z80:H2	2.41	0.56
1:C:28:THR:HB	1:C:256:LEU:HD21	1.88	0.56
1:D:79:ILE:HD11	1:D:131:GLU:HB3	1.86	0.56
1:I:79:ILE:HD11	1:I:131:GLU:HB3	1.87	0.56
1:G:227:SER:OG	1:G:228:PHE:N	2.38	0.56
1:J:155:GLU:HA	1:J:158:ASP:HB2	1.88	0.56
1:B:238:LEU:HB3	1:B:273:ILE:HD13	1.86	0.55
1:C:51:PRO:HD2	1:C:56:LEU:HD23	1.89	0.55
1:E:151:ASN:CG	1:E:155:GLU:OE2	2.49	0.55
1:F:227:SER:O	1:F:231:ARG:HD3	2.05	0.55
1:J:155:GLU:OE1	2:J:401:Z80:H15	2.07	0.55
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.89	0.55
1:B:249:THR:HG23	1:B:253:LEU:HD22	1.88	0.55
1:J:299:ARG:HA	1:J:301:ARG:HG3	1.89	0.55
1:G:210:LEU:HB3	1:G:211:PRO:HD3	1.88	0.55
1:F:151:ASN:ND2	1:F:155:GLU:OE1	2.40	0.55
1:H:151:ASN:CG	1:H:155:GLU:OE2	2.50	0.55
1:D:216:ILE:O	1:D:219:SER:HB3	2.07	0.55
1:F:81:VAL:O	1:J:105:ARG:NH2	2.40	0.55
1:B:14:VAL:O	1:B:141:ARG:N	2.31	0.55
1:D:238:LEU:HB3	1:D:273:ILE:HD13	1.87	0.55
1:E:79:ILE:HD11	1:E:131:GLU:HB3	1.89	0.55
1:I:28:THR:HB	1:I:256:LEU:HD21	1.89	0.55
1:A:155:GLU:HG3	1:A:161:TRP:HD1	1.67	0.55
1:B:105:ARG:NH2	1:C:81:VAL:O	2.40	0.55
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.26	0.54
1:I:224:TRP:NE1	1:I:301:ARG:HB3	2.22	0.54
1:J:126:PHE:CZ	2:J:401:Z80:H2	2.42	0.54
1:G:227:SER:O	1:G:231:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLU:HG3	1:D:161:TRP:NE1	2.20	0.54
1:E:294:ASP:HB3	1:E:297:ILE:CG2	2.37	0.54
1:A:152:ILE:HA	1:A:155:GLU:OE2	2.07	0.54
1:I:227:SER:O	1:I:231:ARG:HD3	2.07	0.54
1:A:147:VAL:HG11	2:A:401:Z80:H4	1.90	0.54
1:H:227:SER:O	1:H:231:ARG:HD3	2.08	0.54
1:B:167:SER:HB2	1:B:194:ARG:HG3	1.89	0.54
1:C:224:TRP:NE1	1:C:301:ARG:HB3	2.23	0.54
1:E:174:ARG:HH11	1:E:187:GLU:HG3	1.73	0.54
1:H:155:GLU:HG3	1:H:161:TRP:NE1	2.21	0.54
1:A:284:HIS:CE1	1:A:291:VAL:HG13	2.43	0.53
1:A:287:GLN:N	1:A:287:GLN:OE1	2.41	0.53
1:G:79:ILE:HD11	1:G:131:GLU:HB3	1.89	0.53
1:F:153:ASP:H	1:F:155:GLU:CD	2.16	0.53
1:J:287:GLN:HG2	1:J:289:ASN:O	2.08	0.53
1:H:28:THR:HB	1:H:256:LEU:HD21	1.89	0.53
1:H:151:ASN:ND2	2:H:401:Z80:H15	2.23	0.53
1:H:64:GLU:HA	1:H:67:ILE:HD12	1.91	0.53
1:A:28:THR:HB	1:A:256:LEU:HD21	1.90	0.53
1:A:81:VAL:O	1:E:105:ARG:NH2	2.42	0.53
1:A:240:LEU:HD23	1:E:241:THR:HA	1.91	0.53
1:G:14:VAL:O	1:G:141:ARG:N	2.35	0.53
1:J:151:ASN:ND2	1:J:162:ILE:HG12	2.22	0.53
1:J:119:PHE:CB	1:J:260:THR:HB	2.38	0.53
1:B:152:ILE:HA	1:B:155:GLU:OE2	2.07	0.53
1:I:119:PHE:CB	1:I:260:THR:HB	2.39	0.53
1:J:284:HIS:HE1	1:J:291:VAL:HG13	1.74	0.53
1:E:28:THR:HB	1:E:256:LEU:HD21	1.91	0.53
1:E:158:ASP:OD2	2:E:401:Z80:H13	2.09	0.53
1:G:122:ASP:HB3	1:G:124:GLN:OE1	2.09	0.52
1:A:238:LEU:HB3	1:A:273:ILE:HD13	1.91	0.52
1:G:119:PHE:HB3	1:G:260:THR:HB	1.91	0.52
1:J:28:THR:HB	1:J:256:LEU:HD21	1.91	0.52
1:H:209:ILE:HG23	1:H:265:MET:HE1	1.91	0.52
1:F:294:ASP:HB3	1:F:297:ILE:CG2	2.40	0.52
1:I:88:GLY:HA2	1:J:84:SER:HB3	1.92	0.52
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.90	0.52
1:E:161:TRP:O	1:E:198:VAL:N	2.38	0.52
1:G:119:PHE:CB	1:G:260:THR:HB	2.39	0.52
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.45	0.52
1:A:147:VAL:CG1	2:A:401:Z80:H4	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:238:LEU:HB3	1:G:273:ILE:HD13	1.92	0.52
1:H:294:ASP:HB3	1:H:297:ILE:CG2	2.40	0.52
1:A:151:ASN:HA	1:A:155:GLU:OE2	2.11	0.51
1:A:155:GLU:HG3	1:A:161:TRP:NE1	2.24	0.51
1:B:122:ASP:HB2	1:B:199:ARG:HB2	1.92	0.51
1:D:279:LEU:HD22	1:D:297:ILE:HD11	1.91	0.51
1:J:126:PHE:HE1	1:J:197:ALA:HB3	1.75	0.51
1:A:126:PHE:HE1	1:A:197:ALA:HB3	1.75	0.51
1:C:66:TRP:CE3	1:C:71:LEU:HD12	2.45	0.51
1:E:155:GLU:HB3	2:E:401:Z80:C16	2.39	0.51
1:F:95:PHE:HE1	1:F:101:ILE:HD12	1.75	0.51
1:C:79:ILE:HD11	1:C:131:GLU:HB3	1.93	0.51
1:D:119:PHE:HB3	1:D:260:THR:HB	1.93	0.51
1:D:161:TRP:O	1:D:198:VAL:N	2.41	0.51
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.93	0.51
1:H:147:VAL:HG13	2:H:401:Z80:H4	1.92	0.51
1:F:289:ASN:O	1:F:290:GLY:C	2.53	0.51
1:D:263:ASP:O	1:D:267:ILE:HG12	2.11	0.51
1:F:155:GLU:HB3	2:F:401:Z80:C15	2.39	0.51
1:F:161:TRP:HB2	1:F:198:VAL:HB	1.92	0.51
1:G:153:ASP:H	1:G:155:GLU:CD	2.18	0.51
1:C:205:LEU:HD23	1:C:209:ILE:HG13	1.92	0.51
1:C:253:LEU:HD21	1:C:262:ILE:HD12	1.93	0.51
1:F:208:PHE:O	1:F:245:TYR:OH	2.28	0.51
1:F:238:LEU:HB3	1:F:273:ILE:HD13	1.92	0.51
1:I:161:TRP:O	1:I:198:VAL:N	2.40	0.51
1:J:155:GLU:HB3	2:J:401:Z80:H15	1.91	0.51
1:D:127:VAL:HG22	1:D:194:ARG:HB3	1.93	0.51
1:G:208:PHE:O	1:G:245:TYR:OH	2.28	0.51
1:H:66:TRP:HE3	1:H:71:LEU:HD12	1.76	0.51
1:J:56:LEU:HD13	1:J:57:ILE:N	2.26	0.51
1:A:161:TRP:O	1:A:198:VAL:N	2.37	0.51
1:B:287:GLN:N	1:B:287:GLN:OE1	2.43	0.50
1:C:66:TRP:HE3	1:C:71:LEU:HD12	1.75	0.50
1:A:93:MET:HB2	1:A:101:ILE:HB	1.93	0.50
1:C:14:VAL:O	1:C:141:ARG:N	2.38	0.50
1:E:153:ASP:H	1:E:155:GLU:CD	2.18	0.50
1:G:247:PHE:CD2	1:H:247:PHE:HE2	2.28	0.50
1:G:167:SER:HB2	1:G:194:ARG:O	2.12	0.50
1:D:161:TRP:HB2	1:D:198:VAL:HB	1.92	0.50
1:I:51:PRO:HD2	1:I:56:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:PHE:HB3	1:I:260:THR:HB	1.93	0.50
1:I:127:VAL:HG22	1:I:194:ARG:HB3	1.92	0.50
1:A:14:VAL:O	1:A:141:ARG:N	2.39	0.50
1:A:158:ASP:OD2	2:A:401:Z80:H14	2.12	0.50
1:D:28:THR:HB	1:D:256:LEU:HD21	1.94	0.50
1:G:91:ARG:HD3	1:H:134:SER:HB3	1.93	0.50
1:A:122:ASP:HB3	1:A:124:GLN:OE1	2.12	0.50
1:B:119:PHE:HB3	1:B:260:THR:HB	1.94	0.50
1:D:224:TRP:HE1	1:D:301:ARG:HB3	1.76	0.50
1:H:66:TRP:CE3	1:H:71:LEU:HD12	2.46	0.50
1:I:287:GLN:N	1:I:287:GLN:OE1	2.45	0.50
1:E:155:GLU:HG3	1:E:161:TRP:NE1	2.26	0.50
1:F:205:LEU:HD23	1:F:209:ILE:HG13	1.93	0.50
1:G:71:LEU:HD11	1:G:94:LEU:HD21	1.93	0.50
1:F:161:TRP:N	1:F:198:VAL:O	2.30	0.49
1:H:119:PHE:HB3	1:H:260:THR:HB	1.94	0.49
1:A:151:ASN:HD22	2:A:401:Z80:H15	1.77	0.49
1:B:216:ILE:O	1:B:219:SER:HB3	2.12	0.49
1:E:126:PHE:HE1	1:E:197:ALA:HB3	1.78	0.49
1:I:91:ARG:HD3	1:J:134:SER:HB3	1.93	0.49
1:I:112:ASN:ND2	1:I:125:GLN:O	2.46	0.49
1:A:88:GLY:HA2	1:B:84:SER:HB3	1.93	0.49
1:C:284:HIS:HE1	1:C:291:VAL:HG13	1.77	0.49
1:G:159:GLU:HB3	1:G:160:TRP:CD1	2.47	0.49
1:J:294:ASP:HB3	1:J:297:ILE:CG2	2.42	0.49
1:E:161:TRP:HB2	1:E:198:VAL:HB	1.95	0.49
1:F:159:GLU:HB3	1:F:160:TRP:CD1	2.47	0.49
1:F:301:ARG:HH12	1:G:285:HIS:HE2	1.60	0.49
1:G:284:HIS:HE1	1:G:291:VAL:HG13	1.75	0.49
1:A:91:ARG:HD3	1:B:134:SER:HB3	1.95	0.49
1:B:38:TYR:CZ	1:B:105:ARG:HD2	2.48	0.49
1:G:162:ILE:HA	1:G:197:ALA:HA	1.95	0.49
1:E:294:ASP:HB3	1:E:297:ILE:HG22	1.94	0.49
1:F:224:TRP:NE1	1:F:301:ARG:HB3	2.28	0.49
1:H:56:LEU:HD13	1:H:57:ILE:N	2.28	0.49
1:D:159:GLU:HB3	1:D:160:TRP:CD1	2.47	0.49
1:B:155:GLU:HB3	2:B:401:Z80:H13	1.94	0.49
1:E:216:ILE:O	1:E:219:SER:HB3	2.13	0.49
1:H:162:ILE:HA	1:H:197:ALA:HA	1.95	0.49
1:E:249:THR:HG23	1:E:253:LEU:HD22	1.94	0.48
1:F:294:ASP:HB3	1:F:297:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ASP:HB3	1:C:297:ILE:CG2	2.43	0.48
1:D:157:ILE:HD11	1:E:117:ARG:NE	2.29	0.48
1:F:162:ILE:HA	1:F:197:ALA:HA	1.95	0.48
1:G:216:ILE:O	1:G:219:SER:HB3	2.13	0.48
1:H:119:PHE:CB	1:H:260:THR:HB	2.43	0.48
1:A:78:PHE:O	1:A:81:VAL:HG12	2.14	0.48
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.31	0.48
1:I:66:TRP:CE3	1:I:71:LEU:HD12	2.49	0.48
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.32	0.48
1:G:294:ASP:HB3	1:G:297:ILE:CG2	2.44	0.48
1:A:216:ILE:O	1:A:219:SER:HB3	2.14	0.48
1:B:28:THR:HB	1:B:256:LEU:HD21	1.96	0.48
1:G:151:ASN:HA	1:G:155:GLU:OE2	2.14	0.48
1:G:179:SER:HB2	1:G:186:ASN:ND2	2.29	0.48
1:G:263:ASP:O	1:G:267:ILE:HG12	2.13	0.48
1:H:151:ASN:ND2	1:H:155:GLU:OE2	2.46	0.48
1:I:14:VAL:O	1:I:141:ARG:N	2.38	0.48
1:A:182:GLN:CD	1:E:93:MET:HE1	2.39	0.48
1:C:155:GLU:HG3	1:C:161:TRP:HD1	1.75	0.48
1:I:95:PHE:HE1	1:I:101:ILE:HD12	1.78	0.48
1:I:123:ARG:C	1:I:124:GLN:NE2	2.72	0.48
1:I:159:GLU:HB3	1:I:160:TRP:CD1	2.48	0.48
1:I:238:LEU:HB3	1:I:273:ILE:HD13	1.96	0.48
1:A:122:ASP:HB2	1:A:199:ARG:HB2	1.96	0.48
1:B:119:PHE:CB	1:B:260:THR:HB	2.44	0.48
1:B:175:TYR:O	1:B:186:ASN:ND2	2.46	0.48
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.31	0.48
1:J:161:TRP:O	1:J:198:VAL:N	2.47	0.48
1:B:205:LEU:HA	1:B:209:ILE:HB	1.96	0.47
1:C:97:ASP:OD2	1:C:99:ARG:NH1	2.47	0.47
1:C:151:ASN:HD22	2:C:401:Z80:H15	1.79	0.47
1:E:162:ILE:HA	1:E:197:ALA:HA	1.95	0.47
1:H:247:PHE:CD2	1:I:247:PHE:HE2	2.31	0.47
1:D:212:LEU:HB2	1:D:245:TYR:CE2	2.48	0.47
1:G:160:TRP:CD1	2:G:401:Z80:H1	2.50	0.47
1:H:153:ASP:H	1:H:155:GLU:CD	2.22	0.47
1:B:235:SER:HB3	1:B:277:ILE:HD11	1.96	0.47
1:D:294:ASP:HB3	1:D:297:ILE:HG22	1.94	0.47
1:A:56:LEU:HD13	1:A:57:ILE:N	2.29	0.47
1:B:294:ASP:HB3	1:B:297:ILE:CG2	2.44	0.47
1:B:56:LEU:HD13	1:B:57:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:LEU:HD11	1:D:94:LEU:HD21	1.97	0.47
1:G:56:LEU:HD13	1:G:57:ILE:N	2.29	0.47
1:H:78:PHE:O	1:H:81:VAL:HG12	2.14	0.47
1:A:134:SER:OG	1:E:59:GLU:OE2	2.33	0.47
1:F:21:ASN:HD21	1:F:38:TYR:HE1	1.61	0.47
1:F:126:PHE:CZ	2:F:401:Z80:H2	2.50	0.47
1:B:247:PHE:CD2	1:C:247:PHE:HE2	2.33	0.47
1:C:161:TRP:O	1:C:198:VAL:N	2.43	0.47
1:D:14:VAL:HG21	1:D:138:GLN:NE2	2.30	0.47
1:D:76:LEU:HB3	1:D:130:LEU:HD11	1.96	0.47
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.62	0.47
1:E:238:LEU:HB3	1:E:273:ILE:HD13	1.96	0.47
1:F:247:PHE:HA	1:J:248:TYR:HD1	1.79	0.47
1:F:289:ASN:OD1	1:F:292:GLU:HB2	2.15	0.47
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.33	0.47
1:J:27:ASN:HB3	1:J:32:THR:HB	1.96	0.47
1:J:154:ASN:C	1:J:156:GLU:H	2.21	0.47
1:J:161:TRP:HB2	1:J:198:VAL:HB	1.96	0.47
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.50	0.47
1:D:155:GLU:HB3	2:D:401:Z80:H13	1.95	0.47
1:I:114:MET:HE2	1:I:116:PHE:CZ	2.49	0.47
1:I:141:ARG:HD2	1:I:142:PHE:CE2	2.50	0.47
1:A:159:GLU:HB3	1:A:160:TRP:CD1	2.49	0.47
1:G:268:ALA:HB1	1:G:308:PHE:CE1	2.50	0.47
1:I:38:TYR:CZ	1:I:105:ARG:HD2	2.50	0.47
1:J:119:PHE:HB2	1:J:260:THR:HB	1.97	0.47
1:C:294:ASP:O	1:C:297:ILE:HG22	2.16	0.46
1:D:78:PHE:O	1:D:81:VAL:HG12	2.14	0.46
1:D:114:MET:HE2	1:D:116:PHE:CZ	2.50	0.46
1:F:126:PHE:CE1	2:F:401:Z80:H18	2.50	0.46
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.97	0.46
1:H:178:LEU:HD13	1:H:178:LEU:HA	1.75	0.46
1:I:56:LEU:HD13	1:I:57:ILE:N	2.29	0.46
1:I:208:PHE:O	1:I:245:TYR:OH	2.30	0.46
1:A:66:TRP:CE3	1:A:71:LEU:HD12	2.50	0.46
1:A:224:TRP:HE1	1:A:301:ARG:HB3	1.79	0.46
1:A:263:ASP:O	1:A:267:ILE:HG12	2.15	0.46
1:D:56:LEU:HD13	1:D:57:ILE:N	2.31	0.46
1:E:155:GLU:OE1	2:E:401:Z80:H12	2.15	0.46
1:F:174:ARG:HH11	1:F:187:GLU:HG3	1.80	0.46
1:F:216:ILE:O	1:F:219:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:119:PHE:HB3	1:J:260:THR:HB	1.97	0.46
1:C:56:LEU:HD13	1:C:57:ILE:N	2.30	0.46
1:F:93:MET:HB2	1:F:101:ILE:HB	1.96	0.46
1:F:220:TRP:CE3	1:F:305:PRO:HG3	2.50	0.46
1:D:284:HIS:CE1	1:D:291:VAL:HG13	2.50	0.46
1:F:114:MET:HE2	1:F:116:PHE:CZ	2.50	0.46
1:I:301:ARG:HH12	1:J:285:HIS:HE2	1.63	0.46
1:A:95:PHE:HE1	1:A:101:ILE:HD12	1.79	0.46
1:E:287:GLN:OE1	1:E:287:GLN:N	2.48	0.46
1:H:294:ASP:HB3	1:H:297:ILE:HG22	1.97	0.46
1:I:147:VAL:HG13	2:I:401:Z80:H4	1.98	0.46
1:E:151:ASN:HA	1:E:155:GLU:OE2	2.16	0.46
1:F:284:HIS:CE1	1:F:291:VAL:HG13	2.51	0.46
1:I:216:ILE:O	1:I:219:SER:HB3	2.15	0.46
1:J:114:MET:HE2	1:J:116:PHE:CZ	2.50	0.46
1:J:147:VAL:HG13	2:J:401:Z80:H4	1.98	0.46
1:H:173:ILE:O	1:H:187:GLU:HA	2.14	0.46
1:A:66:TRP:HE3	1:A:71:LEU:HD12	1.81	0.46
1:B:151:ASN:ND2	1:B:162:ILE:H	2.14	0.46
1:C:88:GLY:HA2	1:D:84:SER:HB3	1.98	0.46
1:C:225:LEU:HB2	1:C:231:ARG:HG3	1.98	0.46
1:G:260:THR:O	1:G:264:GLN:HG3	2.16	0.46
1:H:248:TYR:HE1	1:I:250:SER:OG	1.99	0.46
1:I:226:GLU:OE2	1:J:284:HIS:NE2	2.49	0.46
1:J:72:TRP:CZ3	1:J:74:PRO:HB3	2.51	0.46
1:C:147:VAL:CG1	2:C:401:Z80:H4	2.42	0.46
1:A:294:ASP:HB3	1:A:297:ILE:HG22	1.97	0.45
1:C:301:ARG:HH12	1:D:285:HIS:HE2	1.64	0.45
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.81	0.45
1:F:155:GLU:OE2	1:F:161:TRP:CD1	2.69	0.45
1:G:28:THR:HB	1:G:256:LEU:HD21	1.97	0.45
1:J:263:ASP:O	1:J:267:ILE:HG12	2.16	0.45
1:C:28:THR:HA	1:C:116:PHE:CE1	2.51	0.45
1:D:208:PHE:O	1:D:245:TYR:OH	2.32	0.45
1:G:294:ASP:HB3	1:G:297:ILE:HG22	1.97	0.45
1:J:141:ARG:HD2	1:J:142:PHE:CE2	2.51	0.45
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.34	0.45
1:C:263:ASP:O	1:C:267:ILE:HG12	2.17	0.45
1:E:114:MET:HE2	1:E:116:PHE:CZ	2.52	0.45
1:G:66:TRP:CE3	1:G:71:LEU:HD12	2.52	0.45
1:I:78:PHE:O	1:I:81:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASP:HB3	1:D:297:ILE:CG2	2.46	0.45
1:G:153:ASP:N	1:G:155:GLU:OE2	2.49	0.45
1:H:141:ARG:HD2	1:H:142:PHE:CE2	2.52	0.45
1:J:158:ASP:OD2	2:J:401:Z80:H13	2.16	0.45
1:A:167:SER:CB	1:A:194:ARG:HG3	2.46	0.45
1:B:263:ASP:O	1:B:267:ILE:HG12	2.16	0.45
1:D:114:MET:HE2	1:D:116:PHE:HZ	1.82	0.45
2:J:401:Z80:H9	2:J:401:Z80:H16	1.63	0.45
1:B:132:PRO:HD2	1:B:189:SER:O	2.16	0.45
1:B:167:SER:CB	1:B:194:ARG:HG3	2.46	0.45
1:D:119:PHE:CB	1:D:260:THR:HB	2.47	0.45
1:E:141:ARG:HD2	1:E:142:PHE:CE2	2.52	0.45
1:G:152:ILE:HA	1:G:155:GLU:OE2	2.16	0.45
1:H:126:PHE:CZ	2:H:401:Z80:H2	2.52	0.45
1:J:151:ASN:ND2	1:J:162:ILE:H	2.14	0.45
1:A:247:PHE:CD2	1:B:247:PHE:HE2	2.35	0.45
1:D:38:TYR:CZ	1:D:105:ARG:HD2	2.52	0.45
1:E:235:SER:HB3	1:E:277:ILE:HD11	1.99	0.45
1:I:66:TRP:HE3	1:I:71:LEU:HD12	1.81	0.45
1:B:211:PRO:HB3	1:C:270:TYR:CE1	2.52	0.45
1:G:132:PRO:HD2	1:G:189:SER:O	2.15	0.45
1:G:149:THR:HB	2:G:401:Z80:H16	1.98	0.45
1:J:151:ASN:CG	1:J:162:ILE:HG12	2.42	0.45
1:J:224:TRP:HE1	1:J:301:ARG:HB3	1.79	0.45
1:A:279:LEU:HD22	1:A:297:ILE:HD11	1.97	0.45
1:C:119:PHE:HB3	1:C:260:THR:HB	1.98	0.45
1:C:208:PHE:O	1:C:245:TYR:OH	2.31	0.45
1:H:126:PHE:HE1	1:H:197:ALA:HB3	1.82	0.45
1:J:216:ILE:O	1:J:219:SER:HB3	2.16	0.45
1:C:155:GLU:HG3	1:C:161:TRP:HE1	1.81	0.44
1:J:294:ASP:HB3	1:J:297:ILE:HG22	1.98	0.44
1:C:123:ARG:HG3	1:C:198:VAL:HG22	1.99	0.44
1:G:141:ARG:HD2	1:G:142:PHE:CE2	2.52	0.44
1:H:157:ILE:HD11	1:I:117:ARG:NE	2.32	0.44
1:B:116:PHE:HB2	1:B:258:TYR:HE1	1.82	0.44
1:F:91:ARG:HD3	1:G:134:SER:HB3	1.98	0.44
1:F:155:GLU:H	1:F:155:GLU:HG2	1.27	0.44
1:G:248:TYR:HD1	1:H:247:PHE:HA	1.82	0.44
1:J:66:TRP:CZ3	1:J:94:LEU:HD13	2.52	0.44
1:J:167:SER:HB2	1:J:194:ARG:HG3	1.99	0.44
1:C:161:TRP:HB2	1:C:198:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:ASP:O	1:F:267:ILE:HG12	2.17	0.44
1:J:294:ASP:O	1:J:297:ILE:HG22	2.17	0.44
1:B:294:ASP:HB3	1:B:297:ILE:HG22	1.99	0.44
1:C:78:PHE:O	1:C:81:VAL:HG12	2.18	0.44
1:D:260:THR:O	1:D:264:GLN:HG3	2.18	0.44
1:E:14:VAL:HG21	1:E:138:GLN:NE2	2.32	0.44
1:G:78:PHE:O	1:G:81:VAL:HG12	2.17	0.44
1:H:114:MET:HE2	1:H:116:PHE:CZ	2.53	0.44
1:H:161:TRP:HB2	1:H:198:VAL:HB	1.99	0.44
1:A:27:ASN:HB3	1:A:32:THR:HB	2.00	0.44
1:B:76:LEU:HB3	1:B:130:LEU:HD11	2.00	0.44
1:B:199:ARG:O	1:B:201:PRO:HD3	2.18	0.44
1:B:301:ARG:HH12	1:C:285:HIS:HE2	1.65	0.44
1:C:141:ARG:HD2	1:C:142:PHE:CE2	2.52	0.44
1:D:284:HIS:HB3	1:D:285:HIS:ND1	2.32	0.44
1:F:151:ASN:ND2	2:F:401:Z80:H15	2.28	0.44
1:J:17:SER:HA	1:J:144:ASP:O	2.17	0.44
1:A:161:TRP:HB2	1:A:198:VAL:HB	2.00	0.44
1:C:114:MET:HE2	1:C:116:PHE:CZ	2.52	0.44
1:G:167:SER:CB	1:G:194:ARG:HG3	2.46	0.44
1:J:76:LEU:HB3	1:J:130:LEU:HD11	2.00	0.44
1:C:248:TYR:HD1	1:D:247:PHE:HA	1.83	0.44
1:D:44:THR:HG23	1:D:99:ARG:HB3	2.00	0.44
1:E:112:ASN:OD1	1:E:113:ASP:N	2.51	0.44
2:G:401:Z80:H9	2:G:401:Z80:H17	1.64	0.44
1:E:44:THR:HG23	1:E:99:ARG:HB3	2.00	0.44
1:E:159:GLU:HB3	1:E:160:TRP:CD1	2.53	0.44
1:G:27:ASN:HB3	1:G:32:THR:HB	2.00	0.44
1:J:44:THR:HG23	1:J:99:ARG:HB3	2.00	0.44
1:A:14:VAL:HG21	1:A:138:GLN:NE2	2.32	0.43
1:A:260:THR:O	1:A:264:GLN:HG3	2.18	0.43
1:E:173:ILE:O	1:E:187:GLU:HA	2.18	0.43
1:H:95:PHE:HE1	1:H:101:ILE:HD12	1.83	0.43
1:B:260:THR:O	1:B:264:GLN:HG3	2.17	0.43
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.53	0.43
1:F:126:PHE:HE1	1:F:197:ALA:HB3	1.83	0.43
1:I:294:ASP:HB3	1:I:297:ILE:CG2	2.48	0.43
1:B:157:ILE:HD11	1:C:117:ARG:NE	2.32	0.43
1:I:126:PHE:HE1	1:I:197:ALA:HB3	1.84	0.43
1:B:91:ARG:HD3	1:C:134:SER:HB3	2.00	0.43
1:D:17:SER:HA	1:D:144:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:VAL:HB	1:G:92:LEU:HB2	1.99	0.43
1:A:157:ILE:HD11	1:B:117:ARG:NE	2.33	0.43
1:G:114:MET:HE2	1:G:116:PHE:CZ	2.54	0.43
1:H:216:ILE:O	1:H:219:SER:HB3	2.18	0.43
1:B:178:LEU:HD13	1:B:178:LEU:HA	1.82	0.43
1:E:178:LEU:HD13	1:E:178:LEU:HA	1.79	0.43
1:F:127:VAL:HG22	1:F:194:ARG:CB	2.48	0.43
1:J:114:MET:HE2	1:J:116:PHE:HZ	1.83	0.43
1:A:151:ASN:ND2	1:A:155:GLU:OE2	2.52	0.43
1:B:162:ILE:HA	1:B:197:ALA:HA	2.01	0.43
1:B:179:SER:HB2	1:B:186:ASN:ND2	2.33	0.43
1:C:212:LEU:HB2	1:C:245:TYR:CE2	2.54	0.43
1:D:88:GLY:HA2	1:E:84:SER:HB3	2.00	0.43
1:G:76:LEU:HB3	1:G:130:LEU:HD11	2.00	0.43
1:B:118:LEU:HA	1:B:261:VAL:HG23	2.00	0.43
1:D:178:LEU:HD13	1:D:178:LEU:HA	1.82	0.43
1:I:256:LEU:HD12	1:I:260:THR:HG22	2.00	0.43
1:J:14:VAL:HG21	1:J:138:GLN:NE2	2.34	0.43
1:J:268:ALA:HB1	1:J:308:PHE:CE1	2.53	0.43
1:A:14:VAL:HG13	1:A:43:TRP:HD1	1.83	0.43
1:B:159:GLU:HG3	1:C:257:PRO:HB3	2.00	0.43
1:F:114:MET:HE2	1:F:116:PHE:HZ	1.84	0.43
1:A:97:ASP:OD2	1:A:99:ARG:NH1	2.52	0.43
1:A:166:ALA:O	1:A:167:SER:C	2.62	0.43
1:C:14:VAL:HG21	1:C:138:GLN:NE2	2.34	0.43
1:F:141:ARG:HD2	1:F:142:PHE:CE2	2.54	0.43
1:H:260:THR:O	1:H:264:GLN:HG3	2.19	0.43
1:I:157:ILE:HD11	1:J:117:ARG:NE	2.34	0.43
1:A:141:ARG:HD2	1:A:142:PHE:CE2	2.53	0.42
1:A:167:SER:HB2	1:A:194:ARG:HG3	2.00	0.42
1:D:253:LEU:HD21	1:D:262:ILE:HD12	2.00	0.42
1:E:78:PHE:O	1:E:81:VAL:HG12	2.19	0.42
1:E:119:PHE:CB	1:E:260:THR:HB	2.49	0.42
1:E:209:ILE:HG23	1:E:265:MET:HE1	2.00	0.42
1:E:224:TRP:HE1	1:E:301:ARG:HB3	1.84	0.42
1:F:78:PHE:O	1:F:81:VAL:HG12	2.19	0.42
1:H:72:TRP:CZ3	1:H:74:PRO:HB3	2.54	0.42
1:I:260:THR:N	1:I:263:ASP:HB2	2.34	0.42
1:J:175:TYR:O	1:J:186:ASN:ND2	2.46	0.42
1:A:133:PHE:CE2	1:E:91:ARG:HG2	2.54	0.42
1:B:126:PHE:CE1	2:B:401:Z80:H2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:TRP:CE3	1:D:71:LEU:HD12	2.55	0.42
1:D:95:PHE:HE1	1:D:101:ILE:HD12	1.84	0.42
1:E:27:ASN:HB3	1:E:32:THR:HB	2.01	0.42
1:F:122:ASP:HB2	1:F:199:ARG:HB2	2.01	0.42
1:G:95:PHE:HE1	1:G:101:ILE:HD12	1.85	0.42
1:G:253:LEU:HD21	1:G:262:ILE:HD12	2.01	0.42
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.88	0.42
1:J:273:ILE:O	1:J:277:ILE:HG13	2.19	0.42
1:B:14:VAL:HG21	1:B:138:GLN:NE2	2.34	0.42
1:C:294:ASP:HB3	1:C:297:ILE:HG22	2.01	0.42
1:D:141:ARG:HD2	1:D:142:PHE:CE2	2.54	0.42
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.82	0.42
1:E:160:TRP:CD1	2:E:401:Z80:C5	3.03	0.42
1:F:284:HIS:HB3	1:F:285:HIS:ND1	2.34	0.42
1:G:287:GLN:OE1	1:G:287:GLN:C	2.62	0.42
1:A:285:HIS:HE2	1:E:301:ARG:HH12	1.66	0.42
1:G:14:VAL:HG21	1:G:138:GLN:NE2	2.35	0.42
1:G:93:MET:HB2	1:G:101:ILE:HB	2.01	0.42
1:H:225:LEU:HB2	1:H:231:ARG:HG3	2.01	0.42
1:B:209:ILE:HG23	1:B:265:MET:HE1	2.02	0.42
1:B:212:LEU:HB2	1:B:245:TYR:CE2	2.54	0.42
1:F:151:ASN:HD21	1:F:161:TRP:HA	1.84	0.42
1:F:166:ALA:O	1:F:167:SER:C	2.63	0.42
1:J:16:VAL:HA	1:J:40:VAL:O	2.20	0.42
1:J:78:PHE:O	1:J:81:VAL:HG12	2.18	0.42
1:C:226:GLU:OE2	1:D:284:HIS:NE2	2.50	0.42
1:F:119:PHE:CB	1:F:260:THR:HB	2.50	0.42
1:H:27:ASN:HB3	1:H:32:THR:HB	2.00	0.42
1:H:114:MET:HE2	1:H:116:PHE:HZ	1.85	0.42
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.55	0.42
1:I:119:PHE:HB2	1:I:260:THR:HB	2.02	0.42
1:A:151:ASN:HD21	1:A:161:TRP:HA	1.85	0.42
1:C:157:ILE:HD11	1:D:117:ARG:NE	2.35	0.42
1:D:153:ASP:H	1:D:155:GLU:CD	2.27	0.42
1:F:241:THR:HA	1:G:240:LEU:HD23	2.01	0.42
1:G:167:SER:HB3	1:G:194:ARG:HG3	2.02	0.42
1:H:155:GLU:OE1	2:H:401:Z80:H12	2.19	0.42
1:I:13:ASP:HB3	1:I:141:ARG:HE	1.85	0.42
1:J:155:GLU:HA	1:J:158:ASP:N	2.31	0.42
1:J:179:SER:HB2	1:J:186:ASN:ND2	2.35	0.42
1:J:260:THR:O	1:J:264:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:HE1	1:B:250:SER:OG	2.03	0.42
1:B:208:PHE:O	1:B:245:TYR:OH	2.33	0.42
1:B:225:LEU:HB2	1:B:231:ARG:HG3	2.00	0.42
1:C:179:SER:HB2	1:C:186:ASN:ND2	2.34	0.42
1:E:114:MET:HE2	1:E:116:PHE:HZ	1.83	0.42
1:E:155:GLU:CD	1:E:155:GLU:H	2.14	0.42
1:F:147:VAL:HG13	2:F:401:Z80:CL1	2.57	0.42
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.88	0.42
1:H:238:LEU:HB3	1:H:273:ILE:CD1	2.49	0.42
1:I:72:TRP:CZ3	1:I:74:PRO:HB3	2.55	0.42
1:J:284:HIS:HB3	1:J:285:HIS:ND1	2.34	0.42
1:B:13:ASP:HB3	1:B:141:ARG:HE	1.85	0.42
1:B:224:TRP:HE1	1:B:301:ARG:HB3	1.83	0.42
1:C:287:GLN:HG2	1:C:289:ASN:O	2.20	0.42
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.55	0.42
1:D:27:ASN:HB3	1:D:32:THR:HB	2.01	0.42
1:D:72:TRP:CZ3	1:D:74:PRO:HB3	2.55	0.42
1:D:160:TRP:CD1	2:D:401:Z80:C5	3.02	0.42
1:E:263:ASP:O	1:E:267:ILE:HG12	2.20	0.42
1:F:117:ARG:NE	1:J:157:ILE:HD11	2.34	0.42
1:F:250:SER:OG	1:J:248:TYR:HE1	2.03	0.42
1:F:253:LEU:HD21	1:F:262:ILE:HD12	2.02	0.42
1:H:88:GLY:HA2	1:I:84:SER:HB3	2.01	0.42
1:I:14:VAL:HG21	1:I:138:GLN:NE2	2.35	0.42
1:J:238:LEU:HB3	1:J:273:ILE:CD1	2.48	0.42
1:A:71:LEU:HD11	1:A:94:LEU:HD21	2.01	0.42
1:A:268:ALA:HB1	1:A:308:PHE:CE1	2.55	0.42
1:A:284:HIS:NE2	1:E:226:GLU:OE2	2.53	0.42
1:A:294:ASP:HB3	1:A:297:ILE:CG2	2.49	0.42
1:B:141:ARG:HD2	1:B:142:PHE:CE2	2.55	0.42
1:B:155:GLU:HB2	1:B:161:TRP:CD1	2.55	0.42
1:D:40:VAL:HA	1:D:102:TYR:O	2.20	0.42
1:E:284:HIS:HB3	1:E:285:HIS:ND1	2.34	0.42
1:F:14:VAL:HG21	1:F:138:GLN:NE2	2.35	0.42
1:G:157:ILE:HD11	1:H:117:ARG:NE	2.35	0.42
1:A:133:PHE:HE2	1:E:91:ARG:HG2	1.84	0.41
1:B:78:PHE:O	1:B:81:VAL:HG12	2.19	0.41
1:B:95:PHE:HE1	1:B:101:ILE:HD12	1.84	0.41
1:C:95:PHE:HE1	1:C:101:ILE:HD12	1.84	0.41
1:C:160:TRP:CD1	2:C:401:Z80:C5	3.03	0.41
1:E:225:LEU:HB2	1:E:231:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:SER:HB3	1:J:91:ARG:CD	2.47	0.41
1:F:221:SER:HB2	1:G:281:ILE:CD1	2.50	0.41
1:I:160:TRP:CD1	2:I:401:Z80:C5	3.03	0.41
1:I:232:LEU:O	1:I:235:SER:HB2	2.20	0.41
1:A:178:LEU:HD13	1:A:178:LEU:HA	1.80	0.41
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.85	0.41
1:C:58:VAL:O	1:C:91:ARG:HA	2.20	0.41
1:C:64:GLU:HA	1:C:67:ILE:HD12	2.02	0.41
1:E:119:PHE:HB3	1:E:120:PRO:HD3	2.03	0.41
1:B:155:GLU:HB2	1:B:161:TRP:HD1	1.85	0.41
1:G:126:PHE:CE1	2:G:401:Z80:H2	2.55	0.41
1:I:59:GLU:OE2	1:J:134:SER:OG	2.38	0.41
1:B:114:MET:HE2	1:B:116:PHE:CZ	2.56	0.41
1:B:143:SER:HB2	1:B:170:ILE:HD11	2.02	0.41
1:D:58:VAL:HB	1:D:92:LEU:HB2	2.03	0.41
1:D:151:ASN:ND2	1:D:162:ILE:H	2.19	0.41
1:G:155:GLU:HB3	2:G:401:Z80:C15	2.48	0.41
1:G:178:LEU:HA	1:G:178:LEU:HD13	1.77	0.41
1:H:224:TRP:HE1	1:H:301:ARG:HB3	1.82	0.41
1:H:226:GLU:OE2	1:I:284:HIS:NE2	2.54	0.41
1:A:58:VAL:O	1:A:91:ARG:HA	2.21	0.41
2:B:401:Z80:H16	2:B:401:Z80:H9	1.58	0.41
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.90	0.41
1:E:132:PRO:HD2	1:E:189:SER:O	2.20	0.41
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.55	0.41
1:I:169:HIS:O	1:I:170:ILE:HB	2.20	0.41
1:I:287:GLN:HG2	1:I:289:ASN:O	2.21	0.41
1:I:294:ASP:HB3	1:I:297:ILE:HG22	2.02	0.41
1:A:240:LEU:CD2	1:E:241:THR:HA	2.51	0.41
1:C:13:ASP:HB3	1:C:141:ARG:HE	1.86	0.41
1:C:122:ASP:HB2	1:C:199:ARG:HB2	2.02	0.41
1:C:256:LEU:HD12	1:C:260:THR:HG22	2.02	0.41
1:D:17:SER:HB2	1:D:40:VAL:CG2	2.50	0.41
1:D:167:SER:HB2	1:D:194:ARG:HG3	2.02	0.41
1:G:119:PHE:C	1:G:121:PHE:H	2.28	0.41
1:G:151:ASN:ND2	1:G:162:ILE:H	2.19	0.41
1:B:151:ASN:ND2	1:B:155:GLU:OE1	2.54	0.41
1:C:72:TRP:CZ3	1:C:74:PRO:HB3	2.55	0.41
1:C:155:GLU:CG	1:C:161:TRP:CD1	2.96	0.41
1:C:205:LEU:HA	1:C:209:ILE:HB	2.02	0.41
1:E:56:LEU:HD13	1:E:57:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:TRP:CD1	2:G:401:Z80:C5	3.04	0.41
1:I:173:ILE:O	1:I:187:GLU:HA	2.20	0.41
1:B:153:ASP:O	1:B:155:GLU:HG2	2.20	0.41
1:D:166:ALA:O	1:D:167:SER:C	2.63	0.41
1:F:97:ASP:OD2	1:F:99:ARG:NH1	2.54	0.41
1:I:260:THR:HG23	1:I:263:ASP:OD2	2.21	0.41
1:I:263:ASP:O	1:I:267:ILE:HG12	2.21	0.41
1:A:13:ASP:HB3	1:A:141:ARG:HE	1.85	0.41
1:A:153:ASP:N	1:A:155:GLU:OE2	2.54	0.41
1:A:155:GLU:CD	1:A:155:GLU:H	2.27	0.41
1:A:284:HIS:HB3	1:A:285:HIS:ND1	2.35	0.41
1:D:91:ARG:HD3	1:E:134:SER:HB3	2.02	0.41
1:D:132:PRO:HD2	1:D:189:SER:O	2.21	0.41
1:D:169:HIS:O	1:D:170:ILE:HB	2.20	0.41
1:D:268:ALA:HB1	1:D:308:PHE:CE1	2.56	0.41
1:F:153:ASP:C	1:F:155:GLU:HG2	2.46	0.41
1:F:153:ASP:HB3	1:F:154:ASN:H	1.65	0.41
1:F:167:SER:HB2	1:F:194:ARG:HG3	2.03	0.41
1:G:159:GLU:OE2	1:H:29:LEU:HD21	2.19	0.41
1:H:268:ALA:HB1	1:H:308:PHE:CE1	2.55	0.41
1:J:155:GLU:CG	1:J:161:TRP:HD1	2.29	0.41
1:J:238:LEU:HD13	1:J:238:LEU:HA	1.94	0.41
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.55	0.41
1:F:160:TRP:CD1	2:F:401:Z80:C5	3.04	0.41
1:G:176:ASP:OD1	1:G:176:ASP:N	2.54	0.41
1:H:160:TRP:CD1	2:H:401:Z80:C5	3.04	0.41
1:I:44:THR:HG23	1:I:99:ARG:HB3	2.03	0.41
1:J:178:LEU:HD13	1:J:178:LEU:HA	1.81	0.41
1:C:114:MET:HE2	1:C:116:PHE:HZ	1.87	0.40
1:D:120:PRO:O	1:D:201:PRO:HB3	2.21	0.40
1:D:174:ARG:HH21	1:D:174:ARG:HD3	1.71	0.40
1:F:56:LEU:HD13	1:F:57:ILE:N	2.36	0.40
1:F:66:TRP:HE3	1:F:71:LEU:HD12	1.85	0.40
1:F:248:TYR:HE1	1:G:250:SER:OG	2.03	0.40
1:H:97:ASP:OD2	1:H:99:ARG:NH1	2.54	0.40
1:H:263:ASP:O	1:H:267:ILE:HG12	2.21	0.40
1:E:161:TRP:N	1:E:198:VAL:O	2.34	0.40
1:G:155:GLU:HG3	1:G:161:TRP:NE1	2.36	0.40
1:H:14:VAL:HG21	1:H:138:GLN:NE2	2.35	0.40
1:I:105:ARG:NH2	1:J:81:VAL:O	2.54	0.40
1:I:224:TRP:HE1	1:I:301:ARG:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:CE1	2:A:401:Z80:H18	2.57	0.40
1:E:175:TYR:O	1:E:186:ASN:ND2	2.50	0.40
1:H:92:LEU:HD23	1:H:92:LEU:HA	1.92	0.40
1:H:205:LEU:HA	1:H:209:ILE:HB	2.03	0.40
1:H:240:LEU:HD23	1:H:240:LEU:HA	1.88	0.40
1:I:28:THR:HB	1:I:256:LEU:CD2	2.51	0.40
1:I:28:THR:HA	1:I:116:PHE:CE1	2.57	0.40
1:A:119:PHE:HB3	1:A:120:PRO:HD3	2.03	0.40
1:J:147:VAL:CG1	2:J:401:Z80:H4	2.51	0.40
1:A:162:ILE:HA	1:A:197:ALA:HA	2.03	0.40
1:A:284:HIS:HE1	1:A:291:VAL:HG13	1.83	0.40
1:C:224:TRP:CD1	1:C:224:TRP:N	2.89	0.40
1:D:126:PHE:HE1	1:D:197:ALA:HB3	1.87	0.40
1:E:151:ASN:ND2	1:E:155:GLU:OE2	2.55	0.40
1:F:157:ILE:HD11	1:G:117:ARG:NE	2.37	0.40
1:J:14:VAL:HB	1:J:140:LEU:HD23	2.03	0.40
1:J:154:ASN:C	1:J:156:GLU:N	2.78	0.40

All (1) 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:H:69:ASN:ND2	1:H:288:ALA:O[1_455]	2.19	0.01

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	305/307 (99%)	264 (87%)	39 (13%)	2 (1%)	18	51
1	B	305/307 (99%)	263 (86%)	40 (13%)	2 (1%)	18	51
1	C	305/307 (99%)	265 (87%)	38 (12%)	2 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	305/307 (99%)	265 (87%)	38 (12%)	2 (1%)	18	51
1	E	305/307 (99%)	263 (86%)	40 (13%)	2 (1%)	18	51
1	F	305/307 (99%)	265 (87%)	38 (12%)	2 (1%)	18	51
1	G	305/307 (99%)	266 (87%)	37 (12%)	2 (1%)	18	51
1	H	305/307 (99%)	263 (86%)	40 (13%)	2 (1%)	18	51
1	I	305/307 (99%)	266 (87%)	36 (12%)	3 (1%)	12	45
1	J	305/307 (99%)	265 (87%)	37 (12%)	3 (1%)	12	45
All	All	3050/3070 (99%)	2645 (87%)	383 (13%)	22 (1%)	18	51

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	167	SER
1	J	152	ILE
1	J	155	GLU
1	D	153	ASP
1	E	153	ASP
1	G	170	ILE
1	H	153	ASP
1	I	153	ASP
1	A	153	ASP
1	B	153	ASP
1	C	153	ASP
1	F	153	ASP
1	G	153	ASP
1	D	170	ILE
1	E	170	ILE
1	H	170	ILE
1	I	170	ILE
1	A	170	ILE
1	C	170	ILE
1	F	170	ILE
1	J	170	ILE
1	B	170	ILE

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	274/275 (100%)	274 (100%)	0	100	100
1	B	275/275 (100%)	274 (100%)	1 (0%)	84	80
1	C	275/275 (100%)	274 (100%)	1 (0%)	84	80
1	D	275/275 (100%)	274 (100%)	1 (0%)	84	80
1	E	275/275 (100%)	274 (100%)	1 (0%)	84	80
1	F	275/275 (100%)	274 (100%)	1 (0%)	84	80
1	G	275/275 (100%)	275 (100%)	0	100	100
1	H	275/275 (100%)	274 (100%)	1 (0%)	84	80
1	I	274/275 (100%)	274 (100%)	0	100	100
1	J	275/275 (100%)	274 (100%)	1 (0%)	84	80
All	All	2748/2750 (100%)	2741 (100%)	7 (0%)	86	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	124	GLN
1	C	124	GLN
1	D	124	GLN
1	E	124	GLN
1	F	124	GLN
1	H	124	GLN
1	J	124	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	B	103	ASN
1	B	151	ASN
1	C	62	GLN
1	C	103	ASN
1	C	151	ASN
1	C	177	HIS
1	C	200	ASN

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Mol	Chain	Res	Type
1	D	62	GLN
1	D	151	ASN
1	E	62	GLN
1	E	103	ASN
1	E	151	ASN
1	E	264	GLN
1	F	151	ASN
1	F	177	HIS
1	G	151	ASN
1	G	200	ASN
1	H	62	GLN
1	H	151	ASN
1	H	177	HIS
1	H	287	GLN
1	I	124	GLN
1	I	139	GLN
1	I	177	HIS
1	J	151	ASN
1	J	177	HIS
1	J	182	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	Z80	E	401	-	23,23,23	4.13	5 (21%)	32,32,32	1.73	3 (9%)
2	Z80	F	401	-	23,23,23	4.26	5 (21%)	32,32,32	1.70	5 (15%)
2	Z80	A	401	-	23,23,23	4.17	5 (21%)	32,32,32	1.84	4 (12%)
2	Z80	I	401	-	23,23,23	4.16	5 (21%)	32,32,32	1.68	5 (15%)
2	Z80	J	401	-	23,23,23	4.18	5 (21%)	32,32,32	1.80	3 (9%)
2	Z80	H	401	-	23,23,23	4.20	5 (21%)	32,32,32	1.53	3 (9%)
2	Z80	D	401	-	23,23,23	4.10	5 (21%)	32,32,32	1.49	1 (3%)
2	Z80	C	401	-	23,23,23	4.16	5 (21%)	32,32,32	1.74	4 (12%)
2	Z80	G	401	-	23,23,23	4.22	5 (21%)	32,32,32	1.75	3 (9%)
2	Z80	B	401	-	23,23,23	4.22	5 (21%)	32,32,32	1.82	4 (12%)

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	Z80	E	401	-	-	5/6/18/18	0/3/3/3
2	Z80	F	401	-	-	5/6/18/18	0/3/3/3
2	Z80	A	401	-	-	4/6/18/18	0/3/3/3
2	Z80	I	401	-	-	5/6/18/18	0/3/3/3
2	Z80	J	401	-	-	5/6/18/18	0/3/3/3
2	Z80	H	401	-	-	4/6/18/18	0/3/3/3
2	Z80	D	401	-	-	2/6/18/18	0/3/3/3
2	Z80	C	401	-	-	4/6/18/18	0/3/3/3
2	Z80	G	401	-	-	4/6/18/18	0/3/3/3
2	Z80	B	401	-	-	4/6/18/18	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	Z80	C4-N1	11.46	1.59	1.40
2	F	401	Z80	C4-N1	11.44	1.59	1.40
2	H	401	Z80	C4-N1	11.36	1.59	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	Z80	C4-N1	11.24	1.59	1.40
2	J	401	Z80	C4-N1	11.18	1.59	1.40
2	I	401	Z80	C4-N1	11.11	1.59	1.40
2	C	401	Z80	C4-N1	11.10	1.59	1.40
2	A	401	Z80	C4-N1	11.05	1.59	1.40
2	F	401	Z80	C1-N1	10.89	1.59	1.40
2	D	401	Z80	C4-N1	10.89	1.58	1.40
2	E	401	Z80	C4-N1	10.80	1.58	1.40
2	J	401	Z80	C1-N1	10.77	1.58	1.40
2	B	401	Z80	C1-N1	10.71	1.58	1.40
2	G	401	Z80	C1-N1	10.66	1.58	1.40
2	A	401	Z80	C1-N1	10.61	1.58	1.40
2	H	401	Z80	C1-N1	10.56	1.58	1.40
2	C	401	Z80	C1-N1	10.55	1.58	1.40
2	E	401	Z80	C1-N1	10.53	1.58	1.40
2	I	401	Z80	C1-N1	10.43	1.58	1.40
2	D	401	Z80	C1-N1	10.23	1.57	1.40
2	G	401	Z80	C3-S1	-8.56	1.61	1.76
2	G	401	Z80	C2-S1	-8.40	1.62	1.76
2	I	401	Z80	C3-S1	-8.40	1.62	1.76
2	D	401	Z80	C3-S1	-8.36	1.62	1.76
2	C	401	Z80	C3-S1	-8.36	1.62	1.76
2	E	401	Z80	C2-S1	-8.33	1.62	1.76
2	H	401	Z80	C3-S1	-8.33	1.62	1.76
2	H	401	Z80	C2-S1	-8.33	1.62	1.76
2	E	401	Z80	C3-S1	-8.31	1.62	1.76
2	B	401	Z80	C3-S1	-8.31	1.62	1.76
2	F	401	Z80	C2-S1	-8.31	1.62	1.76
2	F	401	Z80	C3-S1	-8.31	1.62	1.76
2	A	401	Z80	C2-S1	-8.30	1.62	1.76
2	A	401	Z80	C3-S1	-8.26	1.62	1.76
2	I	401	Z80	C2-S1	-8.26	1.62	1.76
2	C	401	Z80	C2-S1	-8.19	1.62	1.76
2	D	401	Z80	C2-S1	-8.18	1.62	1.76
2	J	401	Z80	C3-S1	-8.12	1.62	1.76
2	B	401	Z80	C2-S1	-8.12	1.62	1.76
2	J	401	Z80	C2-S1	-8.00	1.62	1.76
2	J	401	Z80	C17-C1	2.90	1.44	1.39
2	A	401	Z80	C17-C1	2.76	1.43	1.39
2	B	401	Z80	C17-C1	2.75	1.43	1.39
2	I	401	Z80	C17-C1	2.73	1.43	1.39
2	C	401	Z80	C17-C1	2.71	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	Z80	C17-C1	2.70	1.43	1.39
2	E	401	Z80	C17-C1	2.68	1.43	1.39
2	G	401	Z80	C17-C1	2.64	1.43	1.39
2	D	401	Z80	C17-C1	2.57	1.43	1.39
2	H	401	Z80	C17-C1	2.52	1.43	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	Z80	C3-S1-C2	6.38	116.20	100.34
2	G	401	Z80	C3-S1-C2	6.19	115.73	100.34
2	B	401	Z80	C3-S1-C2	6.07	115.44	100.34
2	C	401	Z80	C3-S1-C2	6.00	115.26	100.34
2	J	401	Z80	C3-S1-C2	5.94	115.13	100.34
2	D	401	Z80	C3-S1-C2	5.81	114.79	100.34
2	H	401	Z80	C3-S1-C2	5.75	114.65	100.34
2	I	401	Z80	C3-S1-C2	5.71	114.53	100.34
2	A	401	Z80	C12-N1-C4	-5.69	111.10	119.03
2	E	401	Z80	C3-S1-C2	5.65	114.41	100.34
2	G	401	Z80	C12-N1-C4	-5.41	111.49	119.03
2	E	401	Z80	C12-N1-C4	-5.40	111.50	119.03
2	F	401	Z80	C3-S1-C2	5.35	113.65	100.34
2	C	401	Z80	C12-N1-C4	-5.34	111.58	119.03
2	J	401	Z80	C12-N1-C4	-5.24	111.73	119.03
2	B	401	Z80	C12-N1-C4	-5.09	111.93	119.03
2	I	401	Z80	C12-N1-C4	-4.31	113.02	119.03
2	F	401	Z80	C12-N1-C4	-3.79	113.75	119.03
2	B	401	Z80	C12-N1-C1	-3.21	114.56	119.03
2	F	401	Z80	C14-C13-C12	2.54	121.51	112.91
2	I	401	Z80	C12-N1-C1	-2.53	115.50	119.03
2	E	401	Z80	C8-C9-C10	2.48	121.73	119.24
2	G	401	Z80	C12-N1-C1	-2.46	115.59	119.03
2	A	401	Z80	C8-C9-C10	2.45	121.71	119.24
2	J	401	Z80	C8-C9-C10	2.42	121.68	119.24
2	H	401	Z80	C13-C12-N1	2.40	120.01	112.98
2	I	401	Z80	C13-C14-N2	2.35	119.79	113.71
2	H	401	Z80	C8-C9-C10	2.30	121.56	119.24
2	A	401	Z80	C12-N1-C1	-2.29	115.83	119.03
2	C	401	Z80	C8-C9-C10	2.25	121.51	119.24
2	F	401	Z80	C8-C9-C10	2.25	121.50	119.24
2	B	401	Z80	C14-C13-C12	2.24	120.50	112.91
2	I	401	Z80	C13-C12-N1	2.12	119.20	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	Z80	C1-C2-S1	-2.07	117.08	120.39
2	C	401	Z80	C12-N1-C1	-2.07	116.14	119.03

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	Z80	C13-C12-N1-C4
2	E	401	Z80	C13-C12-N1-C4
2	F	401	Z80	C13-C12-N1-C4
2	G	401	Z80	C13-C12-N1-C4
2	H	401	Z80	C13-C12-N1-C4
2	I	401	Z80	C13-C12-N1-C4
2	J	401	Z80	C13-C12-N1-C4
2	I	401	Z80	C13-C14-N2-C15
2	D	401	Z80	N1-C12-C13-C14
2	A	401	Z80	C13-C12-N1-C4
2	C	401	Z80	C13-C12-N1-C4
2	A	401	Z80	C13-C14-N2-C16
2	C	401	Z80	C13-C14-N2-C16
2	F	401	Z80	C13-C14-N2-C16
2	I	401	Z80	C13-C14-N2-C16
2	J	401	Z80	C13-C14-N2-C16
2	E	401	Z80	C12-C13-C14-N2
2	J	401	Z80	C12-C13-C14-N2
2	B	401	Z80	C12-C13-C14-N2
2	C	401	Z80	N1-C12-C13-C14
2	G	401	Z80	C12-C13-C14-N2
2	H	401	Z80	C12-C13-C14-N2
2	B	401	Z80	C13-C14-N2-C16
2	D	401	Z80	C13-C14-N2-C16
2	H	401	Z80	C13-C14-N2-C16
2	J	401	Z80	N1-C12-C13-C14
2	A	401	Z80	N1-C12-C13-C14
2	G	401	Z80	C13-C14-N2-C16
2	E	401	Z80	C13-C14-N2-C16
2	A	401	Z80	C13-C14-N2-C15
2	F	401	Z80	C13-C14-N2-C15
2	C	401	Z80	C13-C14-N2-C15
2	F	401	Z80	C13-C12-N1-C1
2	I	401	Z80	C13-C12-N1-C1
2	G	401	Z80	C13-C12-N1-C1

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Mol	Chain	Res	Type	Atoms
2	J	401	Z80	C13-C12-N1-C1
2	E	401	Z80	N1-C12-C13-C14
2	I	401	Z80	N1-C12-C13-C14
2	F	401	Z80	C12-C13-C14-N2
2	E	401	Z80	C13-C12-N1-C1
2	B	401	Z80	C13-C12-N1-C1
2	H	401	Z80	C13-C12-N1-C1

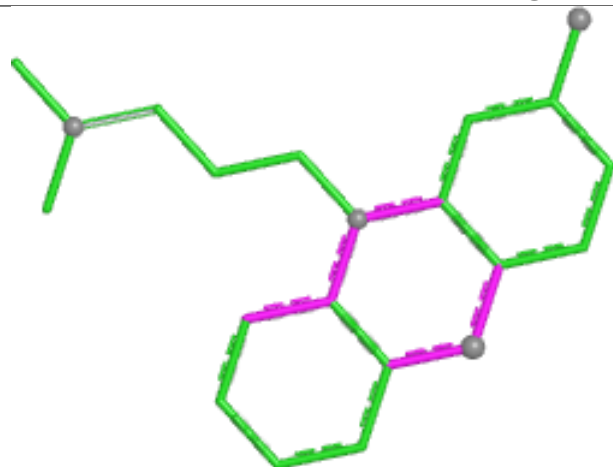
There are no ring outliers.

10 monomers are involved in 62 short contacts:

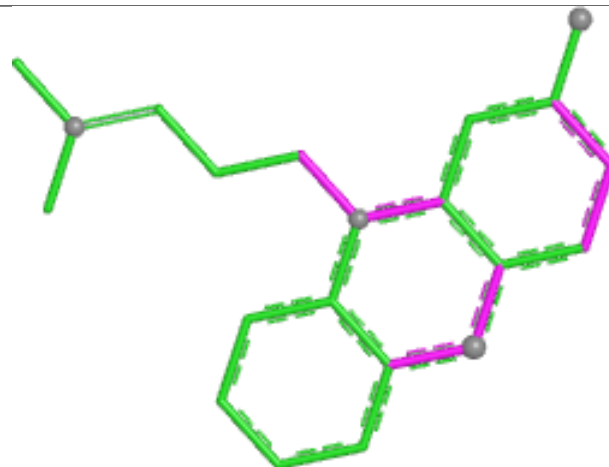
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	Z80	7	0
2	F	401	Z80	8	0
2	A	401	Z80	7	0
2	I	401	Z80	3	0
2	J	401	Z80	7	0
2	H	401	Z80	6	0
2	D	401	Z80	4	0
2	C	401	Z80	5	0
2	G	401	Z80	9	0
2	B	401	Z80	6	0

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.

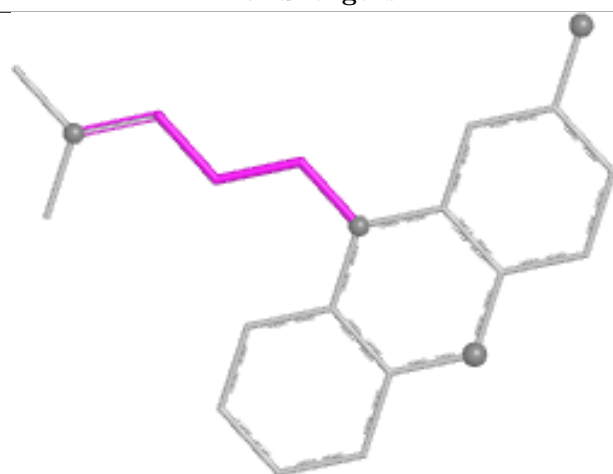
Ligand Z80 E 401



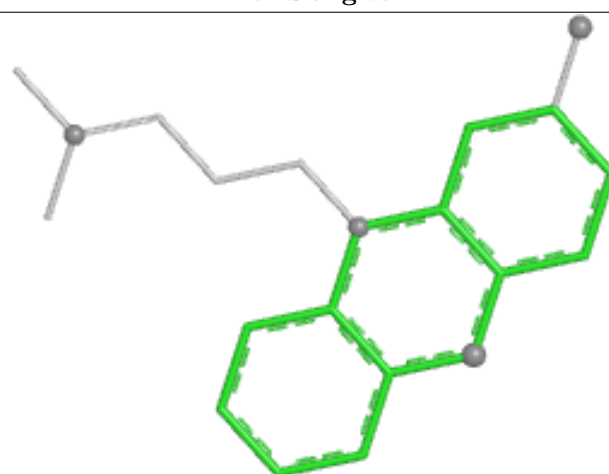
Bond lengths



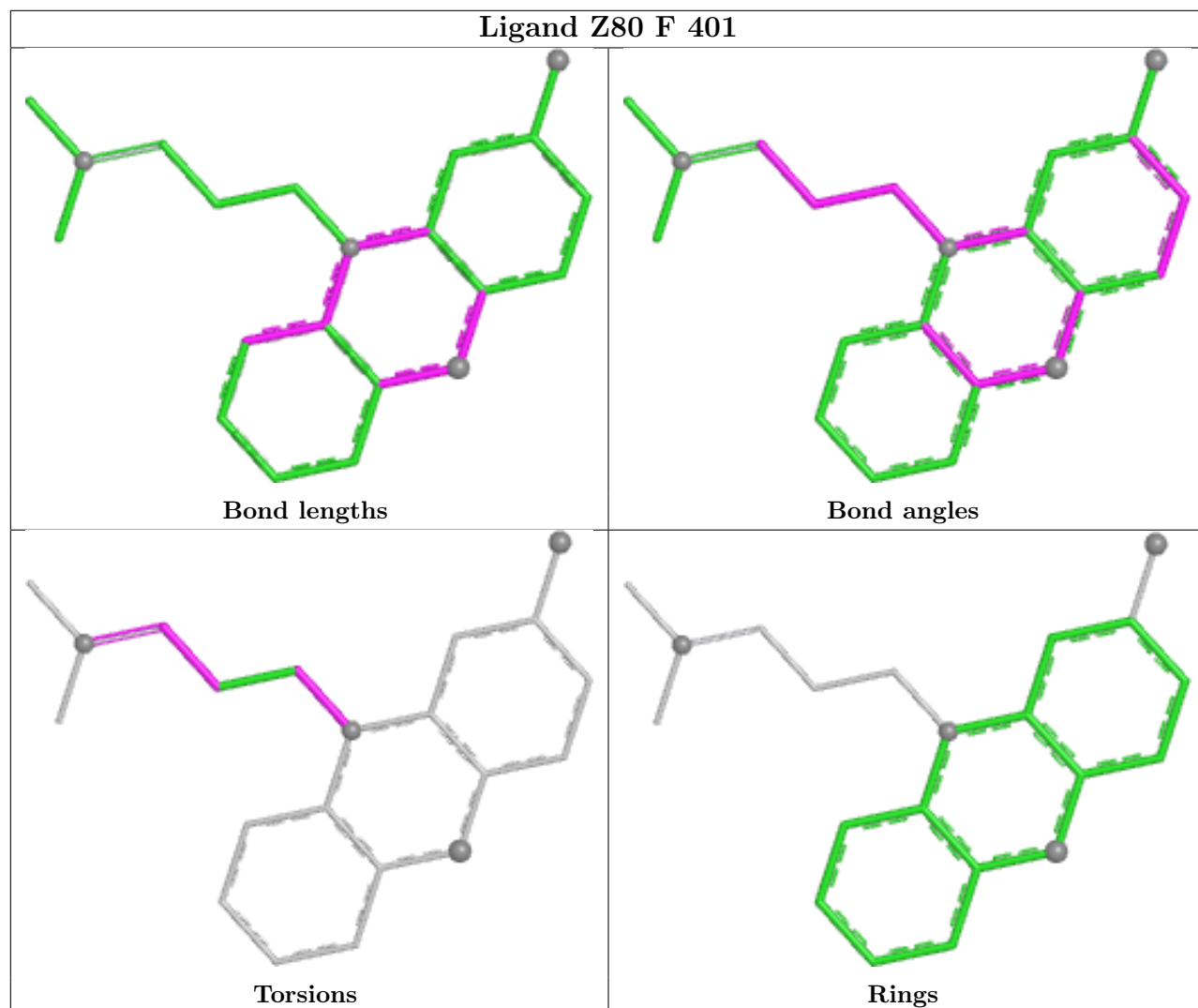
Bond angles



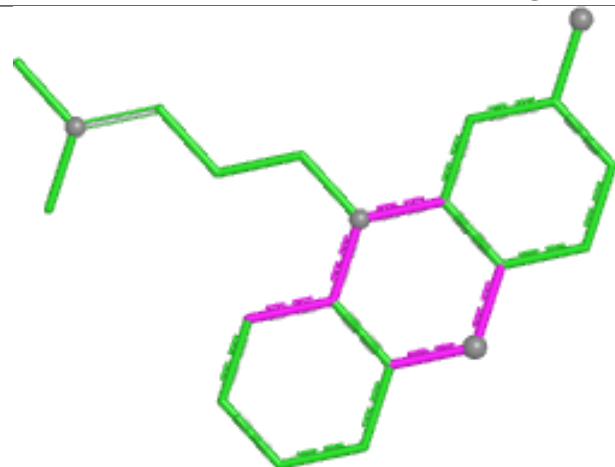
Torsions



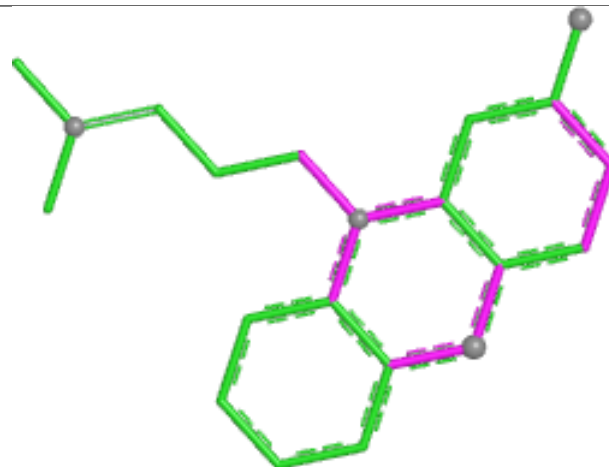
Rings



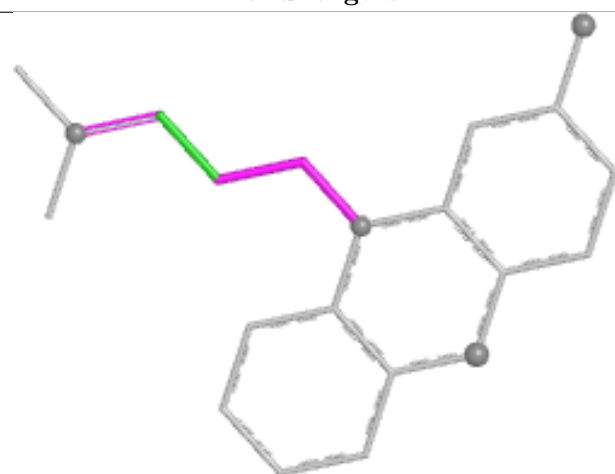
Ligand Z80 A 401



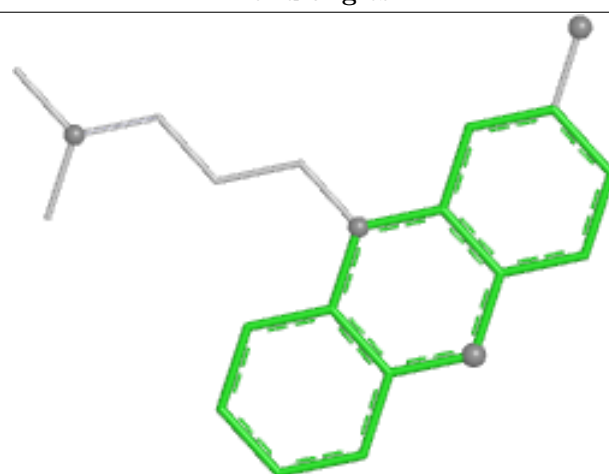
Bond lengths



Bond angles

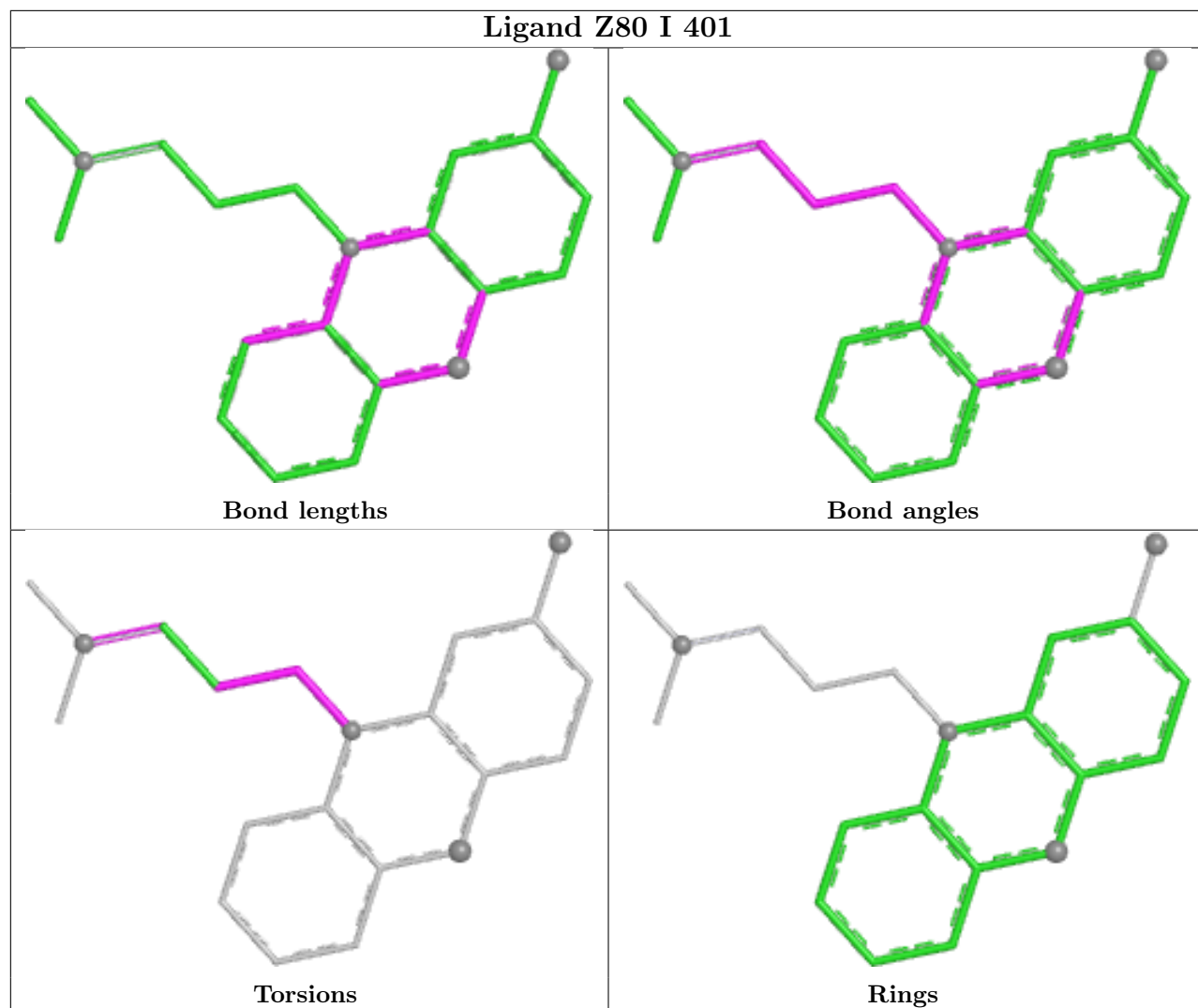


Torsions

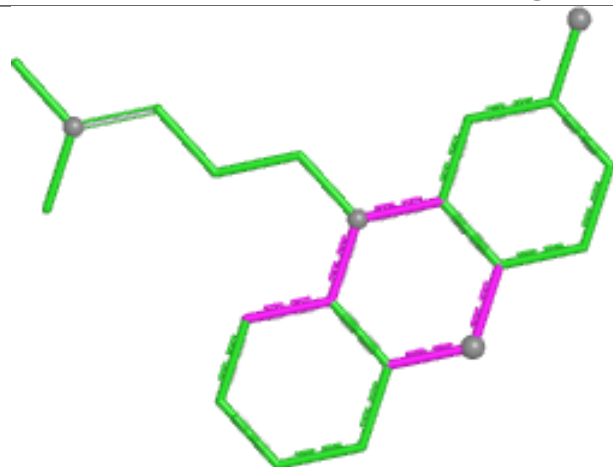


Rings

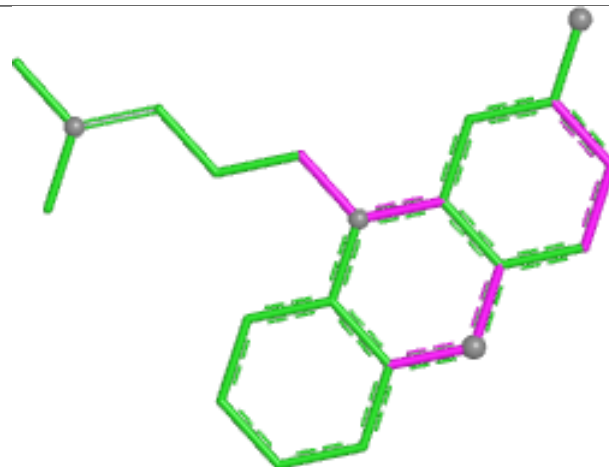
Ligand Z80 I 401



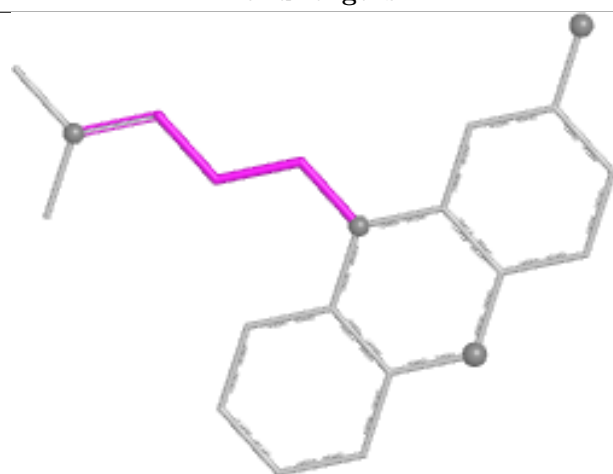
Ligand Z80 J 401



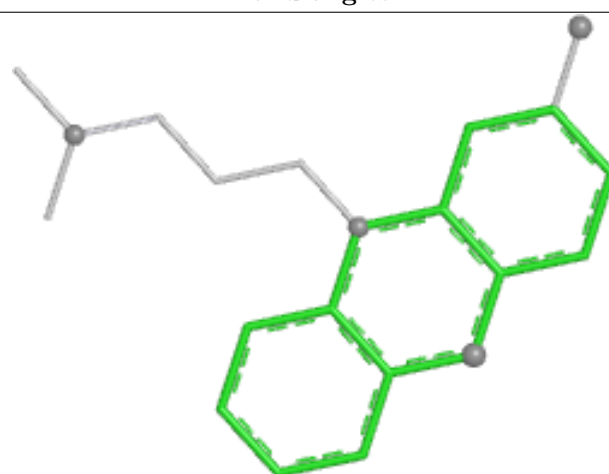
Bond lengths



Bond angles

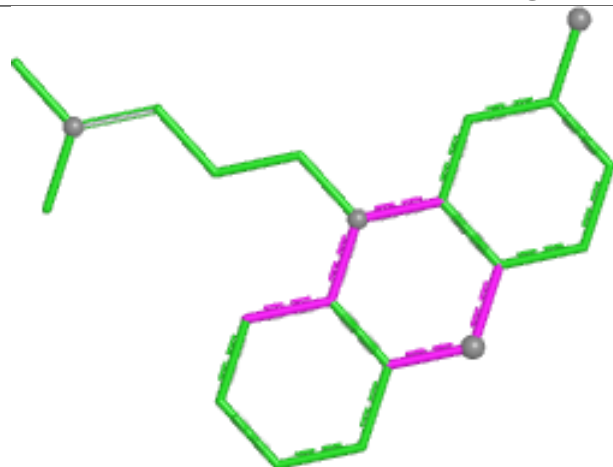


Torsions

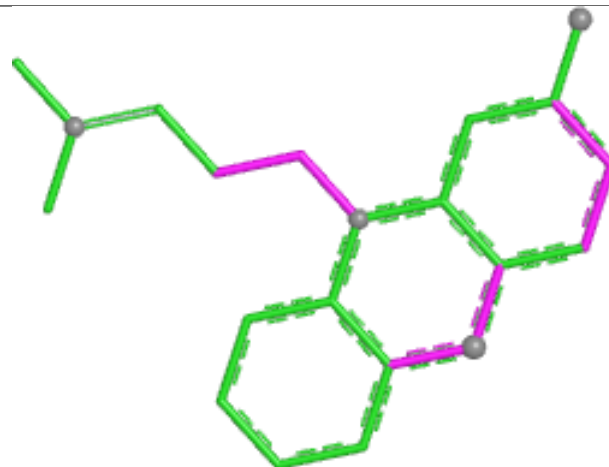


Rings

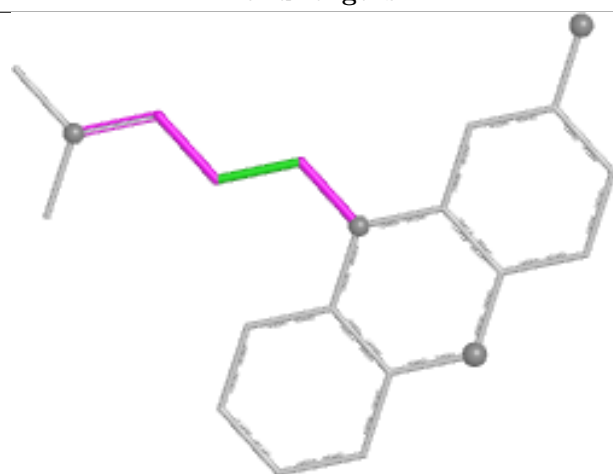
Ligand Z80 H 401



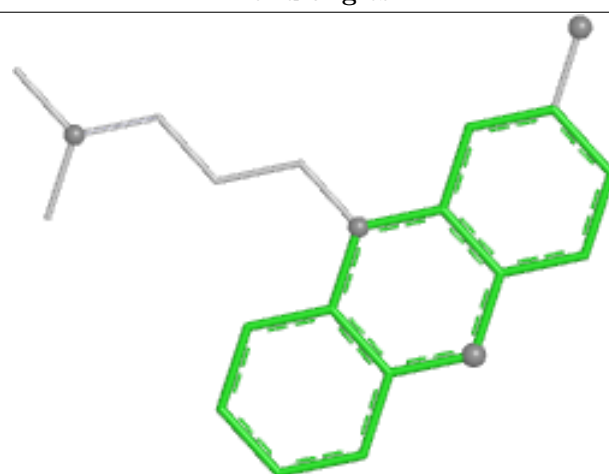
Bond lengths



Bond angles

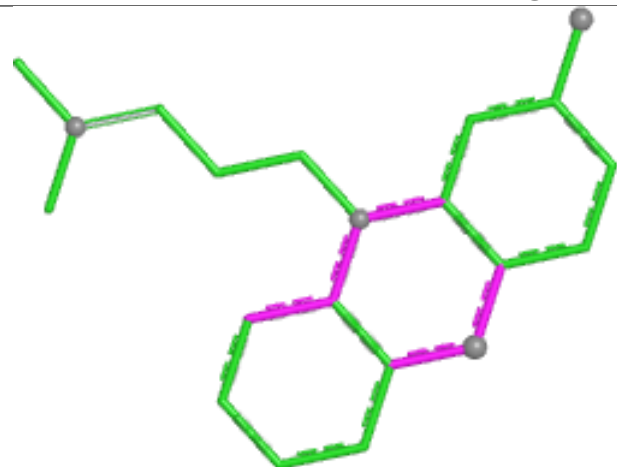


Torsions

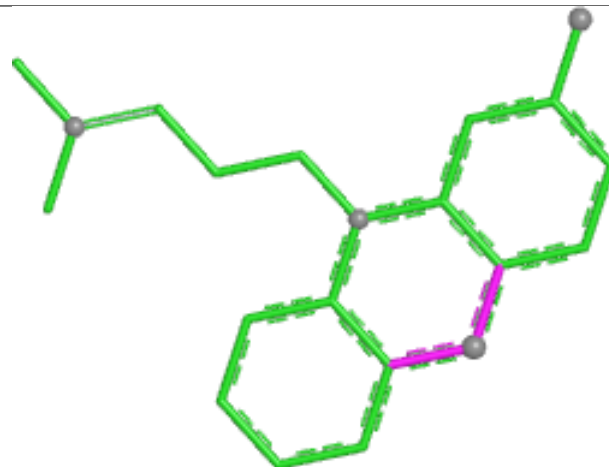


Rings

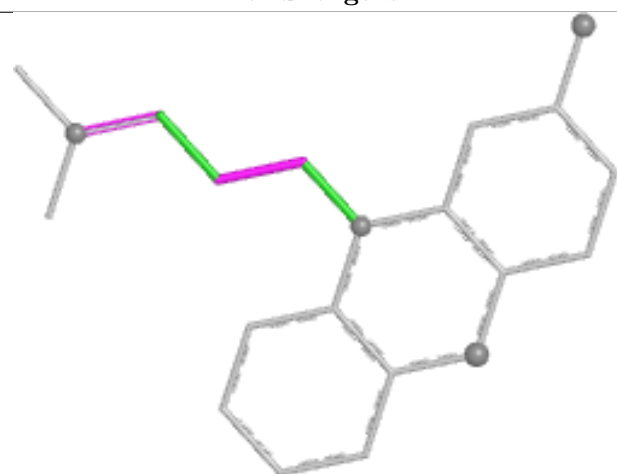
Ligand Z80 D 401



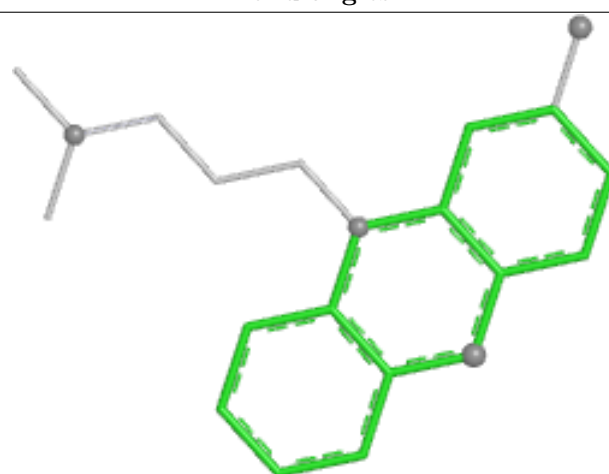
Bond lengths



Bond angles

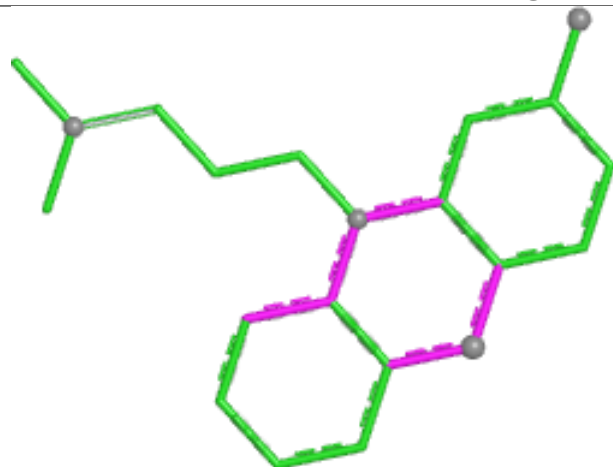


Torsions

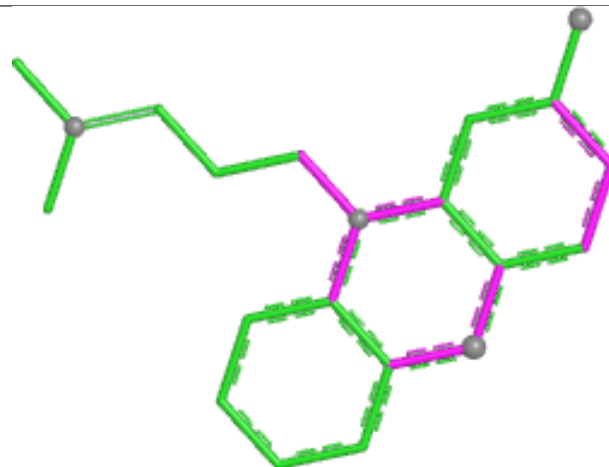


Rings

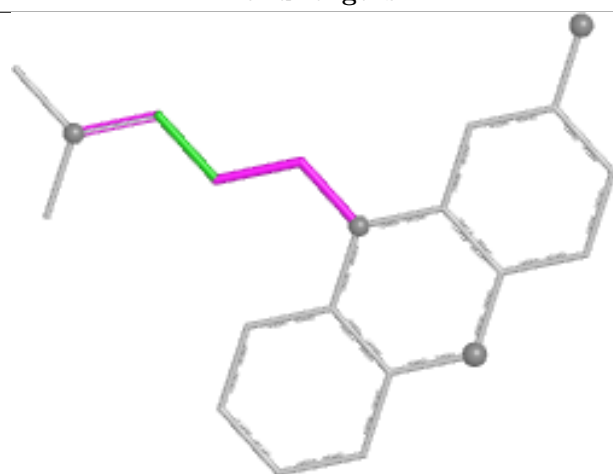
Ligand Z80 C 401



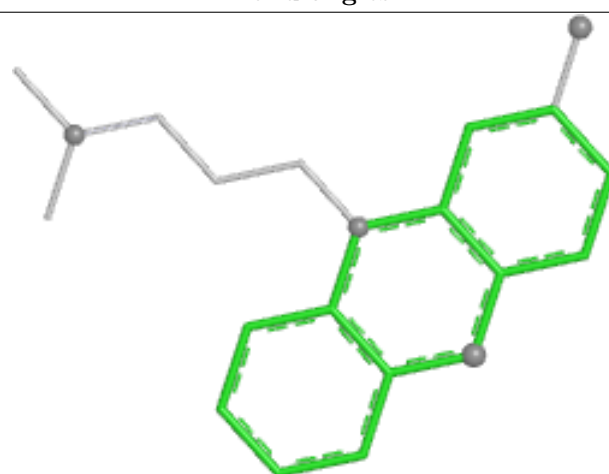
Bond lengths



Bond angles

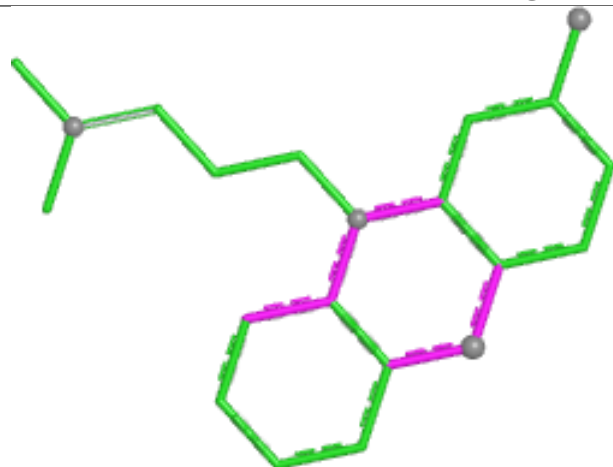


Torsions

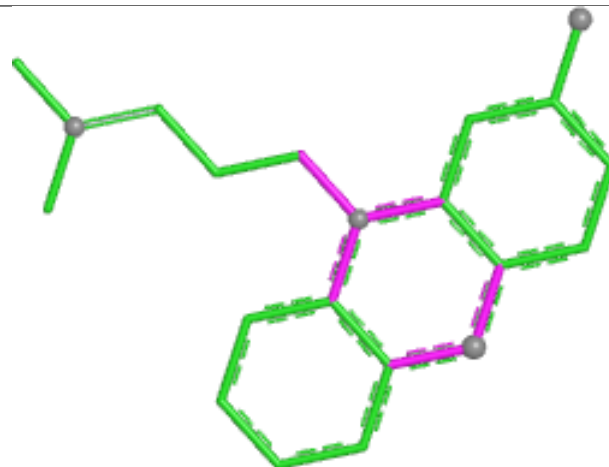


Rings

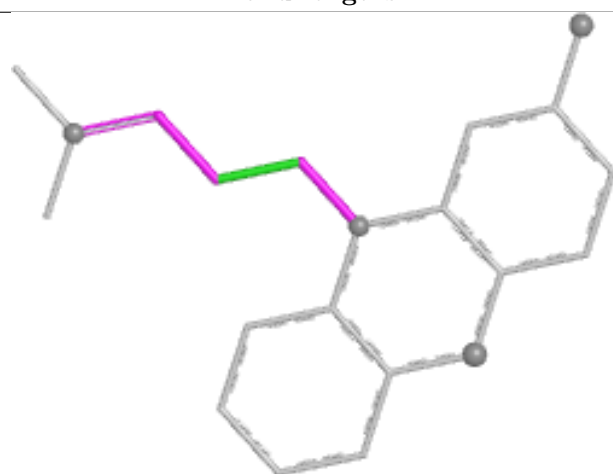
Ligand Z80 G 401



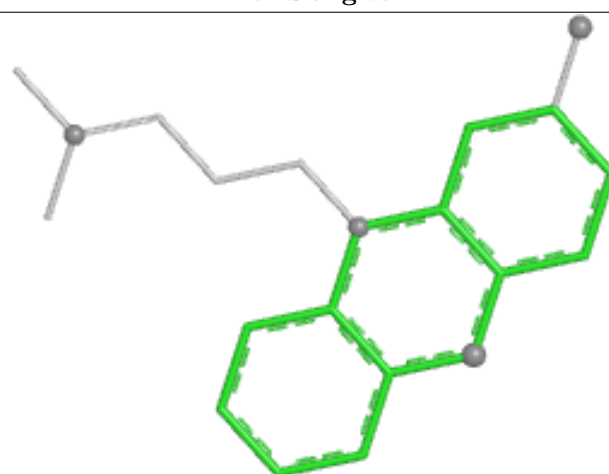
Bond lengths



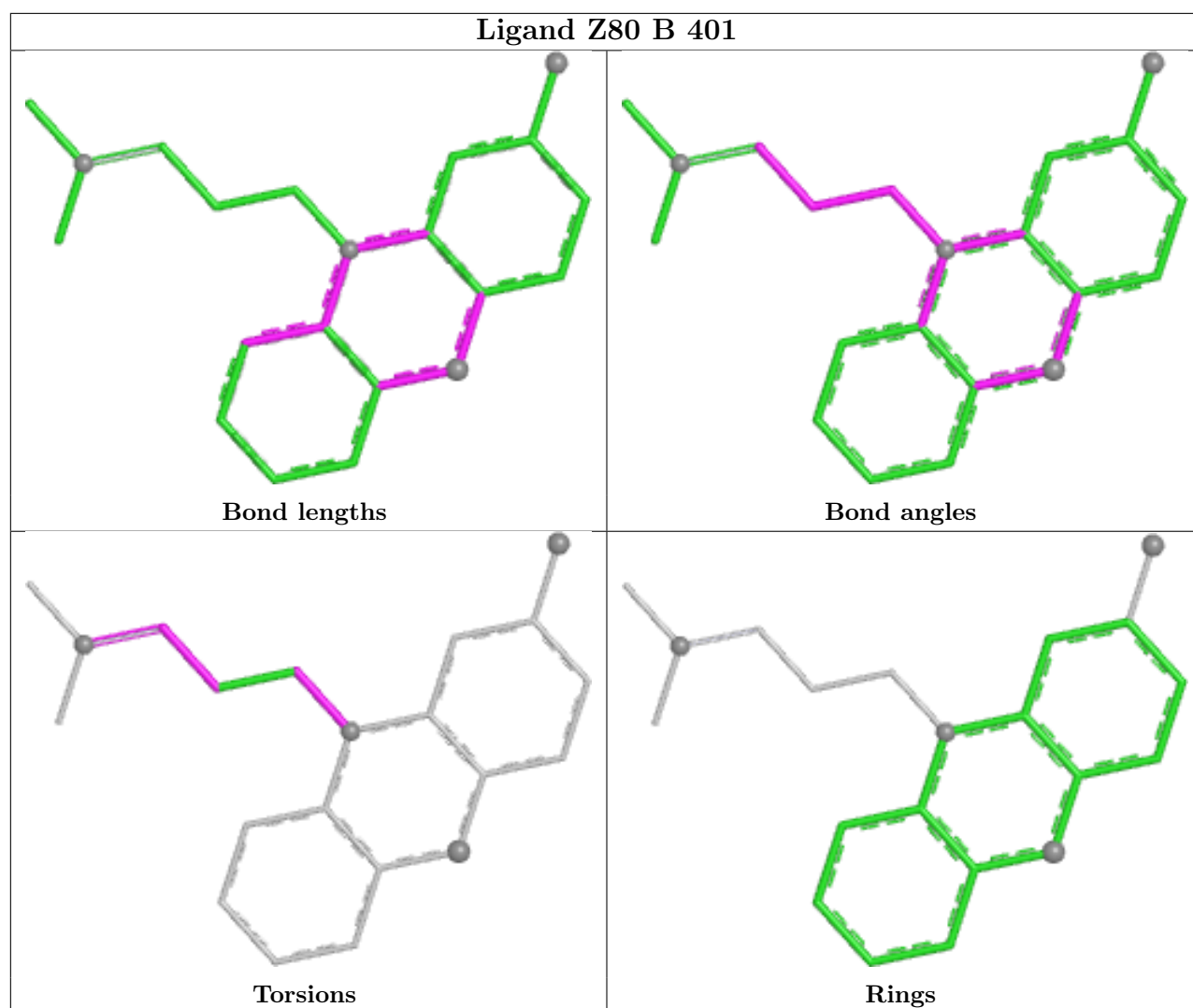
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	307/307 (100%)	0.15	11 (3%)	46	25	49, 88, 191, 243	0
1	B	307/307 (100%)	0.43	31 (10%)	12	8	48, 87, 193, 241	0
1	C	307/307 (100%)	0.38	22 (7%)	21	13	46, 86, 192, 243	0
1	D	307/307 (100%)	0.30	23 (7%)	20	13	44, 86, 192, 241	0
1	E	307/307 (100%)	0.32	19 (6%)	26	15	48, 86, 192, 242	0
1	F	307/307 (100%)	0.11	10 (3%)	49	27	52, 89, 191, 242	0
1	G	307/307 (100%)	0.33	18 (5%)	28	16	49, 87, 192, 241	0
1	H	307/307 (100%)	0.15	15 (4%)	35	19	49, 88, 194, 257	0
1	I	307/307 (100%)	0.29	19 (6%)	26	15	45, 88, 191, 242	0
1	J	307/307 (100%)	0.37	22 (7%)	21	13	48, 89, 196, 242	0
All	All	3070/3070 (100%)	0.28	190 (6%)	26	15	44, 87, 194, 257	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	VAL	7.0
1	H	291	VAL	6.5
1	C	316	VAL	6.0
1	E	290	GLY	6.0
1	I	164	GLY	5.8
1	C	312	GLY	5.4
1	E	166	ALA	5.1
1	D	226	GLU	5.0
1	B	166	ALA	4.9
1	C	317	ILE	4.6
1	C	313	CYS	4.6
1	B	148	TYR	4.5
1	I	169	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	230	GLU	4.2
1	J	178	LEU	4.2
1	C	302	LEU	4.1
1	E	289	ASN	4.1
1	H	289	ASN	4.0
1	J	181	VAL	4.0
1	A	164	GLY	4.0
1	G	255	ARG	4.0
1	B	164	GLY	3.9
1	D	164	GLY	3.9
1	G	166	ALA	3.9
1	D	176	ASP	3.9
1	D	148	TYR	3.9
1	J	305	PRO	3.8
1	J	102	TYR	3.8
1	I	148	TYR	3.7
1	E	178	LEU	3.7
1	I	291	VAL	3.6
1	A	11	PRO	3.6
1	B	302	LEU	3.6
1	B	125	GLN	3.6
1	D	169	HIS	3.6
1	A	177	HIS	3.5
1	H	166	ALA	3.4
1	J	148	TYR	3.4
1	D	163	ARG	3.4
1	J	104	ALA	3.3
1	F	166	ALA	3.3
1	E	164	GLY	3.3
1	F	164	GLY	3.3
1	B	33	TYR	3.3
1	D	166	ALA	3.3
1	G	169	HIS	3.2
1	G	164	GLY	3.2
1	J	164	GLY	3.2
1	E	288	ALA	3.2
1	I	181	VAL	3.2
1	B	194	ARG	3.1
1	C	306	LEU	3.1
1	B	181	VAL	3.0
1	C	164	GLY	3.0
1	A	291	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	291	VAL	3.0
1	B	126	PHE	3.0
1	J	80	ASN	3.0
1	J	129	GLU	3.0
1	B	145	ILE	3.0
1	H	312	GLY	3.0
1	F	178	LEU	2.9
1	D	179	SER	2.9
1	G	157	ILE	2.9
1	G	178	LEU	2.9
1	G	167	SER	2.9
1	A	288	ALA	2.9
1	C	121	PHE	2.9
1	H	147	VAL	2.8
1	G	11	PRO	2.8
1	D	178	LEU	2.8
1	H	164	GLY	2.8
1	I	229	SER	2.8
1	C	68	ASN	2.8
1	J	180	SER	2.7
1	F	305	PRO	2.7
1	I	49	LYS	2.7
1	B	136	ASN	2.7
1	F	147	VAL	2.7
1	B	288	ALA	2.7
1	I	252	ILE	2.7
1	B	291	VAL	2.7
1	C	139	GLN	2.7
1	H	152	ILE	2.7
1	J	39	ILE	2.7
1	A	175	TYR	2.7
1	A	183	PRO	2.6
1	G	315	LEU	2.6
1	C	315	LEU	2.6
1	H	178	LEU	2.6
1	J	307	GLY	2.6
1	G	196	ASP	2.6
1	C	138	GLN	2.6
1	H	288	ALA	2.6
1	B	149	THR	2.6
1	I	165	LYS	2.6
1	B	178	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	165	LYS	2.5
1	F	11	PRO	2.5
1	G	177	HIS	2.5
1	J	157	ILE	2.5
1	E	165	LYS	2.5
1	C	314	VAL	2.5
1	D	175	TYR	2.5
1	B	146	GLN	2.5
1	J	183	PRO	2.5
1	B	25	GLY	2.5
1	J	315	LEU	2.5
1	A	297	ILE	2.4
1	A	178	LEU	2.4
1	E	302	LEU	2.4
1	E	167	SER	2.4
1	D	152	ILE	2.4
1	B	127	VAL	2.4
1	B	165	LYS	2.4
1	E	149	THR	2.4
1	F	206	TRP	2.3
1	B	206	TRP	2.3
1	D	181	VAL	2.3
1	D	227	SER	2.3
1	J	11	PRO	2.3
1	I	147	VAL	2.3
1	I	180	SER	2.3
1	D	69	ASN	2.3
1	G	149	THR	2.3
1	I	68	ASN	2.3
1	B	183	PRO	2.3
1	D	230	GLU	2.2
1	D	147	VAL	2.2
1	E	194	ARG	2.2
1	I	69	ASN	2.2
1	B	152	ILE	2.2
1	J	79	ILE	2.2
1	D	182	GLN	2.2
1	H	148	TYR	2.2
1	I	70	GLY	2.2
1	B	196	ASP	2.2
1	B	289	ASN	2.2
1	B	144	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	293	ASP	2.2
1	F	165	LYS	2.2
1	D	206	TRP	2.2
1	F	141	ARG	2.2
1	C	145	ILE	2.2
1	B	295	LEU	2.2
1	E	11	PRO	2.2
1	D	301	ARG	2.1
1	C	255	ARG	2.1
1	E	287	GLN	2.1
1	C	148	TYR	2.1
1	G	150	GLU	2.1
1	J	306	LEU	2.1
1	B	112	ASN	2.1
1	B	195	ILE	2.1
1	E	317	ILE	2.1
1	H	62	GLN	2.1
1	B	169	HIS	2.1
1	C	165	LYS	2.1
1	I	163	ARG	2.1
1	C	158	ASP	2.1
1	H	158	ASP	2.1
1	I	178	LEU	2.1
1	C	11	PRO	2.1
1	H	292	GLU	2.1
1	I	233	GLN	2.1
1	B	58	VAL	2.1
1	H	296	LEU	2.1
1	D	70	GLY	2.1
1	A	220	TRP	2.1
1	D	305	PRO	2.1
1	G	72	TRP	2.1
1	J	206	TRP	2.1
1	E	177	HIS	2.0
1	H	165	LYS	2.0
1	J	165	LYS	2.0
1	C	166	ALA	2.0
1	E	295	LEU	2.0
1	A	169	HIS	2.0
1	D	145	ILE	2.0
1	I	152	ILE	2.0
1	G	156	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	288	ALA	2.0
1	G	298	GLN	2.0
1	E	150	GLU	2.0
1	E	206	TRP	2.0
1	F	205	LEU	2.0
1	G	155	GLU	2.0
1	C	41	ALA	2.0
1	C	144	ASP	2.0
1	J	147	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

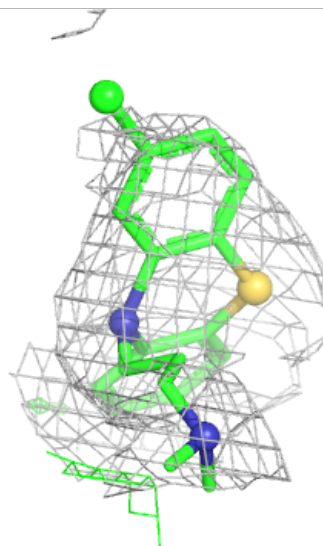
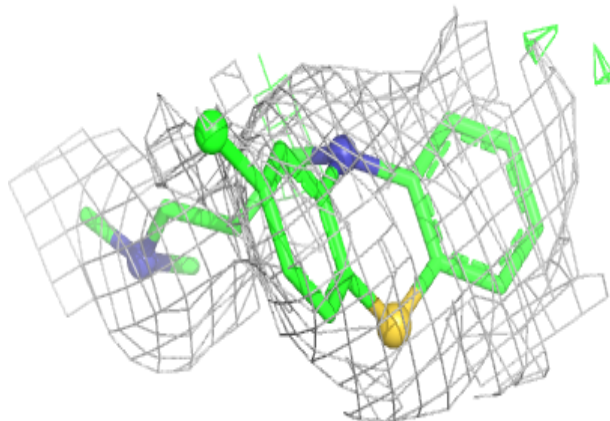
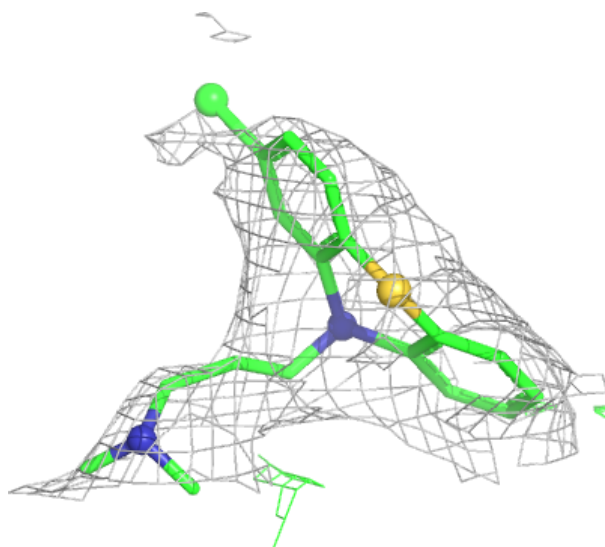
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Z80	E	401	21/21	0.88	0.14	53,83,143,202	0
2	Z80	B	401	21/21	0.90	0.29	53,125,138,159	21
2	Z80	D	401	21/21	0.92	0.18	50,84,133,254	21
2	Z80	C	401	21/21	0.92	0.12	64,107,145,306	0
2	Z80	F	401	21/21	0.92	0.13	23,94,128,261	0
2	Z80	H	401	21/21	0.92	0.14	61,95,146,229	0
2	Z80	I	401	21/21	0.92	0.18	50,103,145,284	21
2	Z80	J	401	21/21	0.92	0.12	29,73,109,228	21
2	Z80	G	401	21/21	0.93	0.23	15,111,180,217	21
2	Z80	A	401	21/21	0.94	0.11	56,101,149,209	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.

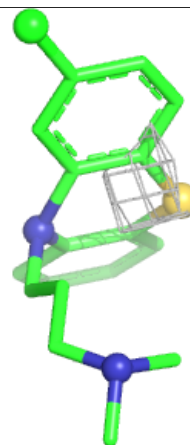
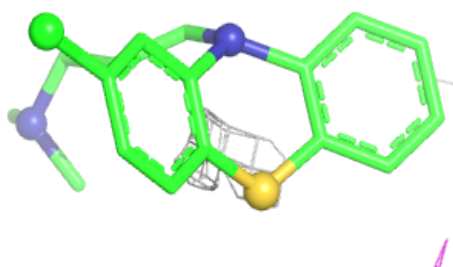
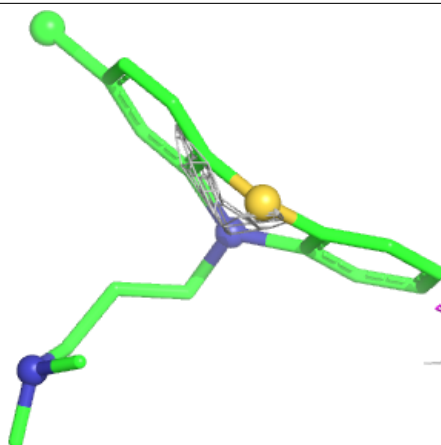
Electron density around Z80 E 401:

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



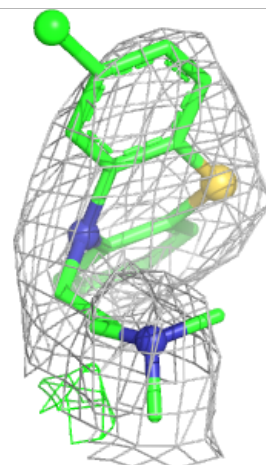
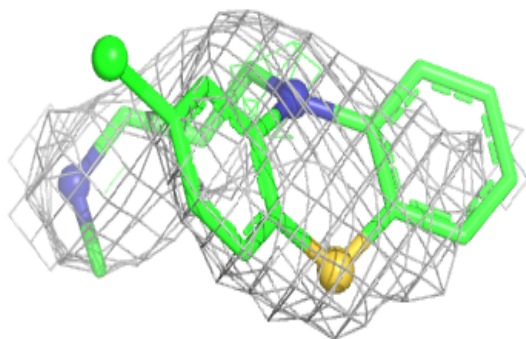
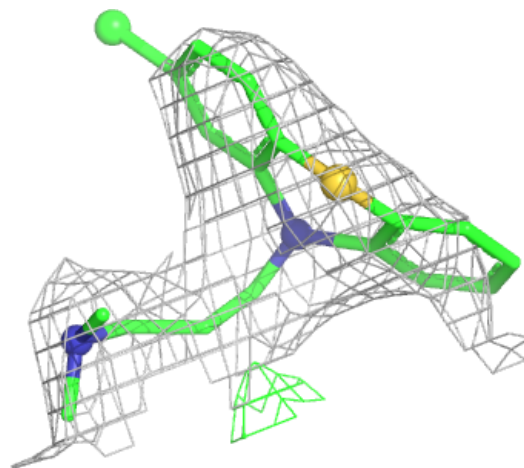
Electron density around Z80 B 401:

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



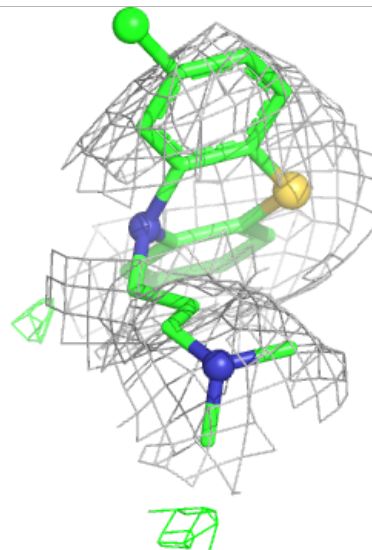
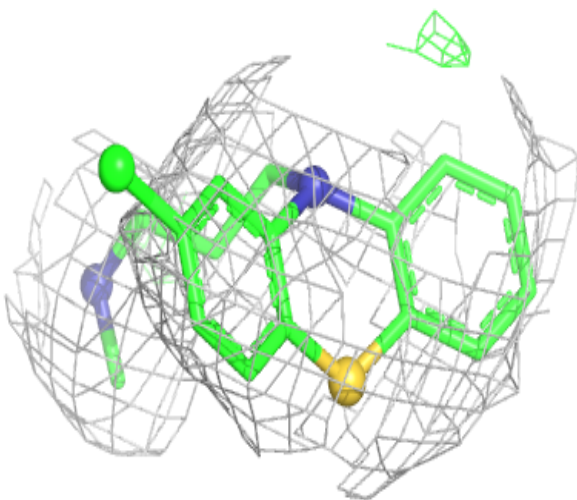
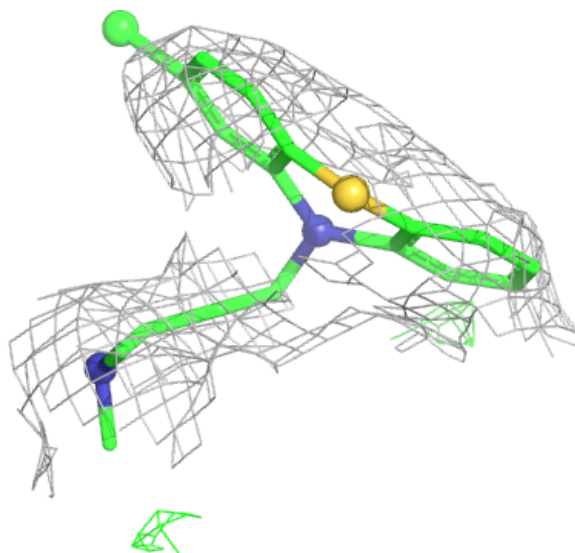
Electron density around Z80 D 401:

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



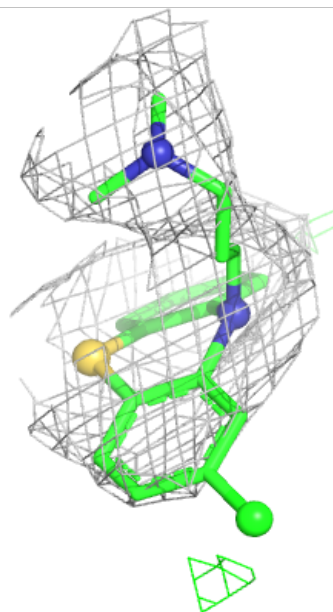
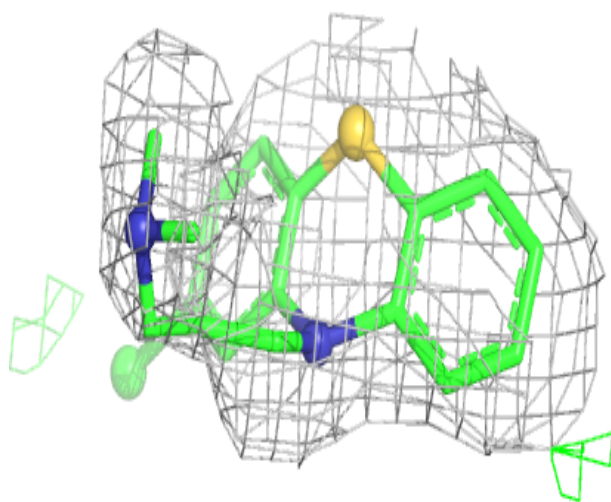
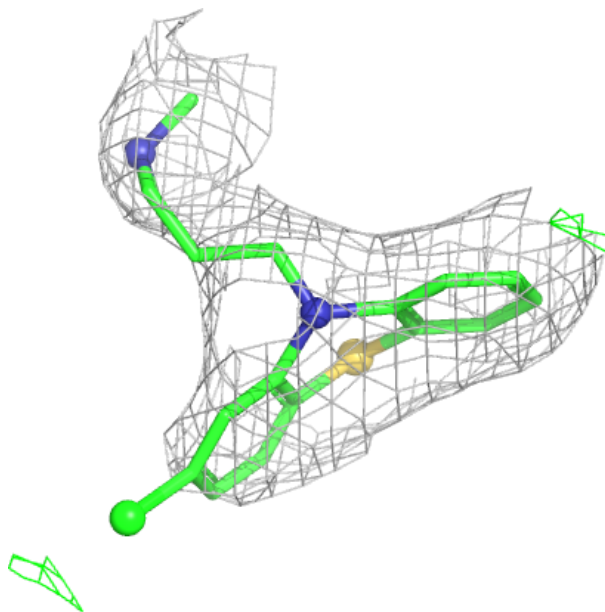
Electron density around Z80 C 401:

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



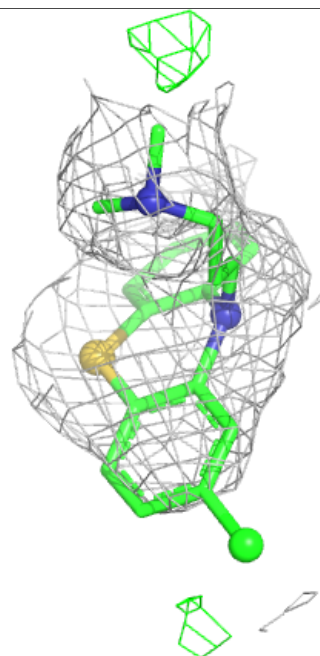
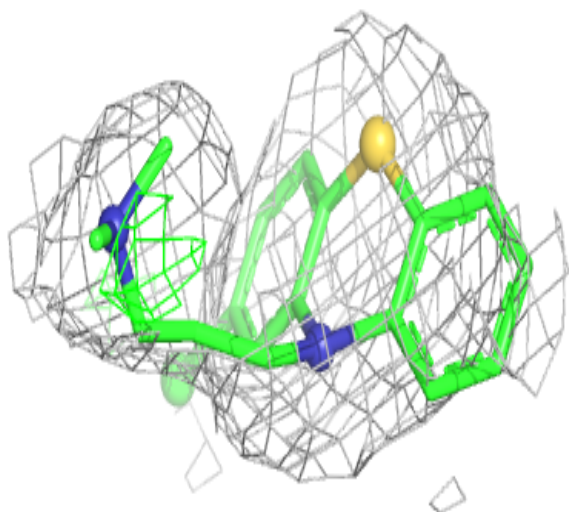
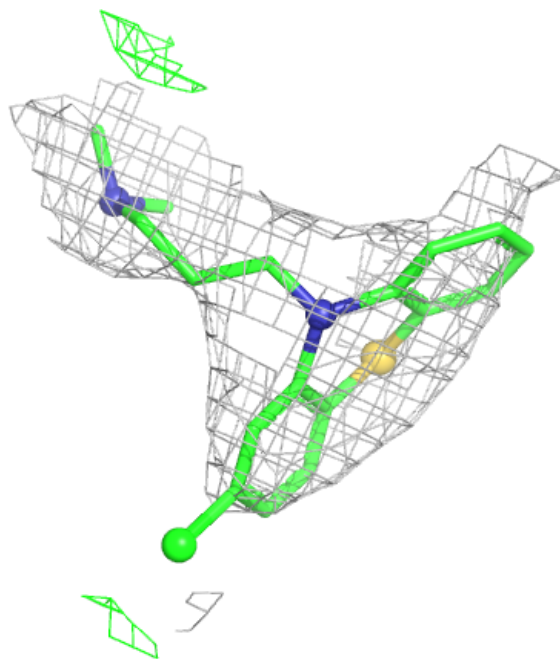
Electron density around Z80 F 401:

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



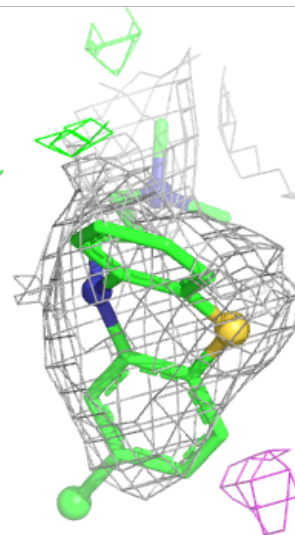
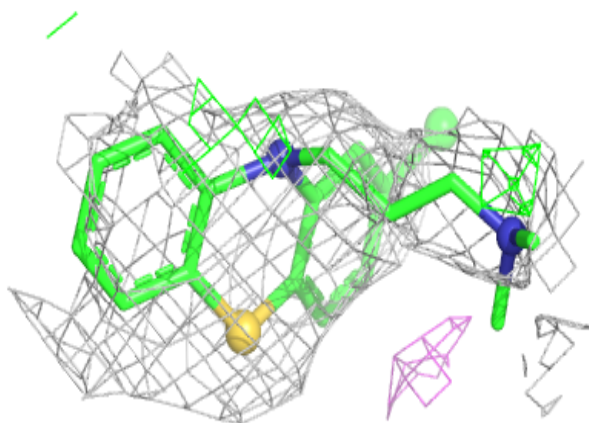
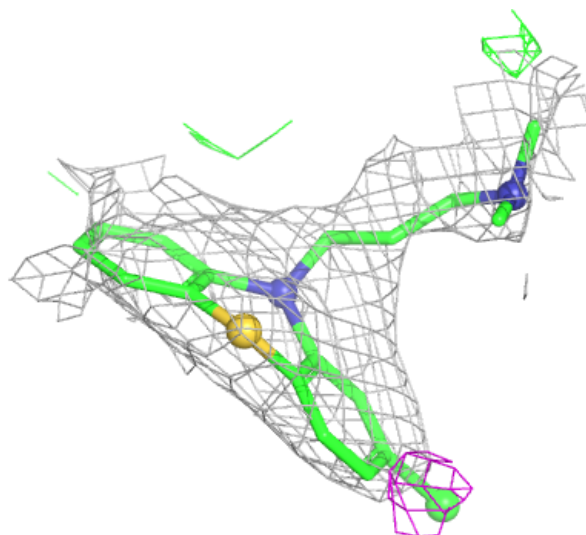
Electron density around Z80 H 401:

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



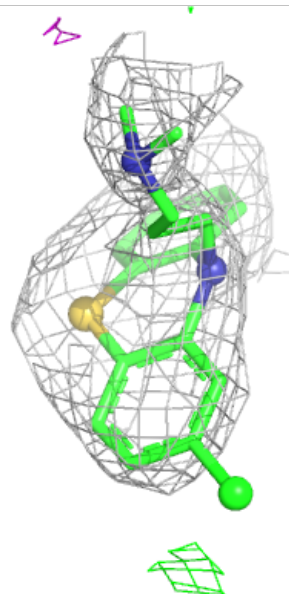
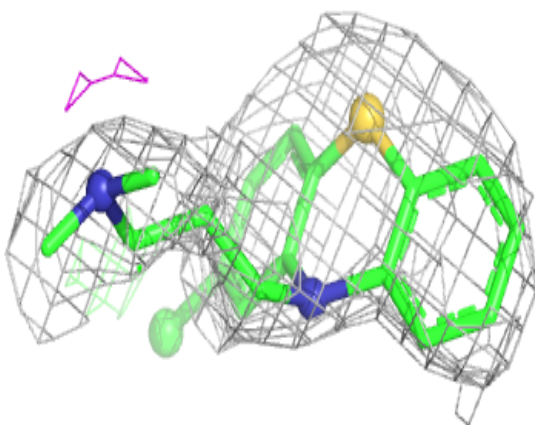
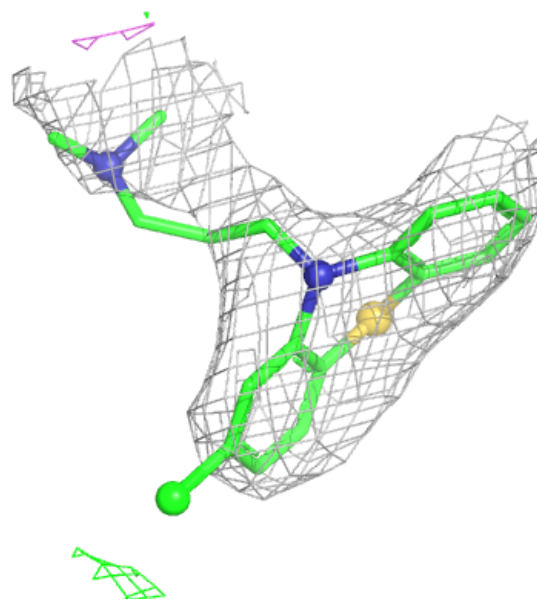
Electron density around Z80 I 401:

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



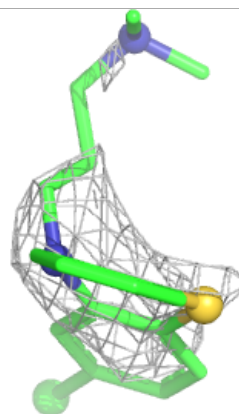
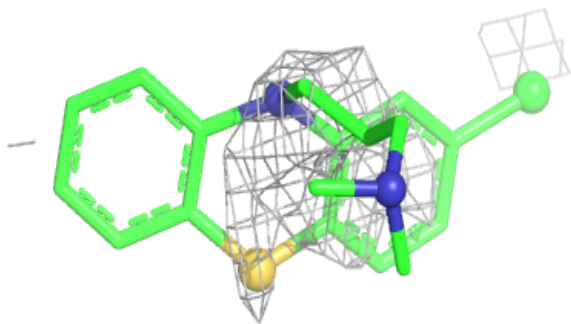
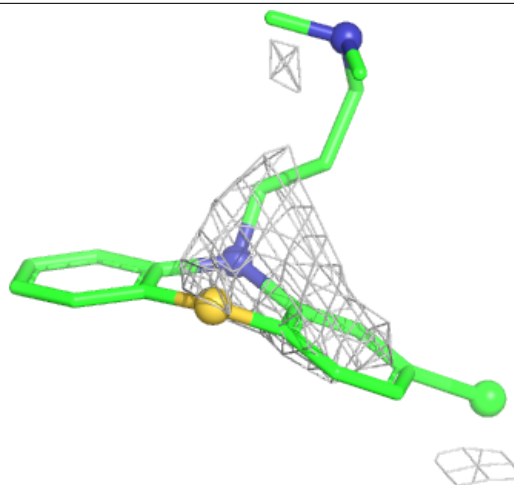
Electron density around Z80 J 401:

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



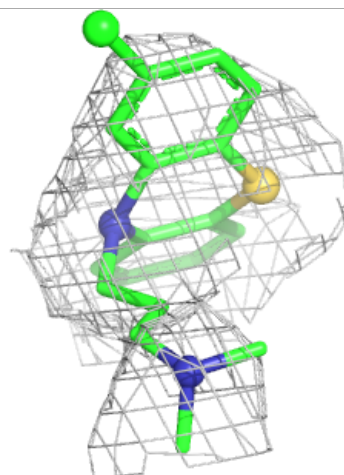
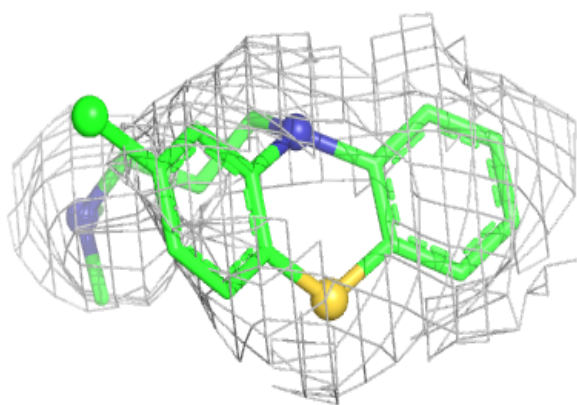
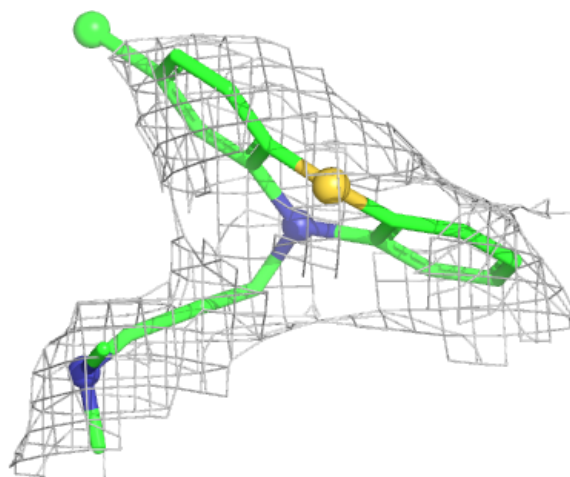
Electron density around Z80 G 401:

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



Electron density around Z80 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.