



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 AM UTC

PDB ID : 4A97 / pdb_00004a97
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with zopiclone
Authors : Spurny, R.; Brams, M.; Ulens, C.
Deposited on : 2011-11-24
Resolution : 3.34 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

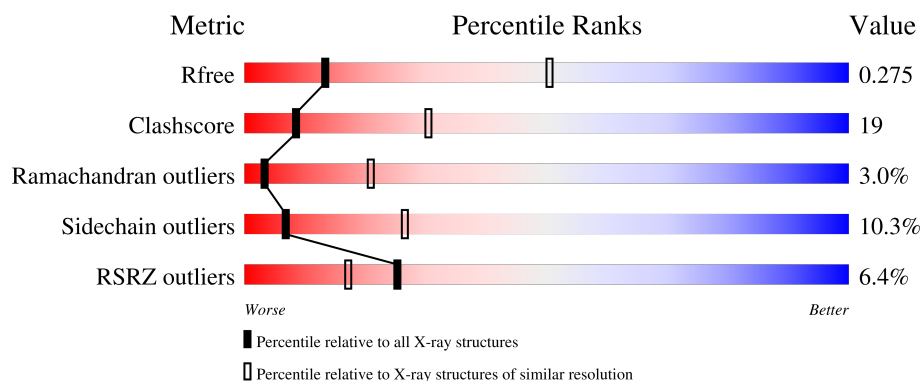
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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% 57% 35% 7%
1	B	307	7% 52% 36% 10%
1	C	307	7% 54% 37% 7%
1	D	307	3% 53% 37% 9%
1	E	307	6% 55% 38% 6%

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Mol	Chain	Length	Quality of chain
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	

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	ZPC	A	1318	-	-	X	-
2	ZPC	D	1318	-	-	X	-
2	ZPC	F	1318	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25290 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	A	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			

There are 20 discrepancies between the modelled and reference sequences:

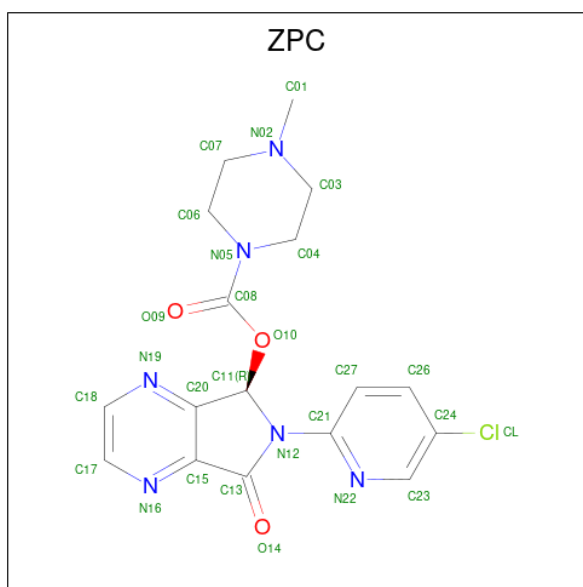
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	289	ASN	MET	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is (5R)-6-(5-chloropyridin-2-yl)-7-oxo-6,7-dihydro-5H-pyrrolo[3,4-b]pyrazin-5-yl 4-methylpiperazine-1-carboxylate (CCD ID: ZPC) (formula: C₁₇H₁₇ClN₆O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	B	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	C	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	D	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	E	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		

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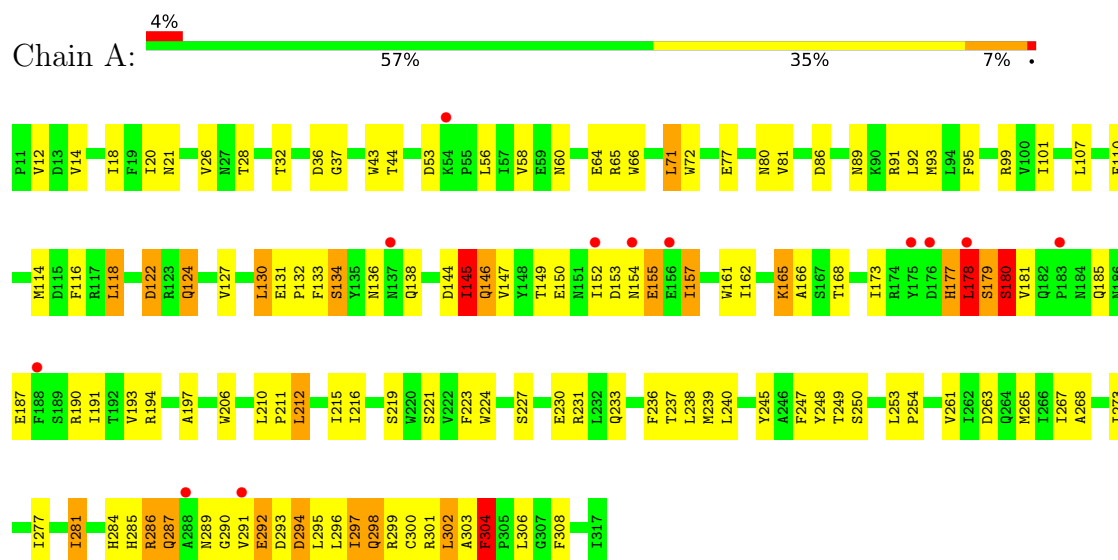
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	G	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	H	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	I	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	J	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		

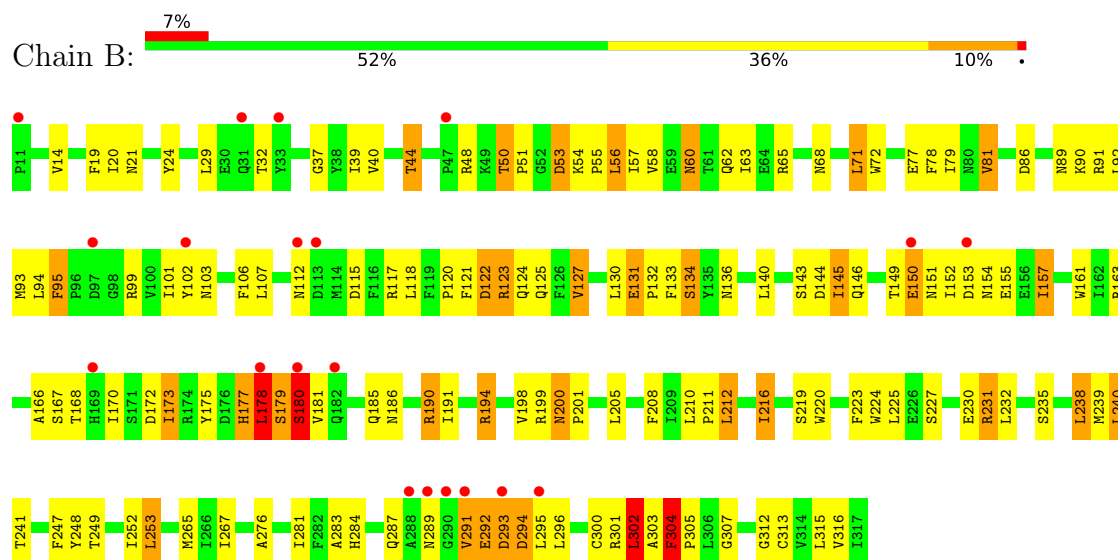
3 Residue-property plots [i](#)

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

• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

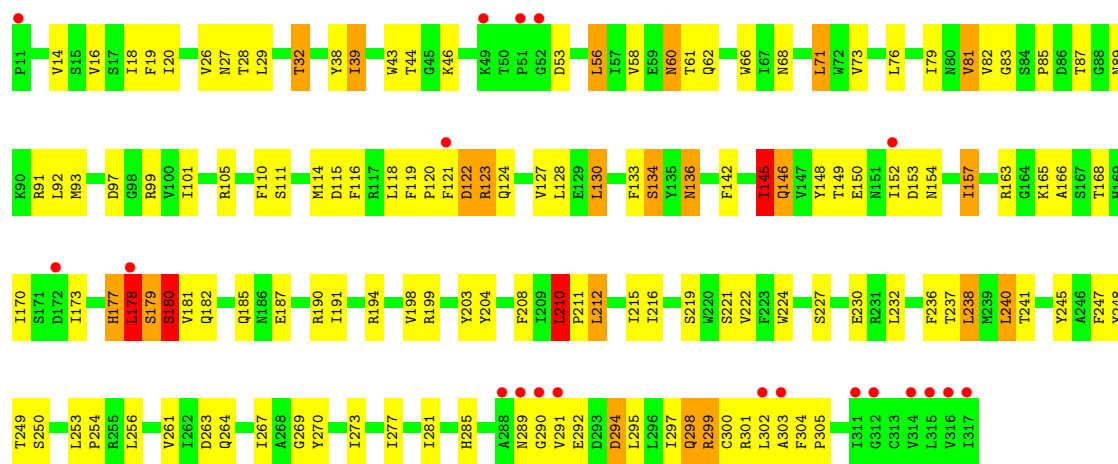


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

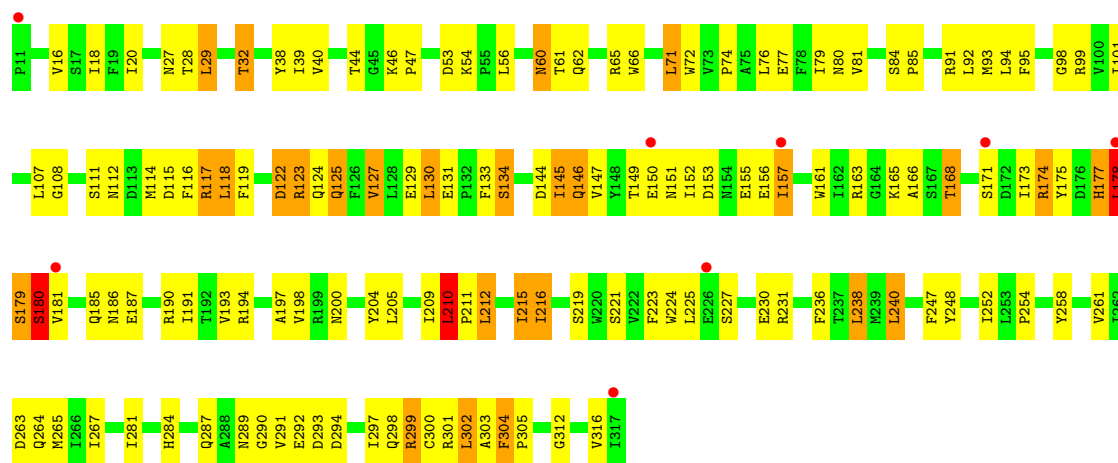


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

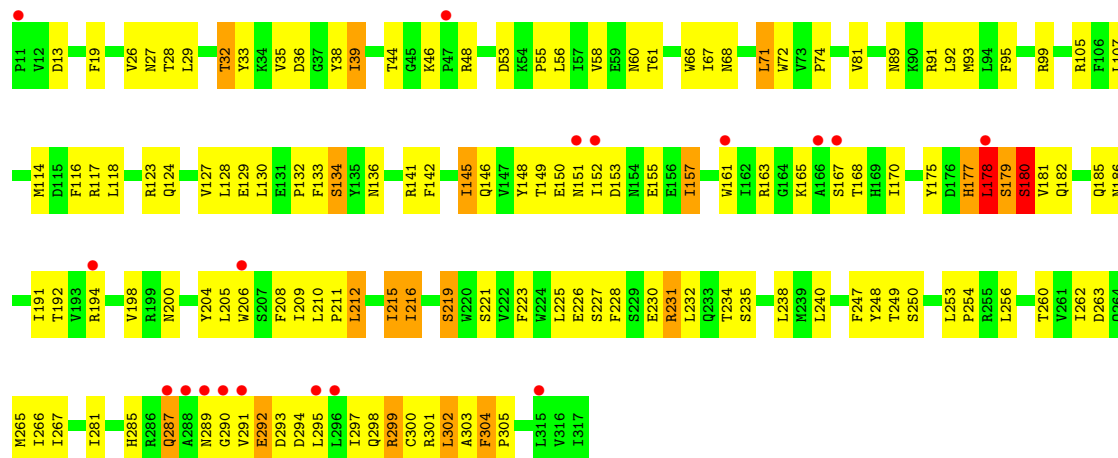




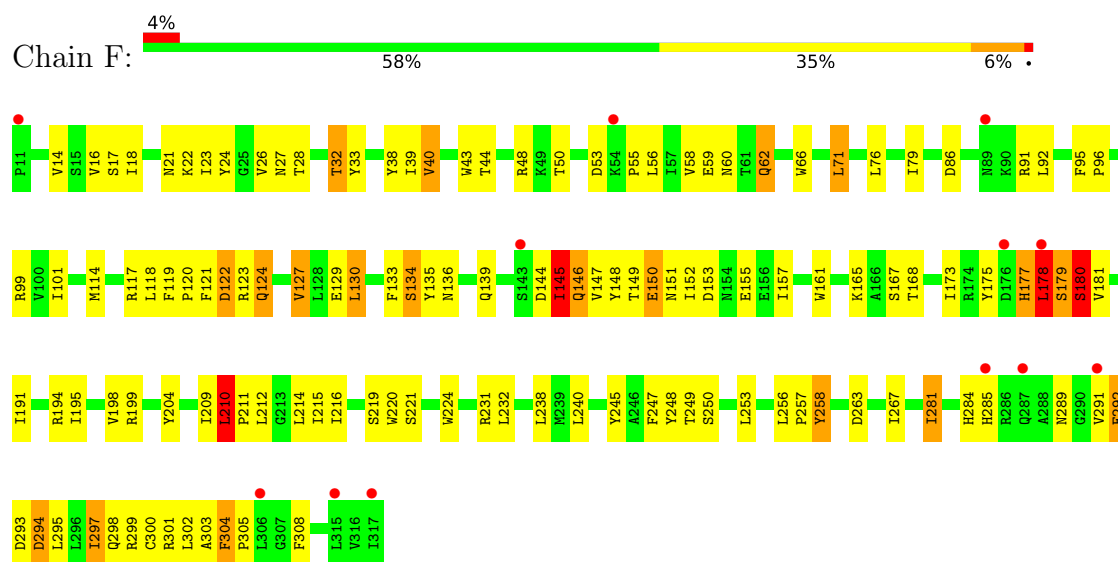
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



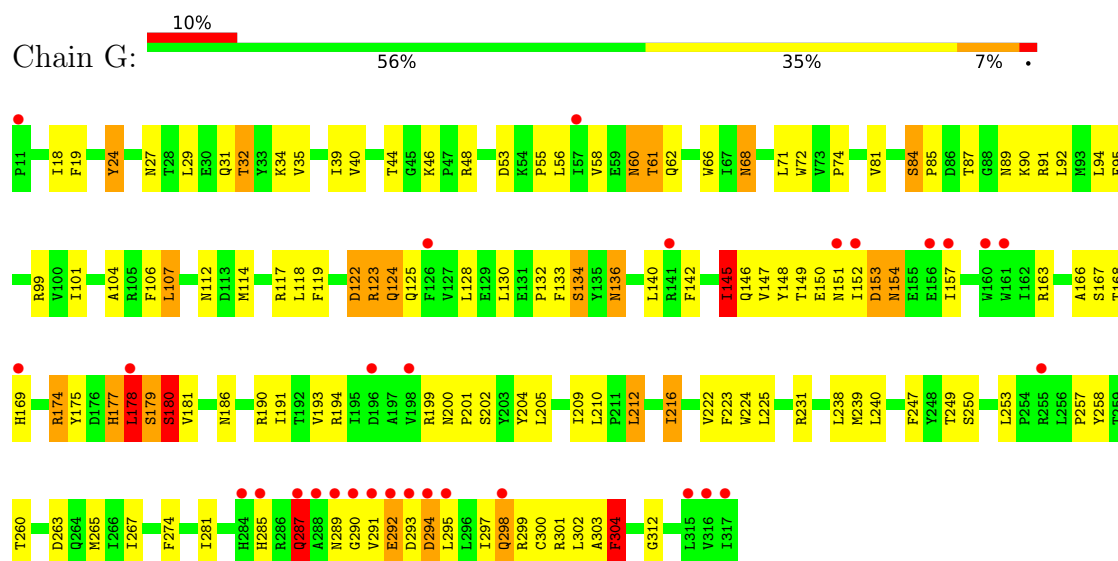
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



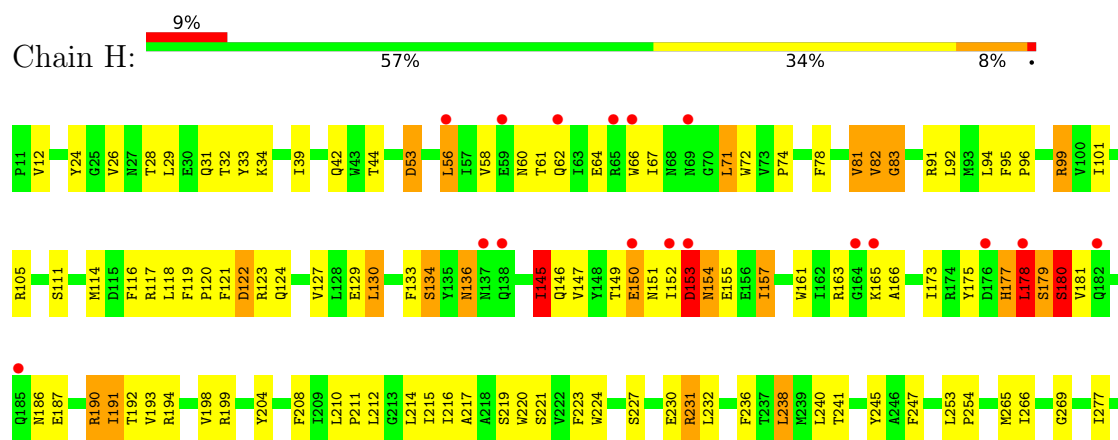
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



- Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

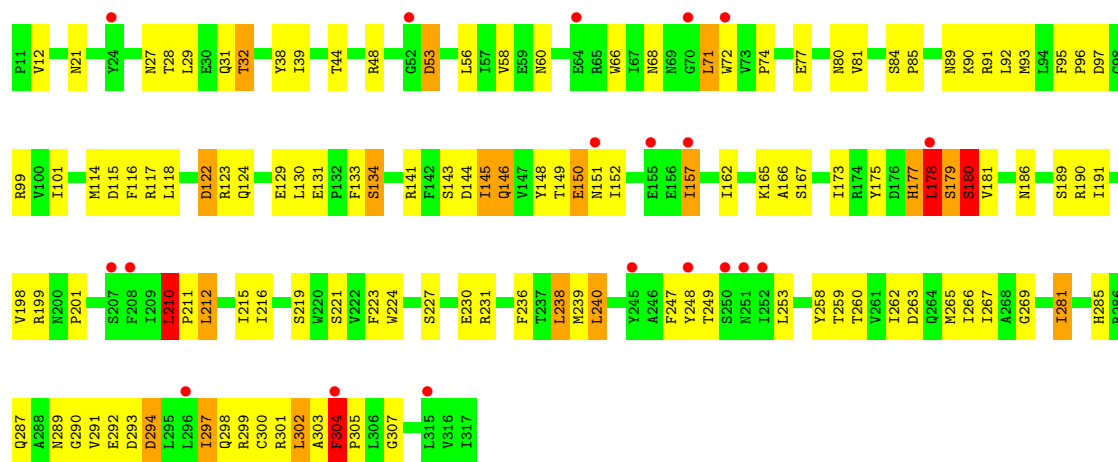


- Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

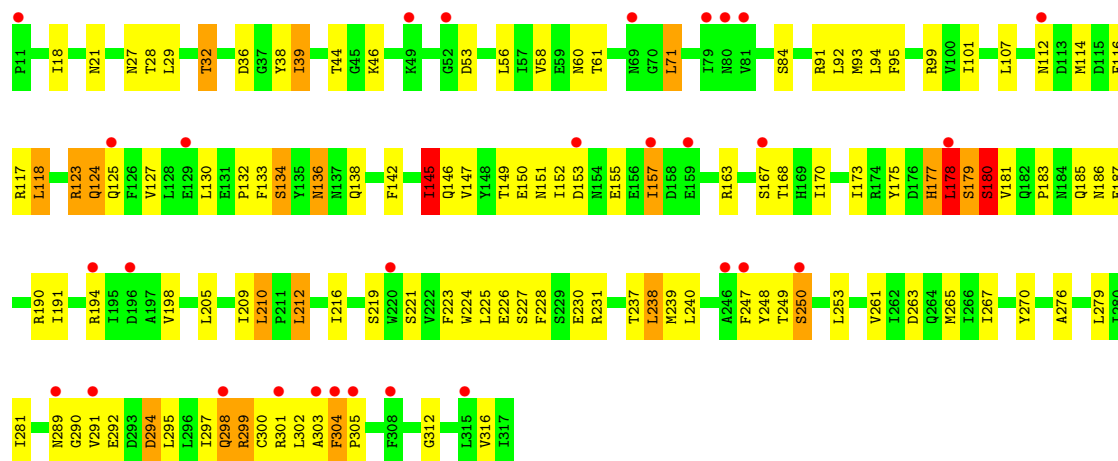




● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.40Å 266.83Å 110.76Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	43.47 – 3.34 43.47 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.47-3.34) 99.4 (43.47-3.34)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.205 , 0.259 0.226 , 0.275	Depositor DCC
R_{free} test set	4134 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 64.9	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	0.90	EDS
Total number of atoms	25290	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: ZPC

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	0.71	0/2570	1.15	11/3503 (0.3%)
1	B	0.87	0/2570	1.33	27/3503 (0.8%)
1	C	0.78	0/2570	1.17	10/3503 (0.3%)
1	D	0.86	0/2570	1.27	22/3503 (0.6%)
1	E	0.76	0/2570	1.16	6/3503 (0.2%)
1	F	0.72	0/2570	1.15	8/3503 (0.2%)
1	G	0.84	0/2570	1.25	22/3503 (0.6%)
1	H	0.78	0/2570	1.16	8/3503 (0.2%)
1	I	0.83	0/2570	1.16	10/3503 (0.3%)
1	J	0.77	1/2570 (0.0%)	1.15	12/3503 (0.3%)
All	All	0.79	1/25700 (0.0%)	1.20	136/35030 (0.4%)

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	2
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	170	ILE	CA-CB	-5.49	1.47	1.54

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	LEU	CA-C-N	-10.09	108.49	119.19
1	B	210	LEU	C-N-CA	-10.09	108.49	119.19
1	J	39	ILE	CB-CA-C	-8.70	97.58	110.81
1	B	95	PHE	CA-C-N	8.65	128.36	119.19
1	B	95	PHE	C-N-CA	8.65	128.36	119.19
1	H	12	VAL	N-CA-C	8.20	119.66	108.84
1	A	287	GLN	N-CA-C	7.76	120.70	109.14
1	D	174	ARG	CA-C-N	7.68	135.53	121.70
1	D	174	ARG	C-N-CA	7.68	135.53	121.70
1	B	293	ASP	N-CA-C	-7.45	98.64	109.59
1	D	46	LYS	CA-C-N	7.37	127.41	119.89
1	D	46	LYS	C-N-CA	7.37	127.41	119.89
1	G	84	SER	CA-C-N	7.27	127.27	119.78
1	G	84	SER	C-N-CA	7.27	127.27	119.78
1	G	145	ILE	N-CA-C	7.08	117.97	108.27
1	E	46	LYS	CA-C-N	7.07	127.11	119.90
1	E	46	LYS	C-N-CA	7.07	127.11	119.90
1	B	304	PHE	CA-C-N	-6.93	111.35	119.05
1	B	304	PHE	C-N-CA	-6.93	111.35	119.05
1	A	210	LEU	CA-C-N	-6.75	112.03	119.19
1	A	210	LEU	C-N-CA	-6.75	112.03	119.19
1	D	210	LEU	CA-C-N	-6.73	111.87	119.28
1	D	210	LEU	C-N-CA	-6.73	111.87	119.28
1	F	127	VAL	N-CA-C	6.65	118.06	108.48
1	F	145	ILE	N-CA-C	6.63	117.35	108.27
1	H	298	GLN	N-CA-C	-6.60	104.49	112.54
1	I	210	LEU	CA-C-N	-6.56	112.07	119.28
1	I	210	LEU	C-N-CA	-6.56	112.07	119.28
1	B	216	ILE	CB-CA-C	-6.46	103.41	112.14
1	D	215	ILE	CB-CA-C	-6.44	103.76	111.81
1	J	298	GLN	N-CA-C	-6.42	104.71	112.54
1	B	123	ARG	N-CA-C	-6.42	98.74	109.07
1	D	20	ILE	CB-CA-C	-6.37	103.63	111.08
1	E	215	ILE	CB-CA-C	-6.33	103.90	111.81
1	B	127	VAL	N-CA-C	6.32	117.58	108.48
1	B	200	ASN	CA-C-N	6.30	127.45	120.45
1	B	200	ASN	C-N-CA	6.30	127.45	120.45
1	E	39	ILE	CB-CA-C	-6.29	101.25	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	GLY	N-CA-C	-6.21	106.65	114.16
1	H	190	ARG	N-CA-C	6.19	118.50	108.41
1	G	190	ARG	N-CA-C	6.06	118.29	108.41
1	B	253	LEU	CA-C-N	6.04	125.80	119.76
1	B	253	LEU	C-N-CA	6.04	125.80	119.76
1	J	145	ILE	N-CA-C	6.03	116.53	108.27
1	D	197	ALA	N-CA-C	6.02	118.44	108.99
1	G	210	LEU	CA-C-N	-6.00	112.67	119.28
1	G	210	LEU	C-N-CA	-6.00	112.67	119.28
1	B	62	GLN	N-CA-C	5.96	119.81	112.54
1	B	44	THR	N-CA-C	5.92	118.55	108.90
1	D	54	LYS	CA-C-N	5.90	125.92	119.90
1	D	54	LYS	C-N-CA	5.90	125.92	119.90
1	D	117	ARG	CB-CG-CD	-5.87	97.81	111.30
1	G	60	ASN	N-CA-C	5.87	123.29	110.80
1	C	210	LEU	CA-C-N	-5.84	112.85	119.28
1	C	210	LEU	C-N-CA	-5.84	112.85	119.28
1	D	216	ILE	CB-CA-C	-5.83	104.51	111.97
1	C	154	ASN	N-CA-C	5.81	119.41	111.39
1	A	250	SER	N-CA-C	5.78	118.52	111.82
1	G	285	HIS	N-CA-C	5.75	120.45	113.38
1	F	135	TYR	N-CA-C	5.73	117.86	108.52
1	J	123	ARG	N-CA-C	-5.73	99.08	108.41
1	F	62	GLN	N-CA-C	5.72	119.87	113.01
1	I	90	LYS	N-CA-C	-5.71	101.29	110.14
1	J	190	ARG	N-CA-C	5.71	117.72	108.41
1	A	145	ILE	N-CA-C	5.69	116.06	108.27
1	B	302	LEU	N-CA-C	-5.68	106.98	114.31
1	D	18	ILE	CB-CA-C	-5.66	102.40	110.83
1	D	171	SER	N-CA-C	5.65	116.83	108.86
1	J	237	THR	N-CA-C	-5.64	105.22	111.36
1	J	84	SER	CA-C-N	5.63	125.54	119.85
1	J	84	SER	C-N-CA	5.63	125.54	119.85
1	A	298	GLN	N-CA-C	-5.63	105.67	112.54
1	G	298	GLN	N-CA-C	-5.62	105.68	112.54
1	C	123	ARG	N-CA-C	-5.62	100.02	109.07
1	G	287	GLN	N-CA-C	5.62	117.33	108.96
1	G	123	ARG	N-CA-C	-5.60	100.05	109.07
1	J	46	LYS	N-CA-C	-5.57	103.02	109.93
1	H	82	VAL	N-CA-C	5.56	115.79	107.51
1	C	73	VAL	CA-C-O	5.54	124.65	120.88
1	J	210	LEU	CA-C-N	-5.53	113.19	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	210	LEU	C-N-CA	-5.53	113.19	119.28
1	I	287	GLN	N-CA-C	5.52	116.64	108.86
1	D	284	HIS	N-CA-C	5.51	117.10	111.14
1	B	50	THR	CA-C-N	5.50	125.82	119.93
1	B	50	THR	C-N-CA	5.50	125.82	119.93
1	G	46	LYS	N-CA-C	-5.50	103.12	109.93
1	B	190	ARG	N-CA-C	5.49	117.85	108.90
1	D	123	ARG	N-CA-C	-5.48	99.97	108.90
1	H	83	GLY	N-CA-C	-5.43	102.98	112.53
1	G	24	TYR	N-CA-C	5.42	115.28	108.45
1	I	12	VAL	N-CA-C	5.37	116.18	108.93
1	C	237	THR	N-CA-C	-5.33	105.55	111.36
1	A	304	PHE	N-CA-C	5.33	121.58	109.81
1	B	77	GLU	N-CA-C	5.32	118.60	110.20
1	E	81	VAL	N-CA-C	5.31	115.90	108.89
1	A	237	THR	N-CA-C	-5.30	105.58	111.36
1	B	53	ASP	N-CA-C	-5.30	99.51	110.80
1	G	304	PHE	N-CA-C	5.30	121.52	109.81
1	A	155	GLU	N-CA-C	-5.30	105.67	111.82
1	I	117	ARG	CA-C-N	-5.28	114.69	122.83
1	I	117	ARG	C-N-CA	-5.28	114.69	122.83
1	B	240	LEU	CA-CB-CG	5.28	134.79	116.30
1	B	131	GLU	CA-C-N	-5.28	114.32	119.76
1	B	131	GLU	C-N-CA	-5.28	114.32	119.76
1	H	145	ILE	N-CA-C	5.26	115.48	108.27
1	D	174	ARG	CA-C-O	-5.25	114.67	120.33
1	C	46	LYS	N-CA-C	-5.24	103.04	109.65
1	C	298	GLN	N-CA-C	-5.24	106.14	112.54
1	F	86	ASP	CA-C-N	-5.24	115.80	122.77
1	F	86	ASP	C-N-CA	-5.24	115.80	122.77
1	B	194	ARG	N-CA-C	5.22	116.90	108.34
1	H	153	ASP	N-CA-C	5.21	121.90	110.80
1	A	302	LEU	N-CA-C	-5.20	107.60	114.31
1	E	302	LEU	N-CA-C	-5.17	107.63	114.31
1	D	125	GLN	N-CA-C	5.17	116.84	108.26
1	D	127	VAL	N-CA-C	5.15	115.89	108.48
1	G	68	ASN	N-CA-C	5.14	117.63	111.71
1	J	250	SER	N-CA-C	5.14	116.88	111.28
1	I	304	PHE	N-CA-C	5.13	121.14	109.81
1	A	154	ASN	N-CA-C	5.12	118.27	111.30
1	G	46	LYS	CA-C-N	5.12	125.11	119.89
1	G	46	LYS	C-N-CA	5.12	125.11	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	106	PHE	N-CA-C	5.12	117.16	109.23
1	G	216	ILE	CB-CA-C	-5.12	105.33	111.88
1	I	117	ARG	CB-CG-CD	-5.11	99.55	111.30
1	G	202	SER	N-CA-C	5.10	116.53	111.07
1	F	210	LEU	CA-C-N	-5.10	113.78	119.19
1	F	210	LEU	C-N-CA	-5.10	113.78	119.19
1	D	185	GLN	N-CA-C	5.09	118.41	107.67
1	G	136	ASN	N-CA-C	5.09	117.10	110.53
1	C	145	ILE	N-CA-C	5.08	115.23	108.27
1	C	190	ARG	N-CA-C	5.08	117.19	108.90
1	G	312	GLY	N-CA-C	5.07	119.26	112.77
1	H	99	ARG	N-CA-C	5.06	117.24	110.35
1	I	307	GLY	N-CA-C	-5.04	108.06	114.16
1	D	60	ASN	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	HIS	Peptide
1	A	178	LEU	Peptide
1	B	177	HIS	Peptide
1	B	178	LEU	Peptide
1	C	177	HIS	Peptide
1	C	178	LEU	Peptide
1	D	174	ARG	Peptide
1	D	177	HIS	Peptide
1	D	178	LEU	Peptide
1	E	177	HIS	Peptide
1	E	178	LEU	Peptide
1	F	177	HIS	Peptide
1	F	178	LEU	Peptide
1	G	177	HIS	Peptide
1	G	178	LEU	Peptide
1	H	177	HIS	Peptide
1	H	178	LEU	Peptide
1	I	177	HIS	Peptide
1	I	178	LEU	Peptide
1	J	177	HIS	Peptide
1	J	178	LEU	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	2502	0	2469	118	0
1	B	2502	0	2469	125	0
1	C	2502	0	2469	116	0
1	D	2502	0	2469	107	0
1	E	2502	0	2469	116	0
1	F	2502	0	2469	103	0
1	G	2502	0	2469	98	0
1	H	2502	0	2469	107	0
1	I	2502	0	2469	98	0
1	J	2502	0	2469	88	0
2	A	27	0	17	9	0
2	B	27	0	17	3	0
2	C	27	0	17	8	0
2	D	27	0	17	12	0
2	E	27	0	17	7	0
2	F	27	0	17	11	0
2	G	27	0	17	6	0
2	H	27	0	17	7	0
2	I	27	0	17	8	0
2	J	27	0	17	4	0
All	All	25290	0	24860	954	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (954) 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:J:133:PHE:O	2:J:1318:ZPC:H03A	1.56	1.05
1:H:150:GLU:OE2	2:I:1318:ZPC:H17	1.58	1.01
1:E:13:ASP:OD1	1:E:141:ARG:NH1	1.94	0.99
1:C:91:ARG:NH2	2:D:1318:ZPC:H23	1.79	0.98
1:F:133:PHE:O	2:F:1318:ZPC:H07	1.66	0.96
1:E:155:GLU:OE2	1:E:163:ARG:NH2	2.02	0.92
1:I:91:ARG:NH2	1:I:93:MET:SD	2.43	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ARG:HH22	2:D:1318:ZPC:H23	1.29	0.90
1:H:175:TYR:O	1:H:186:ASN:ND2	2.06	0.88
1:E:161:TRP:HB3	1:E:163:ARG:HH21	1.40	0.87
1:C:249:THR:HG23	1:C:253:LEU:HD22	1.55	0.86
1:I:215:ILE:HD13	1:J:239:MET:HE3	1.58	0.86
1:E:294:ASP:HB2	1:E:297:ILE:HG22	1.58	0.85
1:E:293:ASP:O	1:E:298:GLN:NE2	2.10	0.84
1:I:91:ARG:HD2	1:J:134:SER:HB3	1.58	0.83
1:F:59:GLU:OE2	1:G:134:SER:OG	1.95	0.83
1:J:44:THR:HA	1:J:99:ARG:HA	1.61	0.82
1:E:132:PRO:O	2:E:1318:ZPC:H01A	1.80	0.81
1:J:294:ASP:HB2	1:J:297:ILE:HG22	1.62	0.81
1:F:133:PHE:O	2:F:1318:ZPC:C07	2.28	0.81
1:D:91:ARG:HD2	1:E:134:SER:HB3	1.63	0.81
1:I:91:ARG:HB2	1:J:133:PHE:HE2	1.45	0.81
1:A:133:PHE:O	2:A:1318:ZPC:H07	1.80	0.80
1:C:123:ARG:HD2	1:C:198:VAL:HG22	1.64	0.79
1:C:133:PHE:O	2:C:1318:ZPC:H07	1.82	0.79
1:I:123:ARG:HD2	1:I:198:VAL:HG22	1.65	0.79
1:I:293:ASP:O	1:I:298:GLN:NE2	2.16	0.78
1:H:224:TRP:CH2	1:H:301:ARG:HB3	2.19	0.78
1:B:123:ARG:HD2	1:B:198:VAL:HG22	1.67	0.77
1:E:167:SER:HB3	1:E:194:ARG:HB2	1.67	0.77
1:B:167:SER:HB3	1:B:194:ARG:HB2	1.65	0.76
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.19	0.76
1:F:66:TRP:HB3	1:F:71:LEU:HD12	1.68	0.76
1:G:167:SER:HB3	1:G:194:ARG:HB2	1.67	0.76
1:A:91:ARG:HD2	1:B:134:SER:HB3	1.68	0.75
1:C:91:ARG:HH22	2:D:1318:ZPC:C23	2.00	0.75
1:C:178:LEU:HD12	1:C:180:SER:HB3	1.68	0.75
1:F:177:HIS:O	1:F:179:SER:N	2.20	0.75
1:G:18:ILE:HD13	1:G:39:ILE:HG12	1.67	0.74
1:A:224:TRP:CH2	1:A:301:ARG:HB3	2.23	0.73
1:J:249:THR:HG23	1:J:253:LEU:HD22	1.71	0.72
1:B:122:ASP:OD1	1:B:122:ASP:N	2.22	0.72
1:I:77:GLU:OE1	2:I:1318:ZPC:H01	1.91	0.71
1:D:93:MET:HB3	1:D:101:ILE:HB	1.72	0.71
1:G:294:ASP:HB2	1:G:297:ILE:HG22	1.73	0.71
1:C:122:ASP:OD1	1:C:122:ASP:N	2.22	0.71
1:A:127:VAL:HG22	1:A:194:ARG:HG2	1.74	0.70
1:D:294:ASP:HB2	1:D:297:ILE:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TYR:O	1:B:186:ASN:ND2	2.25	0.69
1:F:212:LEU:O	1:F:216:ILE:HG12	1.92	0.69
1:I:95:PHE:HB2	1:I:99:ARG:HG2	1.74	0.69
1:E:161:TRP:HB3	1:E:163:ARG:NH2	2.08	0.69
1:C:212:LEU:O	1:C:216:ILE:HG12	1.93	0.69
1:E:127:VAL:HG22	1:E:194:ARG:HG2	1.74	0.69
1:G:178:LEU:HD12	1:G:180:SER:HB3	1.72	0.69
1:I:44:THR:HA	1:I:99:ARG:HA	1.73	0.69
1:A:93:MET:HB3	1:A:101:ILE:HB	1.75	0.68
1:D:248:TYR:HE1	1:E:250:SER:HG	1.39	0.68
1:G:44:THR:HA	1:G:99:ARG:HA	1.73	0.68
1:H:44:THR:HA	1:H:99:ARG:HA	1.75	0.68
1:H:181:VAL:HG11	2:H:1318:ZPC:CL	2.30	0.68
1:I:216:ILE:O	1:I:219:SER:HB3	1.93	0.68
1:I:300:CYS:HB2	1:I:303:ALA:HB3	1.76	0.68
1:F:133:PHE:CD1	2:F:1318:ZPC:H07A	2.29	0.68
1:B:208:PHE:HE2	1:B:249:THR:HA	1.59	0.68
1:E:177:HIS:O	1:E:179:SER:N	2.27	0.68
1:F:150:GLU:OE2	2:G:1318:ZPC:H17	1.94	0.68
1:H:101:ILE:HD13	2:I:1318:ZPC:CL	2.31	0.68
1:C:294:ASP:HB2	1:C:297:ILE:HG22	1.75	0.68
1:A:287:GLN:HA	1:A:292:GLU:OE1	1.95	0.67
1:D:212:LEU:O	1:D:216:ILE:HG12	1.94	0.67
1:F:91:ARG:HD2	1:G:134:SER:HB3	1.75	0.67
1:F:150:GLU:OE2	2:G:1318:ZPC:C17	2.42	0.67
1:J:177:HIS:O	1:J:179:SER:N	2.27	0.67
1:H:284:HIS:HE1	1:H:291:VAL:HG13	1.58	0.67
1:B:212:LEU:O	1:B:216:ILE:HG12	1.93	0.67
1:B:40:VAL:HG11	2:C:1318:ZPC:H26	1.75	0.67
1:A:294:ASP:O	1:A:298:GLN:HG2	1.94	0.67
1:F:91:ARG:HH22	2:G:1318:ZPC:H23	1.60	0.67
1:B:40:VAL:HG21	2:C:1318:ZPC:H27	1.77	0.66
1:G:205:LEU:HD23	1:G:209:ILE:HG13	1.77	0.66
1:D:145:ILE:HD12	1:D:191:ILE:HG21	1.78	0.66
1:D:216:ILE:O	1:D:219:SER:HB3	1.96	0.66
1:G:301:ARG:HH12	1:H:285:HIS:CE1	2.13	0.66
1:J:178:LEU:HD12	1:J:180:SER:HB3	1.78	0.66
1:D:175:TYR:O	1:D:186:ASN:ND2	2.28	0.65
1:I:179:SER:O	1:I:181:VAL:N	2.29	0.65
1:G:225:LEU:HD21	1:H:232:LEU:HD22	1.78	0.65
1:J:167:SER:HB3	1:J:194:ARG:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASN:ND2	2:C:1318:ZPC:H06A	2.11	0.65
1:D:179:SER:O	1:D:181:VAL:N	2.30	0.65
1:H:284:HIS:CE1	1:H:291:VAL:HG13	2.31	0.65
1:D:123:ARG:HD2	1:D:198:VAL:HG22	1.77	0.65
1:D:144:ASP:OD1	1:D:146:GLN:NE2	2.29	0.65
1:A:179:SER:O	1:A:181:VAL:N	2.30	0.65
1:A:289:ASN:OD1	1:A:290:GLY:N	2.26	0.65
1:D:173:ILE:O	1:D:187:GLU:HA	1.95	0.65
1:A:221:SER:HB2	1:B:281:ILE:HD11	1.79	0.64
1:B:65:ARG:HD2	1:C:68:ASN:ND2	2.12	0.64
1:B:149:THR:O	1:B:151:ASN:N	2.26	0.64
1:E:216:ILE:O	1:E:219:SER:HB3	1.96	0.64
1:F:133:PHE:HA	2:F:1318:ZPC:C01	2.28	0.64
1:G:289:ASN:OD1	1:G:290:GLY:N	2.28	0.64
1:D:76:LEU:HB3	1:D:130:LEU:HD21	1.78	0.64
1:H:179:SER:O	1:H:181:VAL:N	2.31	0.64
1:F:133:PHE:HA	2:F:1318:ZPC:H01	1.80	0.64
1:G:295:LEU:HA	1:G:298:GLN:OE1	1.97	0.64
1:E:178:LEU:HD12	1:E:180:SER:HB3	1.78	0.64
1:F:284:HIS:HE1	1:J:226:GLU:OE2	1.80	0.64
1:I:212:LEU:O	1:I:216:ILE:HG12	1.98	0.64
1:F:294:ASP:HB2	1:F:297:ILE:HG22	1.79	0.63
1:F:155:GLU:HB3	1:F:161:TRP:CD1	2.34	0.63
1:J:123:ARG:HG2	1:J:198:VAL:HG22	1.81	0.63
1:G:91:ARG:HD2	1:H:134:SER:HB3	1.80	0.63
1:E:27:ASN:HB3	1:E:32:THR:HB	1.81	0.63
1:A:223:PHE:HE2	1:A:304:PHE:CE1	2.17	0.63
1:C:179:SER:O	1:C:181:VAL:N	2.32	0.63
1:D:161:TRP:HB3	1:D:163:ARG:HH21	1.62	0.63
1:F:26:VAL:HG11	1:F:114:MET:HE1	1.80	0.63
1:G:157:ILE:HD11	1:H:117:ARG:HE	1.64	0.63
1:C:136:ASN:H	1:C:136:ASN:HD22	1.46	0.62
1:G:300:CYS:HB2	1:G:303:ALA:HB3	1.81	0.62
1:B:284:HIS:NE2	1:B:291:VAL:HG13	2.13	0.62
1:D:81:VAL:HG21	1:D:85:PRO:HG3	1.82	0.62
1:E:181:VAL:HG11	2:E:1318:ZPC:CL	2.36	0.62
1:D:225:LEU:HD21	1:E:232:LEU:HD22	1.81	0.62
1:E:289:ASN:OD1	1:E:290:GLY:N	2.30	0.62
1:E:294:ASP:HB2	1:E:297:ILE:CG2	2.29	0.62
1:F:175:TYR:CE2	2:F:1318:ZPC:H04A	2.35	0.62
1:F:293:ASP:O	1:F:298:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:SER:OG	1:B:144:ASP:N	2.33	0.61
1:H:66:TRP:HB3	1:H:71:LEU:HD12	1.81	0.61
1:H:123:ARG:HD2	1:H:198:VAL:HG22	1.81	0.61
1:D:177:HIS:O	1:D:179:SER:N	2.33	0.61
1:G:179:SER:O	1:G:181:VAL:N	2.34	0.61
1:C:127:VAL:HG22	1:C:194:ARG:HG2	1.83	0.61
1:F:123:ARG:HD2	1:F:198:VAL:HG22	1.82	0.61
1:E:223:PHE:HE2	1:E:304:PHE:CE1	2.19	0.61
1:C:58:VAL:HB	1:C:92:LEU:HB2	1.81	0.61
1:E:263:ASP:O	1:E:267:ILE:HG12	2.00	0.61
1:G:289:ASN:ND2	1:G:292:GLU:HB2	2.15	0.61
1:B:300:CYS:HB2	1:B:303:ALA:HB3	1.83	0.60
1:F:167:SER:HB3	1:F:194:ARG:HB2	1.81	0.60
1:D:145:ILE:HD12	1:D:191:ILE:CG2	2.31	0.60
1:D:300:CYS:HB2	1:D:303:ALA:HB3	1.84	0.60
1:A:65:ARG:HD2	1:B:68:ASN:ND2	2.15	0.60
1:C:177:HIS:O	1:C:179:SER:N	2.35	0.60
1:D:122:ASP:OD1	1:D:122:ASP:N	2.33	0.60
1:D:133:PHE:O	2:D:1318:ZPC:H07	2.01	0.60
1:E:175:TYR:O	1:E:186:ASN:ND2	2.35	0.60
1:I:294:ASP:HB2	1:I:297:ILE:HG22	1.83	0.60
1:F:91:ARG:HB2	1:G:133:PHE:HE2	1.66	0.60
1:H:127:VAL:HG22	1:H:194:ARG:HG2	1.82	0.60
1:I:212:LEU:CD1	1:I:265:MET:HB3	2.31	0.60
1:H:129:GLU:HG2	1:H:192:THR:HG23	1.84	0.60
1:H:177:HIS:O	1:H:179:SER:N	2.35	0.60
1:H:216:ILE:O	1:H:219:SER:HB3	2.01	0.59
1:D:147:VAL:HG21	1:D:193:VAL:HG13	1.84	0.59
1:E:44:THR:HA	1:E:99:ARG:HA	1.85	0.59
1:B:55:PRO:HG3	1:C:182:GLN:HE21	1.67	0.59
1:E:227:SER:HB3	1:E:230:GLU:HG3	1.83	0.59
2:F:1318:ZPC:H23	1:J:91:ARG:HH22	1.66	0.59
1:C:211:PRO:O	1:C:215:ILE:HG12	2.03	0.59
1:A:249:THR:O	1:A:253:LEU:HB2	2.03	0.59
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.85	0.59
1:D:178:LEU:HD12	1:D:180:SER:HB3	1.85	0.59
1:B:179:SER:O	1:B:181:VAL:N	2.36	0.59
1:G:101:ILE:HD13	2:H:1318:ZPC:CL	2.40	0.59
1:I:175:TYR:O	1:I:186:ASN:ND2	2.36	0.59
1:I:253:LEU:HD21	1:I:262:ILE:HD12	1.85	0.59
1:D:211:PRO:O	1:D:215:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:SER:O	1:E:182:GLN:N	2.36	0.59
1:E:300:CYS:HB2	1:E:303:ALA:HB3	1.85	0.59
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.20	0.59
1:A:300:CYS:HB2	1:A:303:ALA:HB3	1.83	0.59
1:F:249:THR:HG23	1:F:253:LEU:HD22	1.85	0.59
1:F:145:ILE:HD12	1:F:191:ILE:HG21	1.84	0.58
1:F:215:ILE:HD13	1:G:239:MET:HE3	1.84	0.58
1:I:224:TRP:CH2	1:I:301:ARG:HB3	2.38	0.58
1:B:212:LEU:CD1	1:B:265:MET:HB3	2.32	0.58
1:C:101:ILE:HD13	2:D:1318:ZPC:CL	2.40	0.58
1:G:122:ASP:N	1:G:122:ASP:OD1	2.37	0.58
1:A:239:MET:HE3	1:E:215:ILE:HD13	1.85	0.58
1:G:48:ARG:NH1	1:G:48:ARG:HB2	2.18	0.58
1:A:95:PHE:HB2	1:A:99:ARG:HG2	1.86	0.58
1:D:71:LEU:HD11	1:D:94:LEU:HD21	1.86	0.58
1:D:221:SER:HB2	1:E:281:ILE:HD11	1.84	0.58
1:A:268:ALA:HB1	1:A:308:PHE:HE1	1.69	0.58
1:F:44:THR:HA	1:F:99:ARG:HA	1.85	0.58
1:F:224:TRP:CH2	1:F:301:ARG:HB3	2.39	0.58
1:F:179:SER:O	1:F:181:VAL:N	2.37	0.58
1:A:177:HIS:O	1:A:179:SER:N	2.36	0.58
1:H:150:GLU:OE2	2:I:1318:ZPC:C17	2.45	0.58
1:H:91:ARG:HD2	1:I:134:SER:HB3	1.86	0.58
1:F:22:LYS:HE3	1:F:24:TYR:CG	2.39	0.57
1:H:28:THR:HG21	1:H:254:PRO:HB2	1.85	0.57
1:B:19:PHE:CE2	2:C:1318:ZPC:C15	2.87	0.57
1:I:58:VAL:HB	1:I:92:LEU:HB2	1.86	0.57
1:I:91:ARG:HB2	1:J:133:PHE:CE2	2.33	0.57
1:B:216:ILE:O	1:B:219:SER:HB3	2.04	0.57
1:A:122:ASP:OD1	1:A:122:ASP:N	2.34	0.57
1:F:33:TYR:OH	1:F:127:VAL:N	2.37	0.57
1:F:263:ASP:O	1:F:267:ILE:HG12	2.03	0.57
1:H:212:LEU:HD11	1:H:265:MET:HB3	1.87	0.57
1:H:31:GLN:HG2	1:H:114:MET:HB2	1.86	0.57
1:A:178:LEU:HD12	1:A:180:SER:HB3	1.86	0.57
1:A:299:ARG:HA	1:A:301:ARG:HG3	1.86	0.57
1:H:212:LEU:O	1:H:216:ILE:HG12	2.05	0.57
1:J:263:ASP:O	1:J:267:ILE:HG12	2.05	0.57
1:A:289:ASN:OD1	1:A:292:GLU:N	2.38	0.57
1:A:295:LEU:HA	1:A:298:GLN:OE1	2.05	0.57
1:C:136:ASN:HD22	1:C:136:ASN:N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ILE:O	1:C:219:SER:HB3	2.05	0.57
1:F:136:ASN:ND2	1:F:139:GLN:OE1	2.38	0.57
1:I:219:SER:HA	1:I:238:LEU:HD21	1.87	0.56
1:I:173:ILE:HD13	1:I:190:ARG:HB3	1.85	0.56
1:E:123:ARG:HD2	1:E:198:VAL:HG22	1.86	0.56
1:E:262:ILE:O	1:E:266:ILE:HG12	2.05	0.56
1:G:223:PHE:HE2	1:G:304:PHE:CE1	2.22	0.56
1:I:145:ILE:HD12	1:I:191:ILE:CG2	2.35	0.56
1:I:294:ASP:HB2	1:I:297:ILE:CG2	2.35	0.56
1:B:103:ASN:HD21	2:C:1318:ZPC:H06A	1.69	0.56
1:C:26:VAL:HG13	1:C:114:MET:HE1	1.86	0.56
1:C:66:TRP:HB3	1:C:71:LEU:HD12	1.87	0.56
1:E:205:LEU:HD23	1:E:209:ILE:HG13	1.88	0.56
1:A:284:HIS:HE1	1:E:226:GLU:OE2	1.89	0.56
1:E:28:THR:HB	1:E:256:LEU:HD21	1.87	0.56
1:E:145:ILE:HG21	1:E:191:ILE:HG12	1.87	0.56
1:C:145:ILE:HG23	1:C:168:THR:HG21	1.86	0.56
1:A:14:VAL:HG22	1:A:43:TRP:HB3	1.88	0.56
1:C:91:ARG:CD	1:D:134:SER:HB3	2.36	0.55
1:A:212:LEU:O	1:A:216:ILE:HG12	2.06	0.55
1:B:248:TYR:HA	1:C:247:PHE:CE1	2.42	0.55
1:B:20:ILE:HB	1:B:149:THR:HG22	1.87	0.55
1:B:91:ARG:HB2	1:C:133:PHE:HE2	1.70	0.55
1:C:19:PHE:CE1	1:C:148:TYR:CD2	2.95	0.55
1:C:145:ILE:HD12	1:C:191:ILE:HG21	1.88	0.55
1:D:147:VAL:HG21	1:D:193:VAL:CG1	2.36	0.55
1:E:19:PHE:CD1	1:E:148:TYR:HB2	2.41	0.55
1:G:224:TRP:CH2	1:G:301:ARG:HB3	2.41	0.55
1:H:219:SER:HA	1:H:238:LEU:HD21	1.88	0.55
1:I:150:GLU:OE2	2:J:1318:ZPC:H17	2.06	0.55
1:B:150:GLU:OE1	2:C:1318:ZPC:H17	2.06	0.55
1:B:177:HIS:O	1:B:179:SER:N	2.40	0.55
1:E:227:SER:O	1:E:231:ARG:HD3	2.07	0.55
1:C:44:THR:HA	1:C:99:ARG:HA	1.88	0.55
1:F:216:ILE:O	1:F:219:SER:HB3	2.07	0.55
1:J:145:ILE:HD12	1:J:191:ILE:HG21	1.89	0.55
1:C:241:THR:HA	1:D:240:LEU:HD23	1.89	0.55
1:D:149:THR:C	1:D:151:ASN:H	2.15	0.55
1:G:212:LEU:O	1:G:216:ILE:HG12	2.06	0.55
1:C:105:ARG:HD3	1:D:77:GLU:OE2	2.06	0.55
1:F:91:ARG:NH2	2:G:1318:ZPC:H23	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:LEU:HD12	1:F:180:SER:HB3	1.87	0.55
1:H:294:ASP:HB2	1:H:297:ILE:HG22	1.89	0.55
1:I:101:ILE:HD13	2:J:1318:ZPC:CL	2.43	0.55
1:J:205:LEU:HD23	1:J:209:ILE:HG13	1.87	0.55
1:C:294:ASP:HB2	1:C:297:ILE:CG2	2.37	0.55
1:A:58:VAL:HB	1:A:92:LEU:HB2	1.88	0.55
1:A:133:PHE:HA	2:A:1318:ZPC:C01	2.37	0.55
1:E:133:PHE:HA	2:E:1318:ZPC:C01	2.36	0.55
1:F:26:VAL:CG1	1:F:114:MET:HE1	2.37	0.55
1:C:301:ARG:O	1:C:305:PRO:HG2	2.07	0.54
1:B:249:THR:HG23	1:B:253:LEU:HD22	1.89	0.54
1:A:133:PHE:CD1	2:A:1318:ZPC:H07A	2.42	0.54
1:D:79:ILE:N	1:D:129:GLU:O	2.37	0.54
1:F:27:ASN:HB3	1:F:32:THR:HB	1.88	0.54
1:C:81:VAL:HG12	1:C:83:GLY:O	2.07	0.54
1:D:223:PHE:HE2	1:D:304:PHE:CE1	2.26	0.54
1:D:302:LEU:C	1:D:305:PRO:HD2	2.32	0.54
1:A:216:ILE:O	1:A:219:SER:HB3	2.07	0.54
1:G:62:GLN:O	1:G:66:TRP:HD1	1.91	0.54
1:H:122:ASP:OD1	1:H:122:ASP:N	2.40	0.54
1:J:127:VAL:HG22	1:J:194:ARG:HG2	1.88	0.54
1:B:224:TRP:CH2	1:B:301:ARG:HB3	2.42	0.54
1:D:289:ASN:OD1	1:D:290:GLY:N	2.40	0.54
1:G:91:ARG:HB2	1:H:133:PHE:HE2	1.72	0.54
1:H:173:ILE:HD13	1:H:190:ARG:HB3	1.90	0.54
1:J:136:ASN:H	1:J:136:ASN:HD22	1.56	0.54
1:J:149:THR:C	1:J:151:ASN:H	2.16	0.54
1:G:149:THR:C	1:G:151:ASN:H	2.16	0.54
1:A:133:PHE:HE2	1:E:91:ARG:HB2	1.73	0.54
1:B:172:ASP:HB2	1:I:141:ARG:NH2	2.22	0.54
1:D:293:ASP:O	1:D:298:GLN:NE2	2.41	0.54
1:E:133:PHE:O	2:E:1318:ZPC:N02	2.40	0.54
1:E:227:SER:OG	1:E:228:PHE:N	2.39	0.54
1:E:294:ASP:O	1:E:298:GLN:HG2	2.08	0.54
1:F:122:ASP:CG	1:F:199:ARG:HE	2.15	0.53
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.26	0.53
1:G:294:ASP:O	1:G:298:GLN:HG2	2.07	0.53
1:C:91:ARG:HD2	1:D:134:SER:HB3	1.88	0.53
1:F:133:PHE:O	2:F:1318:ZPC:N02	2.42	0.53
1:H:247:PHE:CD2	1:I:247:PHE:HE2	2.25	0.53
1:J:175:TYR:O	1:J:186:ASN:ND2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:MET:HE3	1:E:215:ILE:HA	1.90	0.53
1:C:119:PHE:CE2	1:C:254:PRO:HG3	2.44	0.53
1:D:294:ASP:HB2	1:D:297:ILE:CG2	2.38	0.53
1:I:212:LEU:HD12	1:I:265:MET:HB3	1.90	0.53
1:J:138:GLN:OE1	1:J:185:GLN:HB3	2.07	0.53
1:B:145:ILE:HG22	1:B:170:ILE:HD11	1.91	0.53
1:D:156:GLU:HA	1:D:200:ASN:ND2	2.24	0.53
1:E:212:LEU:HD11	1:E:265:MET:HB3	1.90	0.53
1:F:17:SER:O	1:F:40:VAL:HG23	2.09	0.53
1:I:302:LEU:C	1:I:305:PRO:HD2	2.33	0.53
1:B:55:PRO:HB3	1:B:95:PHE:CE1	2.43	0.53
1:A:134:SER:HB3	1:E:91:ARG:HD2	1.91	0.53
1:D:44:THR:HA	1:D:99:ARG:HA	1.90	0.53
1:E:299:ARG:HA	1:E:301:ARG:HG3	1.89	0.53
1:F:204:TYR:O	1:F:209:ILE:HG12	2.09	0.53
1:A:247:PHE:CD2	1:B:247:PHE:HE2	2.27	0.53
1:B:145:ILE:HD12	1:B:191:ILE:HG21	1.90	0.53
1:H:122:ASP:OD2	1:H:199:ARG:NH2	2.41	0.53
1:C:203:TYR:HB2	1:D:258:TYR:HA	1.91	0.53
1:B:283:ALA:O	1:B:293:ASP:HA	2.09	0.52
1:F:295:LEU:HA	1:F:298:GLN:NE2	2.24	0.52
1:G:119:PHE:HA	1:G:122:ASP:OD1	2.09	0.52
1:I:260:THR:N	1:I:263:ASP:OD2	2.27	0.52
1:A:173:ILE:HD13	1:A:190:ARG:HB3	1.90	0.52
1:B:78:PHE:HB3	1:B:81:VAL:HB	1.91	0.52
1:B:212:LEU:HD12	1:B:265:MET:HB3	1.91	0.52
1:B:248:TYR:HD1	1:C:247:PHE:HA	1.75	0.52
1:E:299:ARG:C	1:E:301:ARG:H	2.18	0.52
1:G:40:VAL:HG11	2:H:1318:ZPC:H26	1.91	0.52
1:H:212:LEU:HD12	1:H:265:MET:SD	2.49	0.52
1:J:93:MET:HB3	1:J:101:ILE:HB	1.92	0.52
1:J:178:LEU:HD12	1:J:180:SER:CB	2.38	0.52
1:A:133:PHE:HA	2:A:1318:ZPC:H01A	1.92	0.52
1:B:227:SER:HB3	1:B:230:GLU:HG3	1.90	0.52
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.92	0.52
1:I:133:PHE:CE1	2:I:1318:ZPC:H07A	2.44	0.52
1:B:248:TYR:CD1	1:C:247:PHE:HA	2.45	0.52
1:G:177:HIS:O	1:G:179:SER:N	2.42	0.52
1:G:224:TRP:CZ3	1:G:301:ARG:HB3	2.45	0.52
1:H:178:LEU:HD12	1:H:180:SER:HB3	1.91	0.52
1:A:295:LEU:O	1:A:299:ARG:NE	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.44	0.52
1:D:65:ARG:HD2	1:E:68:ASN:ND2	2.24	0.52
1:G:224:TRP:HD1	1:H:285:HIS:CD2	2.27	0.52
1:A:212:LEU:HD23	1:A:245:TYR:CD1	2.45	0.52
1:B:95:PHE:HE2	1:B:101:ILE:HD12	1.75	0.52
1:D:178:LEU:HD12	1:D:180:SER:CB	2.39	0.52
1:D:205:LEU:HD23	1:D:209:ILE:HG13	1.92	0.52
1:G:289:ASN:HD21	1:G:292:GLU:HB2	1.75	0.52
1:H:53:ASP:O	1:H:96:PRO:HG3	2.10	0.52
1:J:132:PRO:HD3	1:J:142:PHE:CE2	2.45	0.52
1:B:91:ARG:HD2	1:C:134:SER:CB	2.40	0.52
1:E:145:ILE:HG23	1:E:168:THR:CG2	2.40	0.52
1:C:89:ASN:HB2	1:D:133:PHE:CE1	2.44	0.51
1:D:263:ASP:O	1:D:267:ILE:HG12	2.10	0.51
1:E:33:TYR:OH	1:E:127:VAL:N	2.38	0.51
1:G:212:LEU:CD1	1:G:265:MET:HB3	2.40	0.51
1:G:289:ASN:CG	1:G:292:GLU:HB2	2.36	0.51
1:H:119:PHE:HA	1:H:122:ASP:OD1	2.11	0.51
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.75	0.51
1:F:145:ILE:HG23	1:F:168:THR:HG21	1.91	0.51
1:H:215:ILE:HD13	1:I:239:MET:HE3	1.92	0.51
1:D:227:SER:HB3	1:D:230:GLU:HG3	1.92	0.51
1:E:145:ILE:HD12	1:E:191:ILE:HG21	1.92	0.51
1:G:81:VAL:HG21	1:G:85:PRO:HG3	1.92	0.51
1:B:178:LEU:HD12	1:B:180:SER:HB3	1.92	0.51
1:C:14:VAL:HG22	1:C:43:TRP:HB3	1.93	0.51
1:D:27:ASN:HB3	1:D:32:THR:HB	1.91	0.51
1:E:179:SER:OG	1:E:180:SER:N	2.44	0.51
1:H:211:PRO:O	1:H:215:ILE:HG12	2.09	0.51
1:C:93:MET:HB3	1:C:101:ILE:HB	1.93	0.51
1:D:133:PHE:CE1	2:D:1318:ZPC:H07A	2.46	0.51
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.45	0.51
1:A:249:THR:HG23	1:A:253:LEU:HD22	1.92	0.51
1:F:122:ASP:OD1	1:F:122:ASP:N	2.32	0.51
1:F:144:ASP:OD2	1:F:146:GLN:NE2	2.39	0.51
1:H:42:GLN:HG3	1:H:101:ILE:HG12	1.91	0.51
1:I:249:THR:HG23	1:I:253:LEU:HD22	1.92	0.51
1:A:26:VAL:HG13	1:A:114:MET:HE1	1.93	0.51
2:A:1318:ZPC:H23	1:E:91:ARG:HH22	1.76	0.51
1:B:131:GLU:OE2	2:B:1318:ZPC:H01B	2.10	0.51
1:B:145:ILE:HG23	1:B:168:THR:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TRP:CH2	1:C:301:ARG:HB3	2.46	0.51
1:E:249:THR:HG23	1:E:253:LEU:HD22	1.93	0.51
1:I:177:HIS:O	1:I:179:SER:N	2.42	0.51
1:J:219:SER:HA	1:J:238:LEU:HD11	1.93	0.51
1:A:215:ILE:HD13	1:B:239:MET:HE3	1.92	0.51
1:A:294:ASP:HB2	1:A:297:ILE:HG22	1.92	0.51
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.46	0.51
1:F:250:SER:OG	1:J:248:TYR:HE1	1.94	0.51
1:H:212:LEU:HD21	1:H:266:ILE:HD13	1.93	0.51
1:I:133:PHE:O	2:I:1318:ZPC:H03A	2.11	0.51
1:I:223:PHE:HE2	1:I:304:PHE:CE1	2.29	0.51
1:A:150:GLU:OE2	2:B:1318:ZPC:H17	2.10	0.50
1:C:18:ILE:HD13	1:C:39:ILE:HG23	1.93	0.50
1:E:210:LEU:HB3	1:E:211:PRO:CD	2.42	0.50
1:I:289:ASN:OD1	1:I:290:GLY:N	2.43	0.50
1:D:155:GLU:HB3	1:D:161:TRP:CD1	2.45	0.50
1:H:114:MET:HE2	1:H:116:PHE:HZ	1.76	0.50
1:A:145:ILE:HG23	1:A:168:THR:HG21	1.94	0.50
1:D:219:SER:HA	1:D:238:LEU:HD21	1.93	0.50
1:G:107:LEU:HD23	1:H:83:GLY:N	2.27	0.50
1:G:247:PHE:CD2	1:H:247:PHE:HE2	2.28	0.50
1:H:212:LEU:HD23	1:H:245:TYR:CD1	2.47	0.50
1:C:208:PHE:O	1:C:245:TYR:OH	2.29	0.50
1:H:223:PHE:HE2	1:H:304:PHE:CE1	2.30	0.50
1:H:224:TRP:HD1	1:I:285:HIS:ND1	2.10	0.50
1:A:145:ILE:HD12	1:A:191:ILE:HG21	1.94	0.50
1:B:91:ARG:HD2	1:C:134:SER:HB3	1.94	0.50
1:E:304:PHE:CD1	1:E:304:PHE:C	2.90	0.50
1:F:95:PHE:HE2	1:F:101:ILE:HD12	1.77	0.50
2:F:1318:ZPC:H23	1:J:91:ARG:NH2	2.25	0.50
1:G:204:TYR:O	1:G:209:ILE:HG12	2.11	0.50
1:B:91:ARG:NH2	1:B:93:MET:SD	2.83	0.50
1:B:103:ASN:HD21	2:C:1318:ZPC:C06	2.25	0.50
1:G:132:PRO:O	2:G:1318:ZPC:H01A	2.11	0.50
1:I:227:SER:HB3	1:I:230:GLU:HG3	1.94	0.50
1:C:123:ARG:CD	1:C:198:VAL:HG22	2.37	0.50
1:E:304:PHE:C	1:E:304:PHE:HD1	2.18	0.50
1:J:155:GLU:OE2	1:J:163:ARG:NH1	2.44	0.50
1:J:212:LEU:O	1:J:216:ILE:HG12	2.12	0.50
1:A:253:LEU:HG	1:A:254:PRO:HD2	1.94	0.50
1:B:145:ILE:HG21	1:B:191:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:PHE:CE1	2:F:1318:ZPC:H07A	2.46	0.50
1:F:134:SER:HB3	1:J:91:ARG:HD2	1.93	0.50
1:G:114:MET:HE2	1:G:124:GLN:HG2	1.94	0.50
1:A:212:LEU:HD11	1:A:265:MET:HB3	1.94	0.49
2:A:1318:ZPC:H06	1:E:38:TYR:CE2	2.47	0.49
1:G:145:ILE:HD12	1:G:191:ILE:HG21	1.94	0.49
1:J:149:THR:O	1:J:151:ASN:N	2.44	0.49
1:A:77:GLU:OE2	1:E:105:ARG:HD3	2.12	0.49
1:E:33:TYR:OH	1:E:127:VAL:O	2.27	0.49
1:I:27:ASN:HB3	1:I:32:THR:HB	1.95	0.49
1:G:146:GLN:HG3	1:G:148:TYR:OH	2.12	0.49
1:D:133:PHE:O	2:D:1318:ZPC:C07	2.61	0.49
1:D:264:GLN:HA	1:D:267:ILE:HG12	1.95	0.49
1:E:225:LEU:HD22	1:E:230:GLU:HB3	1.94	0.49
1:F:157:ILE:HD11	1:G:117:ARG:HE	1.77	0.49
1:A:44:THR:HA	1:A:99:ARG:HA	1.95	0.49
1:H:114:MET:HE2	1:H:116:PHE:CZ	2.48	0.49
1:C:210:LEU:HB3	1:C:211:PRO:CD	2.42	0.49
1:D:156:GLU:HA	1:D:200:ASN:HD21	1.78	0.49
1:D:248:TYR:HA	1:E:247:PHE:CE1	2.48	0.49
1:E:204:TYR:O	1:E:208:PHE:HB2	2.12	0.49
1:F:146:GLN:HG3	1:F:148:TYR:OH	2.11	0.49
1:G:212:LEU:HD12	1:G:265:MET:SD	2.53	0.49
1:C:38:TYR:CE2	2:D:1318:ZPC:H06	2.48	0.49
1:F:220:TRP:CE3	1:F:305:PRO:HB3	2.47	0.49
1:I:97:ASP:OD1	1:I:99:ARG:HD3	2.13	0.49
1:I:224:TRP:CZ3	1:I:301:ARG:HB3	2.46	0.49
1:J:71:LEU:HD11	1:J:94:LEU:HD21	1.94	0.49
1:I:146:GLN:HG3	1:I:148:TYR:OH	2.13	0.49
1:C:173:ILE:O	1:C:187:GLU:HA	2.12	0.49
1:E:114:MET:HE2	1:E:116:PHE:CZ	2.48	0.49
1:F:58:VAL:HB	1:F:92:LEU:HB2	1.93	0.49
1:E:66:TRP:HB3	1:E:71:LEU:HD12	1.95	0.49
1:F:232:LEU:HD22	1:J:225:LEU:HD21	1.94	0.49
1:I:131:GLU:OE1	1:I:190:ARG:NH2	2.44	0.49
1:J:173:ILE:O	1:J:187:GLU:HA	2.13	0.49
1:A:118:LEU:HA	1:A:261:VAL:HG23	1.93	0.48
1:A:247:PHE:CE1	1:E:248:TYR:HA	2.48	0.48
1:B:21:ASN:ND2	1:B:37:GLY:HA2	2.28	0.48
1:A:284:HIS:CE1	1:E:226:GLU:OE2	2.67	0.48
1:B:136:ASN:ND2	1:B:185:GLN:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:PHE:HB3	1:C:170:ILE:HD13	1.95	0.48
1:D:127:VAL:HG22	1:D:194:ARG:HG2	1.96	0.48
1:D:145:ILE:HG23	1:D:168:THR:HG21	1.94	0.48
1:E:72:TRP:CZ2	1:E:74:PRO:HB3	2.48	0.48
1:E:179:SER:O	1:E:181:VAL:N	2.45	0.48
1:J:177:HIS:C	1:J:179:SER:H	2.21	0.48
1:D:28:THR:HG21	1:D:254:PRO:HB2	1.95	0.48
1:D:131:GLU:OE1	1:D:190:ARG:NE	2.45	0.48
1:A:224:TRP:CZ3	1:A:301:ARG:HB3	2.48	0.48
1:C:210:LEU:HB3	1:C:211:PRO:HD3	1.95	0.48
1:D:76:LEU:HB3	1:D:130:LEU:CD2	2.43	0.48
1:H:210:LEU:HB3	1:H:211:PRO:CD	2.44	0.48
1:E:232:LEU:O	1:E:235:SER:OG	2.26	0.48
1:A:66:TRP:O	1:A:71:LEU:HB2	2.13	0.48
1:A:145:ILE:HG23	1:A:168:THR:CG2	2.44	0.48
1:A:236:PHE:CD2	1:E:234:THR:HG21	2.47	0.48
1:B:24:TYR:OH	1:B:107:LEU:HD21	2.14	0.48
1:A:133:PHE:CE1	1:E:89:ASN:HB2	2.49	0.48
1:B:14:VAL:HG21	1:B:140:LEU:HD21	1.95	0.48
1:C:163:ARG:HA	1:C:163:ARG:HD3	1.58	0.48
1:G:205:LEU:HA	1:G:209:ILE:CG1	2.44	0.48
1:G:249:THR:HG23	1:G:253:LEU:HD22	1.96	0.48
1:J:18:ILE:HB	1:J:147:VAL:HG22	1.95	0.48
1:I:212:LEU:HD11	1:I:265:MET:HB3	1.95	0.48
1:J:228:PHE:HA	1:J:231:ARG:NH1	2.29	0.48
1:D:248:TYR:O	1:D:252:ILE:HG12	2.14	0.48
1:D:299:ARG:HA	1:D:301:ARG:HG3	1.95	0.48
1:E:72:TRP:CH2	1:E:74:PRO:HG3	2.49	0.48
1:H:149:THR:C	1:H:151:ASN:H	2.20	0.48
1:C:127:VAL:C	1:C:128:LEU:HD12	2.39	0.47
1:E:129:GLU:HG2	1:E:192:THR:HG23	1.95	0.47
1:F:294:ASP:O	1:F:298:GLN:HG2	2.14	0.47
1:H:105:ARG:HD3	1:I:77:GLU:OE2	2.13	0.47
1:I:53:ASP:O	1:I:96:PRO:HG3	2.14	0.47
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.95	0.47
1:A:149:THR:OG1	1:A:165:LYS:HE2	2.14	0.47
1:E:36:ASP:HB2	1:E:107:LEU:HD13	1.97	0.47
1:G:112:ASN:ND2	1:G:125:GLN:O	2.46	0.47
1:G:299:ARG:HA	1:G:301:ARG:HG3	1.95	0.47
1:A:80:ASN:ND2	1:A:110:PHE:HB3	2.28	0.47
1:A:91:ARG:HH22	2:B:1318:ZPC:H23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HD13	1:B:190:ARG:HB3	1.96	0.47
1:G:122:ASP:OD2	1:G:199:ARG:NH2	2.47	0.47
1:H:253:LEU:HG	1:H:254:PRO:HD2	1.96	0.47
1:J:36:ASP:HB2	1:J:107:LEU:HD13	1.95	0.47
1:A:286:ARG:HA	1:A:286:ARG:HD3	1.61	0.47
1:J:136:ASN:HB2	1:J:187:GLU:O	2.15	0.47
1:A:212:LEU:HD23	1:A:245:TYR:CE1	2.50	0.47
1:B:131:GLU:OE1	1:B:190:ARG:NH2	2.46	0.47
1:B:293:ASP:O	1:B:295:LEU:N	2.47	0.47
1:E:285:HIS:O	1:E:287:GLN:NE2	2.43	0.47
1:F:300:CYS:HB2	1:F:303:ALA:HB3	1.96	0.47
1:H:91:ARG:NH2	2:I:1318:ZPC:H23	2.28	0.47
1:H:227:SER:HB3	1:H:230:GLU:CG	2.44	0.47
1:C:157:ILE:HA	1:C:157:ILE:HD13	1.70	0.47
1:C:263:ASP:O	1:C:267:ILE:HG12	2.14	0.47
1:F:48:ARG:HB2	1:F:48:ARG:NH1	2.30	0.47
1:C:110:PHE:CE2	1:C:128:LEU:HG	2.49	0.47
1:D:47:PRO:HA	1:D:98:GLY:HA2	1.95	0.47
1:E:48:ARG:NH1	1:E:48:ARG:HB2	2.30	0.47
1:E:211:PRO:O	1:E:215:ILE:HG12	2.14	0.47
1:F:22:LYS:HG2	1:F:24:TYR:CD1	2.50	0.47
1:H:82:VAL:HG23	1:H:111:SER:HB2	1.97	0.47
1:H:95:PHE:HB2	1:H:99:ARG:HG2	1.97	0.47
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.50	0.47
1:H:302:LEU:C	1:H:305:PRO:HD2	2.40	0.47
1:I:294:ASP:O	1:I:298:GLN:HG2	2.14	0.47
1:A:247:PHE:HA	1:E:248:TYR:HD1	1.80	0.47
1:B:132:PRO:HG3	1:B:140:LEU:HD22	1.97	0.47
1:B:313:CYS:HA	1:B:316:VAL:HG23	1.97	0.47
1:E:133:PHE:HA	2:E:1318:ZPC:H01	1.95	0.47
1:H:232:LEU:HD23	1:H:236:PHE:HE2	1.79	0.47
1:J:304:PHE:CD1	1:J:304:PHE:C	2.92	0.47
1:J:300:CYS:HB2	1:J:303:ALA:HB3	1.96	0.47
1:H:241:THR:HA	1:I:240:LEU:HD23	1.97	0.47
1:I:48:ARG:HB2	1:I:48:ARG:NH1	2.29	0.47
1:A:81:VAL:O	1:E:105:ARG:NH2	2.48	0.46
1:A:157:ILE:HD11	1:B:117:ARG:HE	1.79	0.46
1:C:145:ILE:HG23	1:C:168:THR:CG2	2.45	0.46
1:D:125:GLN:NE2	1:D:194:ARG:HD3	2.30	0.46
1:F:91:ARG:HB2	1:G:133:PHE:CE2	2.48	0.46
1:F:224:TRP:CZ2	1:F:301:ARG:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:ILE:HG21	1:H:191:ILE:HG12	1.97	0.46
1:C:178:LEU:HD12	1:C:180:SER:CB	2.41	0.46
1:D:294:ASP:O	1:D:298:GLN:HG2	2.15	0.46
1:D:299:ARG:C	1:D:301:ARG:H	2.23	0.46
1:E:136:ASN:ND2	1:E:185:GLN:HB2	2.29	0.46
1:E:253:LEU:HG	1:E:254:PRO:HD2	1.97	0.46
1:G:287:GLN:HB3	1:G:292:GLU:HB3	1.98	0.46
1:C:157:ILE:HD11	1:D:115:ASP:CG	2.40	0.46
1:J:21:ASN:HD21	1:J:38:TYR:HE1	1.61	0.46
1:I:212:LEU:HD12	1:I:265:MET:SD	2.55	0.46
1:B:225:LEU:HD12	1:B:231:ARG:HA	1.97	0.46
1:C:212:LEU:HB2	1:C:245:TYR:HH	1.81	0.46
1:F:155:GLU:OE2	1:F:161:TRP:HB3	2.16	0.46
1:I:114:MET:HE2	1:I:116:PHE:HZ	1.81	0.46
1:I:149:THR:C	1:I:151:ASN:H	2.24	0.46
1:J:224:TRP:CH2	1:J:301:ARG:HB3	2.51	0.46
1:E:178:LEU:HD13	1:E:178:LEU:HA	1.86	0.46
1:F:149:THR:C	1:F:151:ASN:H	2.23	0.46
1:G:132:PRO:HD3	1:G:142:PHE:CE2	2.51	0.46
1:I:145:ILE:HD12	1:I:191:ILE:HG23	1.98	0.46
1:B:72:TRP:CZ2	1:B:140:LEU:HD12	2.50	0.46
1:D:157:ILE:HD11	1:E:117:ARG:NE	2.31	0.46
1:H:78:PHE:HB3	1:H:81:VAL:HB	1.97	0.46
1:J:58:VAL:HB	1:J:92:LEU:HB2	1.98	0.46
1:J:183:PRO:C	1:J:185:GLN:H	2.23	0.46
1:D:95:PHE:HE1	1:D:101:ILE:HD12	1.81	0.46
1:H:155:GLU:OE2	1:H:161:TRP:HB3	2.16	0.46
1:A:267:ILE:HD12	1:E:206:TRP:O	2.16	0.46
1:B:91:ARG:HB2	1:C:133:PHE:CE2	2.50	0.46
1:C:300:CYS:HB2	1:C:303:ALA:HB3	1.97	0.46
1:H:72:TRP:CZ2	1:H:74:PRO:HB3	2.51	0.46
1:I:66:TRP:O	1:I:71:LEU:HB2	2.15	0.46
1:I:145:ILE:HD12	1:I:191:ILE:HG21	1.97	0.46
1:I:221:SER:HB2	1:J:281:ILE:HD11	1.96	0.46
1:B:225:LEU:HD21	1:C:232:LEU:HD22	1.98	0.45
1:D:107:LEU:HD12	1:D:108:GLY:N	2.31	0.45
1:E:26:VAL:HG22	1:E:33:TYR:HB3	1.98	0.45
1:H:210:LEU:HB3	1:H:211:PRO:HD3	1.98	0.45
1:J:114:MET:CE	1:J:124:GLN:HG2	2.46	0.45
1:B:289:ASN:OD1	1:B:292:GLU:HB2	2.16	0.45
1:D:80:ASN:ND2	1:D:111:SER:O	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.34	0.45
1:G:27:ASN:HB3	1:G:32:THR:HB	1.98	0.45
1:I:143:SER:OG	1:I:144:ASP:N	2.49	0.45
1:B:54:LYS:HB3	1:B:55:PRO:HD2	1.99	0.45
1:B:58:VAL:HB	1:B:92:LEU:HB2	1.98	0.45
1:B:145:ILE:HG23	1:B:168:THR:CG2	2.46	0.45
1:C:227:SER:HB3	1:C:230:GLU:CG	2.45	0.45
1:D:133:PHE:CD1	2:D:1318:ZPC:H07A	2.51	0.45
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.97	0.45
1:G:87:THR:HG21	1:G:90:LYS:HE3	1.98	0.45
1:H:221:SER:HB2	1:I:281:ILE:HD11	1.97	0.45
1:H:295:LEU:O	1:H:299:ARG:HB2	2.16	0.45
1:D:112:ASN:ND2	1:D:125:GLN:O	2.49	0.45
1:F:28:THR:HB	1:F:256:LEU:HD21	1.98	0.45
1:F:289:ASN:OD1	1:F:292:GLU:HB2	2.17	0.45
1:G:212:LEU:HD12	1:G:265:MET:HB3	1.99	0.45
1:H:179:SER:OG	1:H:180:SER:N	2.49	0.45
1:H:216:ILE:HD12	1:H:269:GLY:HA2	1.99	0.45
1:I:199:ARG:O	1:I:201:PRO:HD3	2.16	0.45
1:A:155:GLU:HB3	1:A:161:TRP:CD1	2.52	0.45
1:C:295:LEU:HA	1:C:298:GLN:OE1	2.16	0.45
1:E:92:LEU:HA	1:E:92:LEU:HD23	1.76	0.45
1:F:210:LEU:HB3	1:F:211:PRO:CD	2.47	0.45
1:I:211:PRO:HB3	1:J:270:TYR:CD2	2.52	0.45
1:A:114:MET:HE2	1:A:116:PHE:CZ	2.50	0.45
1:B:312:GLY:O	1:B:315:LEU:HB2	2.17	0.45
1:C:27:ASN:HB3	1:C:32:THR:HB	1.98	0.45
1:D:114:MET:HE2	1:D:116:PHE:CZ	2.51	0.45
1:D:181:VAL:HG11	2:D:1318:ZPC:CL	2.53	0.45
1:I:253:LEU:HD21	1:I:262:ILE:CD1	2.46	0.45
1:C:177:HIS:C	1:C:179:SER:H	2.24	0.45
1:D:92:LEU:HA	1:D:92:LEU:HD23	1.74	0.45
1:F:16:VAL:O	1:F:145:ILE:HA	2.16	0.45
1:F:21:ASN:HD21	1:F:38:TYR:HE1	1.65	0.45
1:J:276:ALA:HB2	1:J:304:PHE:HZ	1.80	0.45
1:J:295:LEU:O	1:J:299:ARG:HB2	2.16	0.45
1:C:146:GLN:HG3	1:C:148:TYR:OH	2.16	0.45
1:D:157:ILE:HD13	1:D:157:ILE:HA	1.76	0.45
1:F:55:PRO:HB3	1:F:95:PHE:CD1	2.52	0.45
1:F:224:TRP:CE2	1:F:301:ARG:HD3	2.52	0.45
1:G:89:ASN:HB2	1:H:133:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:ASN:HD21	1:I:38:TYR:HE1	1.64	0.45
1:I:31:GLN:HG2	1:I:114:MET:HB2	1.98	0.45
1:J:227:SER:O	1:J:231:ARG:HD3	2.17	0.45
1:J:228:PHE:HA	1:J:231:ARG:HH11	1.82	0.45
1:J:304:PHE:C	1:J:304:PHE:HD1	2.24	0.45
1:A:162:ILE:HD13	1:A:197:ALA:HB2	1.98	0.45
1:B:293:ASP:O	1:B:294:ASP:C	2.60	0.45
1:D:62:GLN:NE2	1:E:67:ILE:HG22	2.32	0.45
1:H:33:TYR:OH	1:H:127:VAL:N	2.39	0.45
1:B:252:ILE:HG13	1:C:250:SER:HB3	1.99	0.45
1:H:212:LEU:CD1	1:H:265:MET:HB3	2.46	0.45
1:A:236:PHE:HZ	1:E:221:SER:OG	2.00	0.44
1:A:294:ASP:C	1:A:296:LEU:N	2.75	0.44
1:A:299:ARG:C	1:A:301:ARG:H	2.25	0.44
1:C:20:ILE:HB	1:C:149:THR:HG22	1.98	0.44
1:C:179:SER:OG	1:C:180:SER:N	2.50	0.44
1:F:248:TYR:HE1	1:G:250:SER:OG	2.00	0.44
1:H:299:ARG:C	1:H:301:ARG:H	2.25	0.44
1:B:131:GLU:OE1	1:B:190:ARG:NE	2.46	0.44
1:H:181:VAL:HG21	2:H:1318:ZPC:CL	2.54	0.44
1:I:149:THR:O	1:I:151:ASN:N	2.47	0.44
1:A:132:PRO:O	2:A:1318:ZPC:H01A	2.17	0.44
1:D:66:TRP:HB3	1:D:71:LEU:HD12	1.98	0.44
1:E:149:THR:C	1:E:151:ASN:H	2.25	0.44
1:G:24:TYR:CE2	1:G:34:LYS:HD2	2.53	0.44
1:G:40:VAL:HG21	2:H:1318:ZPC:H27	1.98	0.44
1:H:24:TYR:CE2	1:H:34:LYS:HD2	2.52	0.44
1:I:80:ASN:OD1	1:I:129:GLU:N	2.50	0.44
1:J:179:SER:O	1:J:181:VAL:N	2.50	0.44
1:A:86:ASP:HB3	1:A:107:LEU:HB3	1.99	0.44
1:B:50:THR:HB	1:B:56:LEU:HB2	1.99	0.44
1:B:63:ILE:HD12	1:B:90:LYS:HB3	1.98	0.44
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.76	0.44
1:C:273:ILE:O	1:C:277:ILE:HG12	2.18	0.44
1:G:260:THR:HG23	1:G:263:ASP:OD2	2.18	0.44
1:J:294:ASP:HB2	1:J:297:ILE:CG2	2.41	0.44
1:A:130:LEU:HA	1:A:130:LEU:HD23	1.67	0.44
1:C:295:LEU:O	1:C:299:ARG:HB2	2.17	0.44
1:E:301:ARG:O	1:E:305:PRO:HG2	2.18	0.44
1:F:76:LEU:HB3	1:F:130:LEU:HD21	2.00	0.44
1:A:77:GLU:OE1	2:A:1318:ZPC:H01	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PHE:CG	1:F:120:PRO:HA	2.53	0.44
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.98	0.44
1:F:294:ASP:HB2	1:F:297:ILE:CG2	2.45	0.44
1:J:114:MET:HE3	1:J:124:GLN:HG2	2.00	0.44
1:J:133:PHE:HA	2:J:1318:ZPC:H01A	1.99	0.44
1:B:120:PRO:HD2	1:B:121:PHE:CE2	2.52	0.44
1:E:289:ASN:OD1	1:E:292:GLU:N	2.51	0.44
1:C:227:SER:HB3	1:C:230:GLU:HG3	2.00	0.44
1:C:249:THR:O	1:C:253:LEU:HB2	2.18	0.44
1:E:142:PHE:HB3	1:E:170:ILE:HD13	2.00	0.44
1:G:168:THR:HG22	1:G:169:HIS:N	2.32	0.44
1:H:26:VAL:HG13	1:H:114:MET:HE1	2.00	0.44
1:H:157:ILE:HD11	1:I:115:ASP:CG	2.43	0.44
1:J:112:ASN:ND2	1:J:125:GLN:O	2.51	0.44
1:A:211:PRO:O	1:A:215:ILE:HG12	2.17	0.44
1:A:248:TYR:HA	1:B:247:PHE:CE1	2.52	0.44
1:B:51:PRO:HD2	1:B:56:LEU:HG	2.00	0.44
1:C:120:PRO:HD2	1:C:121:PHE:CE2	2.53	0.44
1:D:224:TRP:CH2	1:D:301:ARG:HB3	2.51	0.44
1:G:147:VAL:HG21	1:G:193:VAL:HG13	1.99	0.44
1:G:174:ARG:HH11	1:G:174:ARG:HB3	1.82	0.44
1:H:157:ILE:HA	1:H:157:ILE:HD13	1.68	0.44
1:I:210:LEU:HB3	1:I:211:PRO:CD	2.47	0.44
1:A:147:VAL:HG21	1:A:193:VAL:HG13	2.00	0.43
1:B:95:PHE:HB2	1:B:99:ARG:HG2	1.99	0.43
1:B:241:THR:HA	1:C:240:LEU:HD23	1.99	0.43
1:C:248:TYR:HA	1:D:247:PHE:CE1	2.53	0.43
1:G:89:ASN:O	1:G:104:ALA:HA	2.17	0.43
1:H:56:LEU:HD12	1:H:94:LEU:HD12	1.99	0.43
1:I:212:LEU:HD21	1:I:266:ILE:HD13	2.00	0.43
1:A:223:PHE:CE2	1:A:304:PHE:CE1	3.02	0.43
1:A:236:PHE:CD2	1:E:234:THR:CG2	3.01	0.43
1:B:155:GLU:OE2	1:B:161:TRP:HB3	2.18	0.43
1:B:157:ILE:HD11	1:C:115:ASP:OD2	2.18	0.43
1:C:28:THR:HG22	1:C:116:PHE:CE2	2.53	0.43
1:C:221:SER:OG	1:D:236:PHE:HZ	2.01	0.43
1:I:95:PHE:HE2	1:I:101:ILE:HD12	1.83	0.43
1:J:95:PHE:HB2	1:J:99:ARG:HG2	1.99	0.43
1:G:263:ASP:O	1:G:267:ILE:HG12	2.17	0.43
1:J:223:PHE:HE2	1:J:304:PHE:CE1	2.36	0.43
1:J:299:ARG:C	1:J:301:ARG:H	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:OE1	1:A:190:ARG:NH2	2.39	0.43
1:A:155:GLU:OE2	1:A:161:TRP:HB3	2.18	0.43
1:A:285:HIS:C	1:A:287:GLN:HG3	2.43	0.43
1:B:220:TRP:CE3	1:B:305:PRO:HB3	2.53	0.43
1:C:212:LEU:HD23	1:C:245:TYR:CD1	2.54	0.43
1:D:149:THR:O	1:D:151:ASN:N	2.45	0.43
1:E:58:VAL:HB	1:E:92:LEU:HB2	1.99	0.43
1:G:157:ILE:HD13	1:G:157:ILE:HA	1.75	0.43
1:H:26:VAL:HG22	1:H:33:TYR:HB3	2.01	0.43
1:A:173:ILE:HD13	1:A:190:ARG:CB	2.49	0.43
1:F:211:PRO:O	1:F:215:ILE:HG12	2.19	0.43
1:G:257:PRO:HG2	1:G:258:TYR:CD2	2.53	0.43
1:H:136:ASN:H	1:H:136:ASN:HD22	1.66	0.43
1:I:178:LEU:HD12	1:I:180:SER:HB3	2.00	0.43
1:J:301:ARG:O	1:J:305:PRO:HG2	2.18	0.43
1:A:227:SER:HB3	1:A:230:GLU:CD	2.43	0.43
1:B:223:PHE:HE2	1:B:304:PHE:CE1	2.36	0.43
1:D:38:TYR:CE2	2:E:1318:ZPC:H06A	2.54	0.43
1:H:163:ARG:HA	1:H:163:ARG:HD3	1.61	0.43
1:H:173:ILE:O	1:H:187:GLU:HA	2.19	0.43
1:I:89:ASN:HB2	1:J:133:PHE:CD1	2.54	0.43
1:A:177:HIS:CE1	1:E:148:TYR:CD1	3.06	0.43
1:A:227:SER:HB3	1:A:230:GLU:HG3	2.00	0.43
1:B:211:PRO:HB3	1:C:270:TYR:CD2	2.53	0.43
1:C:219:SER:HA	1:C:238:LEU:HD21	1.99	0.43
1:I:181:VAL:HG11	2:I:1318:ZPC:CL	2.56	0.43
1:A:89:ASN:HB2	1:B:133:PHE:CE1	2.54	0.43
1:B:125:GLN:NE2	1:B:194:ARG:HD3	2.33	0.43
1:C:150:GLU:OE1	2:D:1318:ZPC:H17	2.19	0.43
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.82	0.43
1:J:279:LEU:HD13	1:J:300:CYS:SG	2.59	0.43
1:A:273:ILE:O	1:A:277:ILE:HG12	2.19	0.43
1:C:76:LEU:HB3	1:C:130:LEU:HD21	2.00	0.43
1:D:119:PHE:HA	1:D:122:ASP:OD1	2.19	0.43
1:D:248:TYR:HE1	1:E:250:SER:OG	1.97	0.43
1:D:312:GLY:O	1:D:316:VAL:HG23	2.18	0.43
1:H:130:LEU:HD23	1:H:130:LEU:HA	1.90	0.43
1:H:136:ASN:HD22	1:H:136:ASN:N	2.16	0.43
1:H:227:SER:HB3	1:H:230:GLU:HG3	2.01	0.43
1:I:162:ILE:HD13	1:I:162:ILE:HA	1.82	0.43
1:I:299:ARG:C	1:I:301:ARG:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.36	0.42
1:B:145:ILE:O	1:B:168:THR:HG21	2.19	0.42
1:B:238:LEU:HD13	1:C:236:PHE:CD2	2.54	0.42
1:F:79:ILE:N	1:F:129:GLU:O	2.44	0.42
1:G:249:THR:O	1:G:253:LEU:HB2	2.19	0.42
1:H:294:ASP:HB2	1:H:297:ILE:CG2	2.48	0.42
1:J:118:LEU:HA	1:J:261:VAL:HG23	2.01	0.42
1:J:157:ILE:HD13	1:J:157:ILE:HA	1.80	0.42
1:A:144:ASP:C	1:A:144:ASP:OD1	2.62	0.42
1:A:277:ILE:O	1:A:281:ILE:HD12	2.20	0.42
1:B:212:LEU:HD11	1:B:265:MET:HB3	2.00	0.42
1:C:28:THR:HB	1:C:256:LEU:CD2	2.49	0.42
1:C:81:VAL:HG11	1:C:85:PRO:HG3	2.00	0.42
1:C:145:ILE:HG12	1:C:146:GLN:N	2.32	0.42
1:D:117:ARG:HH11	1:D:117:ARG:HD3	1.70	0.42
1:D:301:ARG:O	1:D:305:PRO:HG2	2.19	0.42
1:E:117:ARG:O	1:E:260:THR:HA	2.19	0.42
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.80	0.42
1:J:28:THR:HG22	1:J:116:PHE:CZ	2.54	0.42
1:A:145:ILE:HG21	1:A:191:ILE:HG12	2.01	0.42
1:E:177:HIS:C	1:E:179:SER:H	2.26	0.42
1:F:216:ILE:HG21	1:F:308:PHE:CZ	2.54	0.42
1:G:84:SER:HA	1:G:85:PRO:HD3	1.70	0.42
1:A:26:VAL:CG1	1:A:114:MET:HE1	2.49	0.42
1:A:173:ILE:O	1:A:187:GLU:HA	2.18	0.42
1:A:293:ASP:O	1:A:295:LEU:N	2.52	0.42
1:D:210:LEU:HB3	1:D:211:PRO:CD	2.49	0.42
1:E:157:ILE:HD13	1:E:157:ILE:HA	1.89	0.42
1:E:285:HIS:C	1:E:287:GLN:HG3	2.44	0.42
1:F:212:LEU:HD23	1:F:245:TYR:CD2	2.54	0.42
1:G:66:TRP:HB3	1:G:71:LEU:HD12	2.02	0.42
1:G:71:LEU:HD11	1:G:94:LEU:HD21	2.01	0.42
2:G:1318:ZPC:C08	2:G:1318:ZPC:N22	2.83	0.42
1:H:62:GLN:NE2	1:I:68:ASN:OD1	2.43	0.42
1:I:260:THR:O	1:I:263:ASP:HB2	2.19	0.42
1:A:133:PHE:CE2	1:E:91:ARG:HB2	2.54	0.42
1:B:302:LEU:C	1:B:305:PRO:HD2	2.44	0.42
1:F:18:ILE:O	1:F:147:VAL:HA	2.20	0.42
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.85	0.42
1:I:114:MET:HB3	1:I:116:PHE:CE2	2.53	0.42
1:A:21:ASN:ND2	1:A:37:GLY:HA2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASN:HA	1:B:201:PRO:HD3	1.84	0.42
1:D:84:SER:HA	1:D:85:PRO:HD3	1.78	0.42
1:E:93:MET:HE2	1:E:95:PHE:CZ	2.54	0.42
1:F:114:MET:HE2	1:F:124:GLN:HG2	2.01	0.42
1:F:157:ILE:HD13	1:F:157:ILE:HA	1.82	0.42
1:I:157:ILE:HD11	1:J:117:ARG:HE	1.85	0.42
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.74	0.42
1:A:212:LEU:HD12	1:A:265:MET:SD	2.60	0.42
1:B:232:LEU:O	1:B:235:SER:OG	2.35	0.42
1:G:289:ASN:OD1	1:G:292:GLU:HB2	2.19	0.42
1:H:300:CYS:HB2	1:H:303:ALA:HB3	2.02	0.42
1:I:263:ASP:O	1:I:267:ILE:HG12	2.20	0.42
1:J:27:ASN:HB3	1:J:32:THR:HB	2.02	0.42
1:J:145:ILE:HG23	1:J:168:THR:CG2	2.49	0.42
1:B:63:ILE:CD1	1:B:90:LYS:HB3	2.50	0.42
1:F:284:HIS:CE1	1:J:226:GLU:OE2	2.65	0.42
1:G:92:LEU:HA	1:G:92:LEU:HD23	1.78	0.42
1:H:64:GLU:HA	1:H:67:ILE:HD12	2.01	0.42
1:J:289:ASN:OD1	1:J:290:GLY:N	2.48	0.42
1:A:157:ILE:HD12	1:B:115:ASP:HA	2.01	0.42
1:A:206:TRP:O	1:B:267:ILE:HD12	2.20	0.42
1:B:112:ASN:ND2	1:B:125:GLN:O	2.53	0.42
1:C:212:LEU:HD23	1:C:245:TYR:CE1	2.55	0.42
1:C:289:ASN:OD1	1:C:290:GLY:N	2.48	0.42
1:D:29:LEU:HD23	1:D:29:LEU:HA	1.74	0.42
1:D:40:VAL:HG11	2:E:1318:ZPC:C26	2.50	0.42
1:H:155:GLU:HB3	1:H:161:TRP:CD1	2.55	0.42
1:I:216:ILE:HD12	1:I:269:GLY:HA2	2.02	0.42
1:A:138:GLN:OE1	1:A:185:GLN:HB3	2.20	0.42
1:B:155:GLU:HB3	1:B:161:TRP:CD1	2.55	0.42
1:B:163:ARG:HD3	1:B:163:ARG:HA	1.70	0.42
1:C:145:ILE:HG21	1:C:191:ILE:HG23	2.02	0.42
1:C:299:ARG:C	1:C:301:ARG:H	2.28	0.42
1:D:227:SER:HB3	1:D:230:GLU:CG	2.49	0.42
1:F:23:ILE:HD11	1:F:195:ILE:HD13	2.02	0.42
1:F:214:LEU:HD22	1:G:274:PHE:CG	2.55	0.42
1:H:147:VAL:HG21	1:H:193:VAL:HG13	2.02	0.42
1:H:204:TYR:O	1:H:208:PHE:HB2	2.20	0.42
1:H:221:SER:OG	1:I:236:PHE:HZ	2.02	0.42
1:H:277:ILE:O	1:H:281:ILE:HD12	2.19	0.42
1:H:289:ASN:OD1	1:H:290:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:O	1:A:306:LEU:HG	2.20	0.41
2:A:1318:ZPC:C23	1:E:91:ARG:HH22	2.33	0.41
1:B:276:ALA:HB2	1:B:304:PHE:HZ	1.85	0.41
1:E:55:PRO:HB3	1:E:95:PHE:CD2	2.55	0.41
1:F:304:PHE:CD1	1:F:304:PHE:C	2.98	0.41
1:G:19:PHE:CE2	2:H:1318:ZPC:C15	3.03	0.41
1:G:163:ARG:HA	1:G:163:ARG:HD3	1.68	0.41
1:B:89:ASN:HB2	1:C:133:PHE:CE1	2.55	0.41
1:B:223:PHE:CE2	1:B:304:PHE:CE1	3.09	0.41
1:D:72:TRP:CH2	1:D:74:PRO:HG3	2.55	0.41
1:E:114:MET:HE2	1:E:116:PHE:HZ	1.85	0.41
1:F:120:PRO:HD2	1:F:121:PHE:CE2	2.55	0.41
1:G:72:TRP:CZ2	1:G:74:PRO:HB3	2.55	0.41
1:B:44:THR:HA	1:B:99:ARG:HA	2.01	0.41
1:B:60:ASN:OD1	1:B:89:ASN:HA	2.19	0.41
1:F:257:PRO:HD2	1:F:258:TYR:CE1	2.54	0.41
1:F:281:ILE:HD11	1:J:221:SER:HB2	2.01	0.41
1:G:205:LEU:HA	1:G:209:ILE:HG12	2.01	0.41
1:H:120:PRO:HD2	1:H:121:PHE:CE2	2.55	0.41
1:H:295:LEU:HD12	1:H:298:GLN:CD	2.45	0.41
1:I:178:LEU:HD13	1:I:178:LEU:HA	1.84	0.41
1:E:225:LEU:HD13	1:E:230:GLU:O	2.20	0.41
1:F:178:LEU:HD12	1:F:180:SER:CB	2.48	0.41
1:G:175:TYR:O	1:G:186:ASN:ND2	2.40	0.41
1:I:247:PHE:CD2	1:J:247:PHE:CE2	3.07	0.41
1:A:12:VAL:HG11	1:A:72:TRP:CZ3	2.55	0.41
1:C:60:ASN:HB2	1:C:61:THR:H	1.57	0.41
1:H:58:VAL:HB	1:H:92:LEU:HB2	2.01	0.41
1:B:127:VAL:HG22	1:B:194:ARG:HG2	2.02	0.41
1:E:178:LEU:HD12	1:E:180:SER:CB	2.48	0.41
1:E:295:LEU:O	1:E:299:ARG:HB2	2.20	0.41
1:G:18:ILE:CD1	1:G:39:ILE:HG12	2.42	0.41
1:I:248:TYR:HE1	1:J:250:SER:OG	2.03	0.41
1:J:294:ASP:O	1:J:298:GLN:HG2	2.21	0.41
1:A:64:GLU:CG	1:E:61:THR:HG21	2.50	0.41
1:A:263:ASP:O	1:A:267:ILE:HG12	2.20	0.41
1:A:294:ASP:HB3	1:A:297:ILE:H	1.86	0.41
1:B:86:ASP:N	1:B:107:LEU:O	2.49	0.41
1:C:97:ASP:OD1	1:C:99:ARG:HD3	2.20	0.41
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.39	0.41
1:F:14:VAL:HG22	1:F:43:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:HIS:CD2	1:J:224:TRP:HD1	2.39	0.41
1:G:153:ASP:HB3	1:G:154:ASN:OD1	2.20	0.41
1:J:227:SER:HB3	1:J:230:GLU:HG3	2.02	0.41
1:A:146:GLN:CD	1:A:146:GLN:N	2.79	0.41
1:A:216:ILE:HD12	1:A:216:ILE:HG23	1.78	0.41
1:B:71:LEU:HD11	1:B:94:LEU:HD21	2.02	0.41
1:C:232:LEU:HD11	1:C:281:ILE:HD11	2.01	0.41
1:C:261:VAL:HA	1:C:264:GLN:NE2	2.35	0.41
1:D:16:VAL:O	1:D:145:ILE:HA	2.21	0.41
1:G:40:VAL:HG11	2:H:1318:ZPC:C26	2.51	0.41
1:I:114:MET:HE2	1:I:116:PHE:CZ	2.55	0.41
1:A:247:PHE:CG	1:B:247:PHE:CE2	3.08	0.41
1:B:48:ARG:HB2	1:B:48:ARG:NH1	2.36	0.41
1:B:79:ILE:HD13	1:B:79:ILE:HA	1.91	0.41
1:B:102:TYR:CD1	1:B:102:TYR:C	2.99	0.41
1:B:106:PHE:CD1	1:B:106:PHE:C	2.98	0.41
1:B:122:ASP:OD2	1:B:199:ARG:NH2	2.45	0.41
1:B:149:THR:C	1:B:151:ASN:H	2.22	0.41
1:B:294:ASP:O	1:B:296:LEU:N	2.54	0.41
1:C:62:GLN:O	1:C:66:TRP:HD1	2.02	0.41
1:C:82:VAL:HG23	1:C:111:SER:HB2	2.02	0.41
1:C:136:ASN:OD1	1:C:185:GLN:HB2	2.21	0.41
1:F:66:TRP:O	1:F:71:LEU:HB2	2.21	0.41
1:F:114:MET:CE	1:F:124:GLN:HG2	2.50	0.41
1:F:133:PHE:CD1	2:F:1318:ZPC:H01	2.55	0.41
1:G:58:VAL:HB	1:G:92:LEU:HB2	2.02	0.41
1:H:29:LEU:HD23	1:H:29:LEU:HA	1.76	0.41
1:J:212:LEU:CD1	1:J:265:MET:HB3	2.50	0.41
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.77	0.41
1:B:219:SER:HA	1:B:238:LEU:HD21	2.03	0.41
1:D:39:ILE:HG21	1:D:39:ILE:HD13	1.82	0.41
1:D:62:GLN:OE1	1:D:65:ARG:HD3	2.21	0.41
1:G:297:ILE:HD13	1:G:297:ILE:HG21	1.89	0.41
1:H:232:LEU:CD2	1:H:236:PHE:HE2	2.34	0.41
1:J:249:THR:O	1:J:253:LEU:HB2	2.21	0.41
1:C:16:VAL:O	1:C:145:ILE:HA	2.21	0.40
1:C:19:PHE:CE1	1:C:148:TYR:HD2	2.38	0.40
1:C:216:ILE:HD12	1:C:269:GLY:HA2	2.03	0.40
1:E:228:PHE:HA	1:E:231:ARG:NH1	2.37	0.40
1:G:31:GLN:HG2	1:G:114:MET:HB2	2.03	0.40
1:G:61:THR:HG21	1:H:64:GLU:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:LEU:HD13	1:G:178:LEU:HA	1.90	0.40
1:I:84:SER:HA	1:I:85:PRO:HD3	1.78	0.40
1:I:122:ASP:OD1	1:I:122:ASP:N	2.53	0.40
1:I:131:GLU:OE2	1:I:175:TYR:HE2	2.05	0.40
1:I:259:THR:HA	1:I:263:ASP:OD2	2.20	0.40
1:J:149:THR:C	1:J:151:ASN:N	2.79	0.40
1:B:157:ILE:HD13	1:B:157:ILE:HA	1.65	0.40
1:B:224:TRP:HD1	1:C:285:HIS:CD2	2.39	0.40
1:B:227:SER:HB3	1:B:230:GLU:CG	2.51	0.40
1:C:204:TYR:O	1:C:208:PHE:HB2	2.21	0.40
1:D:114:MET:HE2	1:D:116:PHE:HZ	1.85	0.40
1:D:118:LEU:HA	1:D:261:VAL:HG23	2.03	0.40
1:F:50:THR:HG23	1:F:96:PRO:HB3	2.03	0.40
1:G:35:VAL:HG21	1:G:128:LEU:HD11	2.03	0.40
1:H:214:LEU:HD23	1:H:214:LEU:HA	1.86	0.40
1:H:231:ARG:HH11	1:H:231:ARG:HD3	1.73	0.40
1:J:114:MET:HE2	1:J:116:PHE:CZ	2.56	0.40
1:J:312:GLY:O	1:J:316:VAL:HG23	2.21	0.40
1:A:66:TRP:HB3	1:A:71:LEU:HD12	2.04	0.40
1:A:114:MET:HE2	1:A:124:GLN:HG2	2.03	0.40
1:B:249:THR:CG2	1:B:253:LEU:HD22	2.50	0.40
1:C:76:LEU:HB3	1:C:130:LEU:CD2	2.51	0.40
1:G:55:PRO:HB3	1:G:95:PHE:CD1	2.56	0.40
1:H:153:ASP:HB3	1:H:154:ASN:OD1	2.21	0.40
1:A:36:ASP:OD1	1:A:36:ASP:C	2.65	0.40
1:A:233:GLN:O	1:A:236:PHE:HB2	2.20	0.40
1:C:56:LEU:HD22	1:C:56:LEU:HA	1.80	0.40
1:C:122:ASP:CG	1:C:199:ARG:HE	2.29	0.40
1:D:212:LEU:HD12	1:D:265:MET:HB3	2.04	0.40
1:F:133:PHE:CE2	1:J:91:ARG:HB2	2.54	0.40
1:F:299:ARG:C	1:F:301:ARG:H	2.29	0.40
1:G:132:PRO:HG3	1:G:140:LEU:HD22	2.02	0.40
1:G:200:ASN:HA	1:G:201:PRO:HD3	1.96	0.40
1:G:205:LEU:HD23	1:G:205:LEU:HA	1.92	0.40
1:I:238:LEU:HD12	1:I:238:LEU:HA	1.69	0.40
1:I:299:ARG:HA	1:I:301:ARG:HG3	2.04	0.40
1:A:179:SER:OG	1:A:180:SER:N	2.54	0.40
1:A:227:SER:HB3	1:A:230:GLU:CG	2.52	0.40
1:B:157:ILE:HD11	1:C:115:ASP:CG	2.46	0.40
1:D:133:PHE:O	2:D:1318:ZPC:N02	2.55	0.40
1:D:204:TYR:O	1:D:209:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:VAL:HG21	1:E:128:LEU:HD11	2.03	0.40
1:F:117:ARG:HH11	1:F:117:ARG:HD3	1.73	0.40
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.38	0.40
1:H:224:TRP:CE2	1:H:301:ARG:HD3	2.56	0.40

There are no symmetry-related clashes.

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	A	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	3	21
1	B	305/307 (99%)	274 (90%)	21 (7%)	10 (3%)	3	19
1	C	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	3	21
1	D	305/307 (99%)	274 (90%)	22 (7%)	9 (3%)	3	21
1	E	305/307 (99%)	275 (90%)	21 (7%)	9 (3%)	3	21
1	F	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	3	21
1	G	305/307 (99%)	278 (91%)	17 (6%)	10 (3%)	3	19
1	H	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	3	21
1	I	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	3	21
1	J	305/307 (99%)	271 (89%)	25 (8%)	9 (3%)	3	21
All	All	3050/3070 (99%)	2754 (90%)	204 (7%)	92 (3%)	3	21

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	178	LEU
1	A	179	SER

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Mol	Chain	Res	Type
1	A	180	SER
1	B	60	ASN
1	B	166	ALA
1	B	178	LEU
1	B	179	SER
1	B	180	SER
1	C	166	ALA
1	C	178	LEU
1	C	179	SER
1	C	180	SER
1	D	60	ASN
1	D	166	ALA
1	D	178	LEU
1	D	179	SER
1	D	180	SER
1	E	60	ASN
1	E	178	LEU
1	E	179	SER
1	E	180	SER
1	F	60	ASN
1	F	178	LEU
1	F	179	SER
1	F	180	SER
1	G	60	ASN
1	G	166	ALA
1	G	178	LEU
1	G	179	SER
1	G	180	SER
1	H	60	ASN
1	H	166	ALA
1	H	178	LEU
1	H	179	SER
1	H	180	SER
1	I	60	ASN
1	I	166	ALA
1	I	178	LEU
1	I	179	SER
1	I	180	SER
1	J	60	ASN
1	J	178	LEU
1	J	179	SER
1	J	180	SER

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Mol	Chain	Res	Type
1	A	53	ASP
1	B	53	ASP
1	B	152	ILE
1	C	53	ASP
1	C	152	ILE
1	D	152	ILE
1	E	53	ASP
1	E	152	ILE
1	F	53	ASP
1	F	152	ILE
1	G	53	ASP
1	G	152	ILE
1	G	294	ASP
1	H	53	ASP
1	H	153	ASP
1	I	152	ILE
1	J	53	ASP
1	J	152	ILE
1	A	152	ILE
1	A	153	ASP
1	A	294	ASP
1	B	150	GLU
1	B	153	ASP
1	B	294	ASP
1	C	294	ASP
1	D	53	ASP
1	D	150	GLU
1	D	153	ASP
1	E	153	ASP
1	F	294	ASP
1	G	153	ASP
1	H	150	GLU
1	I	53	ASP
1	I	150	GLU
1	J	153	ASP
1	C	153	ASP
1	E	200	ASN
1	F	150	GLU
1	F	153	ASP
1	J	150	GLU
1	J	294	ASP
1	A	166	ALA

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Mol	Chain	Res	Type
1	C	60	ASN
1	G	150	GLU
1	H	152	ILE
1	I	294	ASP
1	E	150	GLU

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%)	245 (89%)	29 (11%)	6	25
1	B	274/275 (100%)	246 (90%)	28 (10%)	7	27
1	C	274/275 (100%)	244 (89%)	30 (11%)	6	24
1	D	274/275 (100%)	246 (90%)	28 (10%)	7	27
1	E	274/275 (100%)	247 (90%)	27 (10%)	7	28
1	F	274/275 (100%)	247 (90%)	27 (10%)	7	28
1	G	274/275 (100%)	246 (90%)	28 (10%)	7	27
1	H	274/275 (100%)	246 (90%)	28 (10%)	7	27
1	I	274/275 (100%)	242 (88%)	32 (12%)	5	21
1	J	274/275 (100%)	249 (91%)	25 (9%)	9	32
All	All	2740/2750 (100%)	2458 (90%)	282 (10%)	7	26

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	20	ILE
1	A	28	THR
1	A	32	THR
1	A	56	LEU
1	A	71	LEU
1	A	118	LEU
1	A	122	ASP

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Mol	Chain	Res	Type
1	A	124	GLN
1	A	130	LEU
1	A	134	SER
1	A	136	ASN
1	A	145	ILE
1	A	146	GLN
1	A	157	ILE
1	A	165	LYS
1	A	178	LEU
1	A	180	SER
1	A	212	LEU
1	A	231	ARG
1	A	238	LEU
1	A	240	LEU
1	A	281	ILE
1	A	286	ARG
1	A	291	VAL
1	A	292	GLU
1	A	297	ILE
1	A	302	LEU
1	A	304	PHE
1	B	29	LEU
1	B	32	THR
1	B	39	ILE
1	B	56	LEU
1	B	57	ILE
1	B	71	LEU
1	B	81	VAL
1	B	118	LEU
1	B	122	ASP
1	B	124	GLN
1	B	130	LEU
1	B	134	SER
1	B	145	ILE
1	B	146	GLN
1	B	154	ASN
1	B	157	ILE
1	B	173	ILE
1	B	178	LEU
1	B	180	SER
1	B	212	LEU
1	B	231	ARG

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Mol	Chain	Res	Type
1	B	238	LEU
1	B	240	LEU
1	B	287	GLN
1	B	291	VAL
1	B	292	GLU
1	B	302	LEU
1	B	304	PHE
1	C	29	LEU
1	C	32	THR
1	C	39	ILE
1	C	56	LEU
1	C	71	LEU
1	C	79	ILE
1	C	81	VAL
1	C	87	THR
1	C	118	LEU
1	C	122	ASP
1	C	124	GLN
1	C	130	LEU
1	C	134	SER
1	C	136	ASN
1	C	145	ILE
1	C	146	GLN
1	C	157	ILE
1	C	165	LYS
1	C	178	LEU
1	C	180	SER
1	C	210	LEU
1	C	212	LEU
1	C	222	VAL
1	C	238	LEU
1	C	240	LEU
1	C	291	VAL
1	C	292	GLU
1	C	299	ARG
1	C	302	LEU
1	C	304	PHE
1	D	29	LEU
1	D	32	THR
1	D	56	LEU
1	D	61	THR
1	D	71	LEU

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Mol	Chain	Res	Type
1	D	118	LEU
1	D	122	ASP
1	D	124	GLN
1	D	130	LEU
1	D	134	SER
1	D	145	ILE
1	D	146	GLN
1	D	157	ILE
1	D	165	LYS
1	D	168	THR
1	D	178	LEU
1	D	180	SER
1	D	210	LEU
1	D	212	LEU
1	D	231	ARG
1	D	238	LEU
1	D	240	LEU
1	D	287	GLN
1	D	291	VAL
1	D	292	GLU
1	D	299	ARG
1	D	302	LEU
1	D	304	PHE
1	E	29	LEU
1	E	32	THR
1	E	39	ILE
1	E	56	LEU
1	E	71	LEU
1	E	118	LEU
1	E	124	GLN
1	E	130	LEU
1	E	134	SER
1	E	145	ILE
1	E	146	GLN
1	E	157	ILE
1	E	165	LYS
1	E	178	LEU
1	E	180	SER
1	E	212	LEU
1	E	216	ILE
1	E	219	SER
1	E	231	ARG

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Mol	Chain	Res	Type
1	E	238	LEU
1	E	240	LEU
1	E	287	GLN
1	E	291	VAL
1	E	292	GLU
1	E	299	ARG
1	E	302	LEU
1	E	304	PHE
1	F	32	THR
1	F	39	ILE
1	F	40	VAL
1	F	56	LEU
1	F	71	LEU
1	F	118	LEU
1	F	122	ASP
1	F	124	GLN
1	F	130	LEU
1	F	134	SER
1	F	145	ILE
1	F	146	GLN
1	F	165	LYS
1	F	173	ILE
1	F	178	LEU
1	F	180	SER
1	F	210	LEU
1	F	231	ARG
1	F	238	LEU
1	F	240	LEU
1	F	258	TYR
1	F	281	ILE
1	F	291	VAL
1	F	292	GLU
1	F	297	ILE
1	F	302	LEU
1	F	304	PHE
1	G	29	LEU
1	G	32	THR
1	G	56	LEU
1	G	61	THR
1	G	107	LEU
1	G	118	LEU
1	G	122	ASP

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Mol	Chain	Res	Type
1	G	123	ARG
1	G	124	GLN
1	G	130	LEU
1	G	134	SER
1	G	136	ASN
1	G	145	ILE
1	G	154	ASN
1	G	174	ARG
1	G	178	LEU
1	G	180	SER
1	G	212	LEU
1	G	222	VAL
1	G	231	ARG
1	G	238	LEU
1	G	240	LEU
1	G	287	GLN
1	G	291	VAL
1	G	292	GLU
1	G	293	ASP
1	G	302	LEU
1	G	304	PHE
1	H	32	THR
1	H	39	ILE
1	H	56	LEU
1	H	61	THR
1	H	71	LEU
1	H	81	VAL
1	H	118	LEU
1	H	122	ASP
1	H	124	GLN
1	H	130	LEU
1	H	134	SER
1	H	136	ASN
1	H	145	ILE
1	H	146	GLN
1	H	154	ASN
1	H	157	ILE
1	H	165	LYS
1	H	178	LEU
1	H	180	SER
1	H	191	ILE
1	H	231	ARG

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Mol	Chain	Res	Type
1	H	238	LEU
1	H	240	LEU
1	H	291	VAL
1	H	292	GLU
1	H	299	ARG
1	H	302	LEU
1	H	304	PHE
1	I	28	THR
1	I	29	LEU
1	I	32	THR
1	I	39	ILE
1	I	56	LEU
1	I	71	LEU
1	I	81	VAL
1	I	118	LEU
1	I	122	ASP
1	I	124	GLN
1	I	130	LEU
1	I	134	SER
1	I	145	ILE
1	I	146	GLN
1	I	157	ILE
1	I	165	LYS
1	I	167	SER
1	I	178	LEU
1	I	180	SER
1	I	189	SER
1	I	210	LEU
1	I	212	LEU
1	I	231	ARG
1	I	238	LEU
1	I	240	LEU
1	I	258	TYR
1	I	281	ILE
1	I	291	VAL
1	I	292	GLU
1	I	297	ILE
1	I	302	LEU
1	I	304	PHE
1	J	29	LEU
1	J	32	THR
1	J	39	ILE

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Mol	Chain	Res	Type
1	J	56	LEU
1	J	61	THR
1	J	71	LEU
1	J	118	LEU
1	J	124	GLN
1	J	130	LEU
1	J	134	SER
1	J	136	ASN
1	J	145	ILE
1	J	146	GLN
1	J	157	ILE
1	J	178	LEU
1	J	180	SER
1	J	210	LEU
1	J	212	LEU
1	J	238	LEU
1	J	240	LEU
1	J	291	VAL
1	J	292	GLU
1	J	299	ARG
1	J	302	LEU
1	J	304	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	136	ASN
1	A	182	GLN
1	A	285	HIS
1	B	21	ASN
1	B	103	ASN
1	B	125	GLN
1	B	182	GLN
1	C	68	ASN
1	C	89	ASN
1	C	136	ASN
1	C	139	GLN
1	C	185	GLN
1	C	284	HIS
1	D	125	GLN
1	D	177	HIS

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Mol	Chain	Res	Type
1	D	182	GLN
1	D	264	GLN
1	D	287	GLN
1	D	298	GLN
1	E	103	ASN
1	E	251	ASN
1	E	285	HIS
1	F	103	ASN
1	F	177	HIS
1	F	233	GLN
1	F	284	HIS
1	F	285	HIS
1	G	136	ASN
1	G	185	GLN
1	G	264	GLN
1	H	136	ASN
1	H	285	HIS
1	H	298	GLN
1	I	125	GLN
1	I	185	GLN
1	I	233	GLN
1	I	284	HIS
1	J	103	ASN
1	J	124	GLN
1	J	136	ASN
1	J	169	HIS
1	J	284	HIS

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

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	ZPC	E	1318	-	29,30,30	2.56	9 (31%)	34,43,43	5.02	26 (76%)
2	ZPC	J	1318	-	29,30,30	2.26	10 (34%)	34,43,43	4.38	21 (61%)
2	ZPC	H	1318	-	29,30,30	2.54	10 (34%)	34,43,43	4.45	21 (61%)
2	ZPC	B	1318	-	29,30,30	2.84	11 (37%)	34,43,43	4.81	20 (58%)
2	ZPC	I	1318	-	29,30,30	2.43	8 (27%)	34,43,43	3.96	23 (67%)
2	ZPC	F	1318	-	29,30,30	2.63	10 (34%)	34,43,43	5.19	24 (70%)
2	ZPC	G	1318	-	29,30,30	2.69	11 (37%)	34,43,43	4.92	25 (73%)
2	ZPC	A	1318	-	29,30,30	2.58	8 (27%)	34,43,43	4.94	20 (58%)
2	ZPC	D	1318	-	29,30,30	2.55	9 (31%)	34,43,43	4.85	19 (55%)
2	ZPC	C	1318	-	29,30,30	2.54	10 (34%)	34,43,43	5.68	21 (61%)

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	ZPC	E	1318	-	-	8/12/38/38	0/4/4/4
2	ZPC	J	1318	-	-	5/12/38/38	0/4/4/4
2	ZPC	H	1318	-	-	9/12/38/38	0/4/4/4
2	ZPC	B	1318	-	-	10/12/38/38	0/4/4/4
2	ZPC	I	1318	-	-	3/12/38/38	0/4/4/4
2	ZPC	F	1318	-	-	6/12/38/38	0/4/4/4
2	ZPC	G	1318	-	-	7/12/38/38	0/4/4/4
2	ZPC	A	1318	-	-	7/12/38/38	0/4/4/4
2	ZPC	D	1318	-	-	5/12/38/38	0/4/4/4
2	ZPC	C	1318	-	-	8/12/38/38	0/4/4/4

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1318	ZPC	C21-N12	6.78	1.51	1.41
2	C	1318	ZPC	C08-N05	6.69	1.47	1.35
2	G	1318	ZPC	C08-N05	6.67	1.47	1.35
2	D	1318	ZPC	C21-N12	6.48	1.50	1.41
2	F	1318	ZPC	C08-N05	6.40	1.46	1.35
2	I	1318	ZPC	C21-N12	6.34	1.50	1.41
2	B	1318	ZPC	C13-N12	6.28	1.49	1.38
2	A	1318	ZPC	C21-N12	6.23	1.50	1.41
2	A	1318	ZPC	C13-N12	6.23	1.49	1.38
2	J	1318	ZPC	C08-N05	6.17	1.46	1.35
2	B	1318	ZPC	C21-N12	6.03	1.50	1.41
2	A	1318	ZPC	C08-N05	6.00	1.46	1.35
2	E	1318	ZPC	C21-N12	5.92	1.49	1.41
2	E	1318	ZPC	C08-N05	5.80	1.45	1.35
2	F	1318	ZPC	C21-N12	5.61	1.49	1.41
2	B	1318	ZPC	C08-N05	5.56	1.45	1.35
2	D	1318	ZPC	C13-N12	5.55	1.48	1.38
2	G	1318	ZPC	C21-N12	5.54	1.49	1.41
2	E	1318	ZPC	C13-N12	5.53	1.48	1.38
2	D	1318	ZPC	C08-N05	5.51	1.45	1.35
2	H	1318	ZPC	C08-N05	5.47	1.45	1.35
2	F	1318	ZPC	C13-N12	5.36	1.48	1.38
2	C	1318	ZPC	C21-N12	5.36	1.49	1.41
2	B	1318	ZPC	C20-C11	5.09	1.55	1.51
2	I	1318	ZPC	C13-N12	5.03	1.47	1.38
2	I	1318	ZPC	C08-N05	4.87	1.44	1.35
2	H	1318	ZPC	C20-N19	4.75	1.40	1.34
2	B	1318	ZPC	C20-N19	4.74	1.40	1.34
2	G	1318	ZPC	C20-C11	4.68	1.55	1.51
2	F	1318	ZPC	C06-N05	-4.67	1.38	1.47
2	J	1318	ZPC	C20-N19	4.59	1.40	1.34
2	E	1318	ZPC	C06-N05	-4.58	1.38	1.47
2	I	1318	ZPC	C06-N05	-4.54	1.38	1.47
2	G	1318	ZPC	C13-N12	4.45	1.46	1.38
2	A	1318	ZPC	O10-C08	4.30	1.42	1.34
2	C	1318	ZPC	O10-C08	4.30	1.42	1.34
2	G	1318	ZPC	C20-N19	4.27	1.39	1.34
2	J	1318	ZPC	C06-N05	-4.19	1.39	1.47
2	J	1318	ZPC	C21-N12	4.13	1.47	1.41
2	D	1318	ZPC	C20-N19	4.13	1.39	1.34
2	B	1318	ZPC	C06-N05	-4.04	1.39	1.47
2	G	1318	ZPC	C27-C26	4.03	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1318	ZPC	C20-N19	3.94	1.39	1.34
2	H	1318	ZPC	O10-C08	3.94	1.42	1.34
2	H	1318	ZPC	C13-N12	3.92	1.45	1.38
2	F	1318	ZPC	O10-C08	3.90	1.42	1.34
2	E	1318	ZPC	C27-C26	3.85	1.45	1.38
2	I	1318	ZPC	C20-N19	3.83	1.39	1.34
2	A	1318	ZPC	C06-N05	-3.82	1.40	1.47
2	B	1318	ZPC	O10-C08	3.82	1.41	1.34
2	C	1318	ZPC	C27-C26	3.76	1.44	1.38
2	D	1318	ZPC	C06-N05	-3.75	1.40	1.47
2	F	1318	ZPC	C27-C26	3.72	1.44	1.38
2	E	1318	ZPC	O10-C08	3.67	1.41	1.34
2	G	1318	ZPC	O10-C08	3.65	1.41	1.34
2	C	1318	ZPC	C13-N12	3.64	1.45	1.38
2	G	1318	ZPC	C26-C24	3.63	1.44	1.38
2	G	1318	ZPC	C06-N05	-3.59	1.40	1.47
2	H	1318	ZPC	C06-N05	-3.57	1.40	1.47
2	C	1318	ZPC	C06-N05	-3.53	1.40	1.47
2	I	1318	ZPC	C27-C26	3.53	1.44	1.38
2	C	1318	ZPC	C26-C24	3.51	1.44	1.38
2	J	1318	ZPC	C13-N12	3.46	1.44	1.38
2	D	1318	ZPC	O10-C08	3.45	1.41	1.34
2	B	1318	ZPC	C26-C24	3.42	1.44	1.38
2	H	1318	ZPC	C27-C26	3.41	1.44	1.38
2	A	1318	ZPC	C27-C26	3.36	1.44	1.38
2	A	1318	ZPC	C20-N19	3.35	1.38	1.34
2	C	1318	ZPC	C20-N19	3.35	1.38	1.34
2	E	1318	ZPC	C20-N19	3.24	1.38	1.34
2	I	1318	ZPC	O10-C08	3.22	1.40	1.34
2	D	1318	ZPC	C27-C26	3.16	1.43	1.38
2	B	1318	ZPC	C27-C26	3.06	1.43	1.38
2	J	1318	ZPC	C11-N12	-3.05	1.44	1.47
2	J	1318	ZPC	C27-C26	2.88	1.43	1.38
2	H	1318	ZPC	C20-C11	2.87	1.53	1.51
2	D	1318	ZPC	C20-C11	2.84	1.53	1.51
2	I	1318	ZPC	C26-C24	2.77	1.43	1.38
2	B	1318	ZPC	C11-N12	-2.74	1.45	1.47
2	H	1318	ZPC	C26-C24	2.67	1.43	1.38
2	J	1318	ZPC	O10-C08	2.67	1.39	1.34
2	F	1318	ZPC	C26-C24	2.58	1.42	1.38
2	A	1318	ZPC	C26-C24	2.54	1.42	1.38
2	C	1318	ZPC	C21-N22	2.53	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1318	ZPC	C20-C11	2.49	1.53	1.51
2	D	1318	ZPC	C26-C24	2.37	1.42	1.38
2	E	1318	ZPC	C18-N19	-2.36	1.29	1.34
2	F	1318	ZPC	C18-C17	2.32	1.44	1.38
2	H	1318	ZPC	C18-C17	2.29	1.44	1.38
2	E	1318	ZPC	C26-C24	2.29	1.42	1.38
2	J	1318	ZPC	C26-C24	2.27	1.42	1.38
2	J	1318	ZPC	C18-C17	2.23	1.44	1.38
2	B	1318	ZPC	C18-C17	2.12	1.44	1.38
2	G	1318	ZPC	C15-C13	-2.10	1.45	1.49
2	C	1318	ZPC	C18-C17	2.09	1.43	1.38
2	G	1318	ZPC	C18-C17	2.02	1.43	1.38

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1318	ZPC	O10-C08-N05	20.28	129.03	111.24
2	F	1318	ZPC	O10-C08-N05	18.30	127.29	111.24
2	E	1318	ZPC	O10-C08-N05	17.32	126.43	111.24
2	D	1318	ZPC	O10-C08-N05	16.30	125.53	111.24
2	A	1318	ZPC	O10-C08-N05	15.64	124.96	111.24
2	H	1318	ZPC	O10-C08-N05	15.04	124.43	111.24
2	J	1318	ZPC	O10-C08-N05	14.80	124.22	111.24
2	B	1318	ZPC	O10-C08-N05	14.39	123.86	111.24
2	G	1318	ZPC	O10-C08-N05	14.17	123.66	111.24
2	B	1318	ZPC	O14-C13-N12	12.74	144.49	126.15
2	A	1318	ZPC	O14-C13-N12	12.41	144.01	126.15
2	E	1318	ZPC	O14-C13-N12	11.91	143.29	126.15
2	F	1318	ZPC	O14-C13-N12	10.90	141.84	126.15
2	G	1318	ZPC	O14-C13-N12	10.43	141.16	126.15
2	D	1318	ZPC	O14-C13-N12	10.38	141.09	126.15
2	C	1318	ZPC	O14-C13-N12	9.33	139.57	126.15
2	I	1318	ZPC	O14-C13-N12	8.90	138.96	126.15
2	G	1318	ZPC	C27-C21-N12	8.89	129.36	122.38
2	F	1318	ZPC	C04-N05-C08	-8.81	96.09	121.75
2	C	1318	ZPC	C04-N05-C08	-8.47	97.08	121.75
2	I	1318	ZPC	O10-C08-N05	8.42	118.62	111.24
2	H	1318	ZPC	C04-N05-C08	-8.21	97.84	121.75
2	J	1318	ZPC	O14-C13-N12	8.17	137.91	126.15
2	J	1318	ZPC	C04-N05-C08	-8.11	98.13	121.75
2	C	1318	ZPC	O09-C08-N05	-7.93	109.61	124.30
2	C	1318	ZPC	C01-N02-C07	7.87	125.63	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1318	ZPC	C06-C07-N02	7.68	123.20	110.86
2	E	1318	ZPC	C04-N05-C08	-7.66	99.45	121.75
2	H	1318	ZPC	O14-C13-N12	7.63	137.12	126.15
2	A	1318	ZPC	C04-N05-C08	-7.43	100.13	121.75
2	I	1318	ZPC	C04-N05-C08	-7.39	100.22	121.75
2	B	1318	ZPC	C04-N05-C08	-7.13	100.98	121.75
2	D	1318	ZPC	N22-C21-N12	7.03	122.33	114.54
2	F	1318	ZPC	C23-N22-C21	6.92	128.74	117.41
2	A	1318	ZPC	C03-C04-N05	6.91	124.15	110.42
2	G	1318	ZPC	C03-C04-N05	6.90	124.14	110.42
2	A	1318	ZPC	C11-O10-C08	6.75	126.20	116.47
2	D	1318	ZPC	C04-N05-C08	-6.74	102.11	121.75
2	C	1318	ZPC	C23-N22-C21	6.57	128.16	117.41
2	D	1318	ZPC	C21-N12-C11	6.56	126.22	118.57
2	C	1318	ZPC	N22-C21-N12	6.53	121.78	114.54
2	F	1318	ZPC	C01-N02-C07	6.48	122.98	110.63
2	J	1318	ZPC	C01-N02-C07	6.47	122.96	110.63
2	H	1318	ZPC	O09-C08-N05	-6.45	112.36	124.30
2	G	1318	ZPC	C21-N12-C11	6.44	126.08	118.57
2	B	1318	ZPC	C01-N02-C07	6.26	122.57	110.63
2	I	1318	ZPC	C11-O10-C08	6.24	125.47	116.47
2	J	1318	ZPC	C21-N12-C11	6.23	125.84	118.57
2	G	1318	ZPC	C26-C24-CL	6.16	128.45	119.36
2	I	1318	ZPC	C01-N02-C07	6.13	122.31	110.63
2	G	1318	ZPC	C23-N22-C21	6.09	127.38	117.41
2	E	1318	ZPC	C03-C04-N05	6.08	122.50	110.42
2	I	1318	ZPC	C21-N12-C11	6.06	125.64	118.57
2	H	1318	ZPC	C11-O10-C08	6.06	125.20	116.47
2	D	1318	ZPC	C23-N22-C21	6.05	127.31	117.41
2	B	1318	ZPC	C23-N22-C21	6.00	127.24	117.41
2	A	1318	ZPC	O09-C08-N05	-5.97	113.25	124.30
2	C	1318	ZPC	O10-C08-O09	-5.96	112.61	124.92
2	B	1318	ZPC	O09-C08-N05	-5.93	113.32	124.30
2	G	1318	ZPC	C04-N05-C08	-5.88	104.62	121.75
2	B	1318	ZPC	O14-C13-C15	-5.85	110.83	128.78
2	D	1318	ZPC	O09-C08-N05	-5.75	113.66	124.30
2	C	1318	ZPC	C04-C03-N02	-5.69	101.71	110.86
2	D	1318	ZPC	C01-N02-C07	5.63	121.36	110.63
2	I	1318	ZPC	C01-N02-C03	5.54	121.18	110.63
2	B	1318	ZPC	C11-O10-C08	5.51	124.41	116.47
2	C	1318	ZPC	C24-C23-N22	-5.49	115.22	122.26
2	A	1318	ZPC	O14-C13-C15	-5.46	112.02	128.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1318	ZPC	C01-N02-C03	5.45	121.01	110.63
2	G	1318	ZPC	O14-C13-C15	-5.44	112.10	128.78
2	F	1318	ZPC	O14-C13-C15	-5.38	112.28	128.78
2	I	1318	ZPC	C03-C04-N05	5.37	121.09	110.42
2	A	1318	ZPC	C23-N22-C21	5.36	126.19	117.41
2	E	1318	ZPC	O09-C08-N05	-5.34	114.42	124.30
2	J	1318	ZPC	C23-N22-C21	5.28	126.05	117.41
2	C	1318	ZPC	C07-N02-C03	5.27	117.93	109.54
2	B	1318	ZPC	C03-C04-N05	5.26	120.87	110.42
2	F	1318	ZPC	C06-C07-N02	5.25	119.30	110.86
2	D	1318	ZPC	O14-C13-C15	-5.23	112.74	128.78
2	C	1318	ZPC	C03-C04-N05	5.21	120.77	110.42
2	H	1318	ZPC	C23-N22-C21	5.19	125.90	117.41
2	E	1318	ZPC	O14-C13-C15	-5.13	113.04	128.78
2	A	1318	ZPC	C01-N02-C07	5.12	120.40	110.63
2	A	1318	ZPC	C01-N02-C03	5.06	120.28	110.63
2	H	1318	ZPC	C03-C04-N05	5.06	120.47	110.42
2	B	1318	ZPC	C24-C23-N22	-5.04	115.80	122.26
2	E	1318	ZPC	C23-N22-C21	5.03	125.65	117.41
2	F	1318	ZPC	C26-C24-CL	5.01	126.75	119.36
2	D	1318	ZPC	C11-O10-C08	4.94	123.59	116.47
2	H	1318	ZPC	C01-N02-C07	4.92	120.01	110.63
2	G	1318	ZPC	C01-N02-C07	4.77	119.73	110.63
2	F	1318	ZPC	C04-C03-N02	-4.76	103.20	110.86
2	G	1318	ZPC	C11-O10-C08	4.74	123.31	116.47
2	I	1318	ZPC	C23-N22-C21	4.74	125.18	117.41
2	A	1318	ZPC	C06-C07-N02	4.74	118.47	110.86
2	A	1318	ZPC	N22-C21-N12	4.72	119.77	114.54
2	F	1318	ZPC	O09-C08-N05	-4.70	115.60	124.30
2	D	1318	ZPC	C06-C07-N02	4.62	118.28	110.86
2	G	1318	ZPC	C07-N02-C03	4.62	116.89	109.54
2	E	1318	ZPC	C26-C24-CL	4.61	126.16	119.36
2	C	1318	ZPC	O14-C13-C15	-4.61	114.65	128.78
2	H	1318	ZPC	C15-C20-C11	-4.60	106.30	109.81
2	F	1318	ZPC	N22-C21-N12	4.60	119.63	114.54
2	G	1318	ZPC	O10-C08-O09	-4.58	115.46	124.92
2	J	1318	ZPC	C03-C04-N05	4.56	119.48	110.42
2	H	1318	ZPC	C07-N02-C03	4.42	116.58	109.54
2	C	1318	ZPC	C06-N05-C08	4.42	134.64	121.75
2	F	1318	ZPC	C07-N02-C03	4.37	116.50	109.54
2	G	1318	ZPC	C23-C24-CL	-4.36	111.80	119.73
2	G	1318	ZPC	O09-C08-N05	-4.34	116.27	124.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1318	ZPC	C07-N02-C03	4.31	116.41	109.54
2	D	1318	ZPC	C06-N05-C08	4.30	134.28	121.75
2	H	1318	ZPC	C27-C21-N12	4.29	125.75	122.38
2	I	1318	ZPC	O14-C13-C15	-4.28	115.65	128.78
2	D	1318	ZPC	C07-N02-C03	4.25	116.30	109.54
2	F	1318	ZPC	C27-C21-N22	-4.20	115.16	123.46
2	J	1318	ZPC	C15-C20-C11	-4.17	106.63	109.81
2	E	1318	ZPC	C01-N02-C07	4.14	118.53	110.63
2	J	1318	ZPC	C11-O10-C08	4.13	122.42	116.47
2	F	1318	ZPC	O10-C08-O09	-4.05	116.55	124.92
2	E	1318	ZPC	C11-O10-C08	4.02	122.27	116.47
2	J	1318	ZPC	O14-C13-C15	-4.00	116.52	128.78
2	D	1318	ZPC	C03-C04-N05	3.98	118.34	110.42
2	E	1318	ZPC	C18-C17-N16	3.98	127.79	122.19
2	E	1318	ZPC	C06-C07-N02	3.93	117.18	110.86
2	I	1318	ZPC	N22-C21-N12	3.91	118.87	114.54
2	D	1318	ZPC	C27-C21-N22	-3.90	115.77	123.46
2	A	1318	ZPC	C26-C24-CL	3.89	125.11	119.36
2	E	1318	ZPC	C01-N02-C03	3.80	117.87	110.63
2	J	1318	ZPC	O10-C08-O09	-3.80	117.08	124.92
2	I	1318	ZPC	C07-N02-C03	3.75	115.51	109.54
2	D	1318	ZPC	C24-C23-N22	-3.75	117.45	122.26
2	H	1318	ZPC	O14-C13-C15	-3.75	117.28	128.78
2	E	1318	ZPC	C27-C21-N12	3.71	125.30	122.38
2	J	1318	ZPC	C06-C07-N02	3.62	116.68	110.86
2	B	1318	ZPC	C26-C24-CL	3.61	124.68	119.36
2	I	1318	ZPC	C26-C24-CL	3.60	124.66	119.36
2	E	1318	ZPC	C23-C24-CL	-3.58	113.23	119.73
2	G	1318	ZPC	C01-N02-C03	3.53	117.37	110.63
2	F	1318	ZPC	C27-C21-N12	3.52	125.14	122.38
2	F	1318	ZPC	C03-C04-N05	3.51	117.41	110.42
2	G	1318	ZPC	C24-C23-N22	-3.47	117.81	122.26
2	B	1318	ZPC	C23-C24-CL	-3.47	113.43	119.73
2	J	1318	ZPC	N22-C21-N12	3.46	118.38	114.54
2	B	1318	ZPC	N22-C21-N12	3.45	118.36	114.54
2	C	1318	ZPC	C27-C21-N12	-3.40	119.71	122.38
2	E	1318	ZPC	C21-N12-C11	3.40	122.54	118.57
2	B	1318	ZPC	C26-C24-C23	3.30	121.88	119.60
2	H	1318	ZPC	C26-C24-CL	3.30	124.22	119.36
2	I	1318	ZPC	C27-C21-N22	-3.29	116.97	123.46
2	E	1318	ZPC	O10-C08-O09	-3.27	118.17	124.92
2	G	1318	ZPC	C06-C07-N02	3.27	116.11	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1318	ZPC	C01-N02-C03	3.25	116.83	110.63
2	H	1318	ZPC	C01-N02-C03	3.25	116.82	110.63
2	F	1318	ZPC	C21-N12-C11	3.22	122.33	118.57
2	B	1318	ZPC	O10-C08-O09	-3.22	118.26	124.92
2	J	1318	ZPC	C26-C24-CL	3.20	124.08	119.36
2	J	1318	ZPC	O09-C08-N05	-3.14	118.48	124.30
2	A	1318	ZPC	C27-C21-N22	-3.12	117.30	123.46
2	E	1318	ZPC	C27-C21-N22	-3.12	117.31	123.46
2	A	1318	ZPC	O10-C08-O09	-3.07	118.57	124.92
2	A	1318	ZPC	C24-C23-N22	-3.07	118.32	122.26
2	F	1318	ZPC	C26-C24-C23	-3.04	117.50	119.60
2	C	1318	ZPC	C11-O10-C08	3.04	120.85	116.47
2	C	1318	ZPC	C27-C26-C24	3.03	122.30	119.24
2	H	1318	ZPC	C27-C21-N22	-3.01	117.52	123.46
2	I	1318	ZPC	O09-C08-N05	-3.01	118.73	124.30
2	H	1318	ZPC	C24-C23-N22	-2.99	118.42	122.26
2	J	1318	ZPC	C27-C21-N22	-2.98	117.58	123.46
2	H	1318	ZPC	C06-N05-C08	2.94	130.32	121.75
2	G	1318	ZPC	C15-C20-C11	-2.91	107.59	109.81
2	I	1318	ZPC	C15-C20-C11	-2.86	107.63	109.81
2	E	1318	ZPC	C24-C23-N22	-2.85	118.61	122.26
2	F	1318	ZPC	C24-C23-N22	-2.77	118.70	122.26
2	H	1318	ZPC	O10-C08-O09	-2.77	119.20	124.92
2	J	1318	ZPC	C24-C23-N22	-2.76	118.72	122.26
2	G	1318	ZPC	C27-C21-N22	-2.73	118.07	123.46
2	E	1318	ZPC	C20-C15-C13	2.71	113.10	108.60
2	A	1318	ZPC	C23-C24-CL	-2.69	114.84	119.73
2	C	1318	ZPC	C27-C21-N22	-2.69	118.15	123.46
2	G	1318	ZPC	C13-C15-N16	-2.69	122.33	125.59
2	E	1318	ZPC	C17-C18-N19	-2.66	118.44	122.19
2	B	1318	ZPC	C15-C20-C11	-2.60	107.83	109.81
2	I	1318	ZPC	C23-C24-CL	-2.58	115.04	119.73
2	E	1318	ZPC	C15-C20-C11	-2.58	107.84	109.81
2	J	1318	ZPC	C07-N02-C03	2.57	113.64	109.54
2	E	1318	ZPC	N22-C21-N12	2.57	117.39	114.54
2	F	1318	ZPC	C06-N05-C08	2.57	129.24	121.75
2	C	1318	ZPC	C01-N02-C03	2.57	115.52	110.63
2	B	1318	ZPC	C27-C21-N22	-2.53	118.46	123.46
2	H	1318	ZPC	C07-C06-N05	-2.52	105.40	110.42
2	H	1318	ZPC	C06-C07-N02	2.52	114.90	110.86
2	I	1318	ZPC	C07-C06-N05	-2.44	105.56	110.42
2	E	1318	ZPC	C17-N16-C15	-2.42	112.08	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1318	ZPC	O10-C08-O09	-2.38	120.00	124.92
2	F	1318	ZPC	C17-N16-C15	-2.36	112.20	116.80
2	F	1318	ZPC	C01-N02-C03	2.36	115.12	110.63
2	B	1318	ZPC	C13-C15-N16	-2.31	122.79	125.59
2	A	1318	ZPC	C06-N05-C08	2.30	128.46	121.75
2	J	1318	ZPC	C04-C03-N02	2.26	114.49	110.86
2	A	1318	ZPC	C06-N05-C04	2.26	117.30	112.68
2	G	1318	ZPC	C17-N16-C15	-2.25	112.41	116.80
2	I	1318	ZPC	C27-C21-N12	2.23	124.13	122.38
2	B	1318	ZPC	C18-C17-N16	2.22	125.31	122.19
2	I	1318	ZPC	C26-C27-C21	2.21	120.71	117.65
2	D	1318	ZPC	C26-C27-C21	2.21	120.71	117.65
2	F	1318	ZPC	C23-C24-CL	-2.19	115.75	119.73
2	I	1318	ZPC	C06-N05-C04	2.17	117.12	112.68
2	A	1318	ZPC	C07-N02-C03	2.17	112.99	109.54
2	E	1318	ZPC	C06-N05-C08	2.14	127.97	121.75
2	F	1318	ZPC	C15-C20-C11	-2.10	108.21	109.81
2	G	1318	ZPC	C06-N05-C08	2.09	127.85	121.75
2	J	1318	ZPC	C27-C21-N12	2.09	124.02	122.38
2	I	1318	ZPC	C27-C26-C24	-2.08	117.14	119.24
2	C	1318	ZPC	C21-N12-C11	2.07	120.99	118.57
2	H	1318	ZPC	C20-C15-C13	2.06	112.02	108.60
2	G	1318	ZPC	C04-C03-N02	2.03	114.12	110.86
2	I	1318	ZPC	C24-C23-N22	-2.02	119.67	122.26
2	D	1318	ZPC	C07-C06-N05	-2.01	106.41	110.42
2	G	1318	ZPC	N22-C21-N12	-2.01	112.31	114.54

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1318	ZPC	O10-C08-N05-C04
2	A	1318	ZPC	N12-C11-O10-C08
2	A	1318	ZPC	N22-C21-N12-C11
2	A	1318	ZPC	C27-C21-N12-C11
2	A	1318	ZPC	N22-C21-N12-C13
2	A	1318	ZPC	C27-C21-N12-C13
2	B	1318	ZPC	O09-C08-N05-C06
2	B	1318	ZPC	O10-C08-N05-C06
2	B	1318	ZPC	N05-C08-O10-C11
2	B	1318	ZPC	N12-C11-O10-C08
2	B	1318	ZPC	C20-C11-O10-C08

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Mol	Chain	Res	Type	Atoms
2	B	1318	ZPC	N22-C21-N12-C11
2	B	1318	ZPC	C27-C21-N12-C11
2	B	1318	ZPC	N22-C21-N12-C13
2	B	1318	ZPC	C27-C21-N12-C13
2	C	1318	ZPC	O10-C08-N05-C04
2	C	1318	ZPC	O10-C08-N05-C06
2	C	1318	ZPC	N12-C11-O10-C08
2	C	1318	ZPC	N22-C21-N12-C11
2	C	1318	ZPC	C27-C21-N12-C11
2	C	1318	ZPC	N22-C21-N12-C13
2	C	1318	ZPC	C27-C21-N12-C13
2	D	1318	ZPC	O09-C08-N05-C04
2	D	1318	ZPC	O10-C08-N05-C04
2	D	1318	ZPC	N12-C11-O10-C08
2	E	1318	ZPC	O09-C08-N05-C06
2	E	1318	ZPC	O10-C08-N05-C06
2	E	1318	ZPC	N12-C11-O10-C08
2	E	1318	ZPC	C20-C11-O10-C08
2	E	1318	ZPC	N22-C21-N12-C11
2	E	1318	ZPC	C27-C21-N12-C11
2	E	1318	ZPC	N22-C21-N12-C13
2	E	1318	ZPC	C27-C21-N12-C13
2	F	1318	ZPC	O10-C08-N05-C04
2	F	1318	ZPC	N12-C11-O10-C08
2	F	1318	ZPC	C20-C11-O10-C08
2	F	1318	ZPC	N22-C21-N12-C11
2	F	1318	ZPC	C27-C21-N12-C11
2	G	1318	ZPC	O09-C08-N05-C06
2	G	1318	ZPC	N12-C11-O10-C08
2	G	1318	ZPC	N22-C21-N12-C11
2	G	1318	ZPC	C27-C21-N12-C11
2	H	1318	ZPC	O09-C08-N05-C06
2	H	1318	ZPC	N12-C11-O10-C08
2	H	1318	ZPC	N22-C21-N12-C11
2	H	1318	ZPC	C27-C21-N12-C11
2	H	1318	ZPC	N22-C21-N12-C13
2	H	1318	ZPC	C27-C21-N12-C13
2	I	1318	ZPC	N12-C11-O10-C08
2	J	1318	ZPC	O09-C08-N05-C06
2	J	1318	ZPC	O10-C08-N05-C06
2	J	1318	ZPC	N12-C11-O10-C08
2	J	1318	ZPC	N22-C21-N12-C11

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Mol	Chain	Res	Type	Atoms
2	C	1318	ZPC	O09-C08-N05-C04
2	A	1318	ZPC	O09-C08-N05-C04
2	F	1318	ZPC	O09-C08-N05-C04
2	G	1318	ZPC	O10-C08-N05-C04
2	H	1318	ZPC	N05-C08-O10-C11
2	H	1318	ZPC	O10-C08-N05-C04
2	I	1318	ZPC	O10-C08-N05-C04
2	G	1318	ZPC	N05-C08-O10-C11
2	D	1318	ZPC	O09-C08-O10-C11
2	I	1318	ZPC	O09-C08-N05-C04
2	D	1318	ZPC	C20-C11-O10-C08
2	H	1318	ZPC	C20-C11-O10-C08
2	G	1318	ZPC	N22-C21-N12-C13
2	B	1318	ZPC	O09-C08-O10-C11
2	J	1318	ZPC	C27-C21-N12-C11

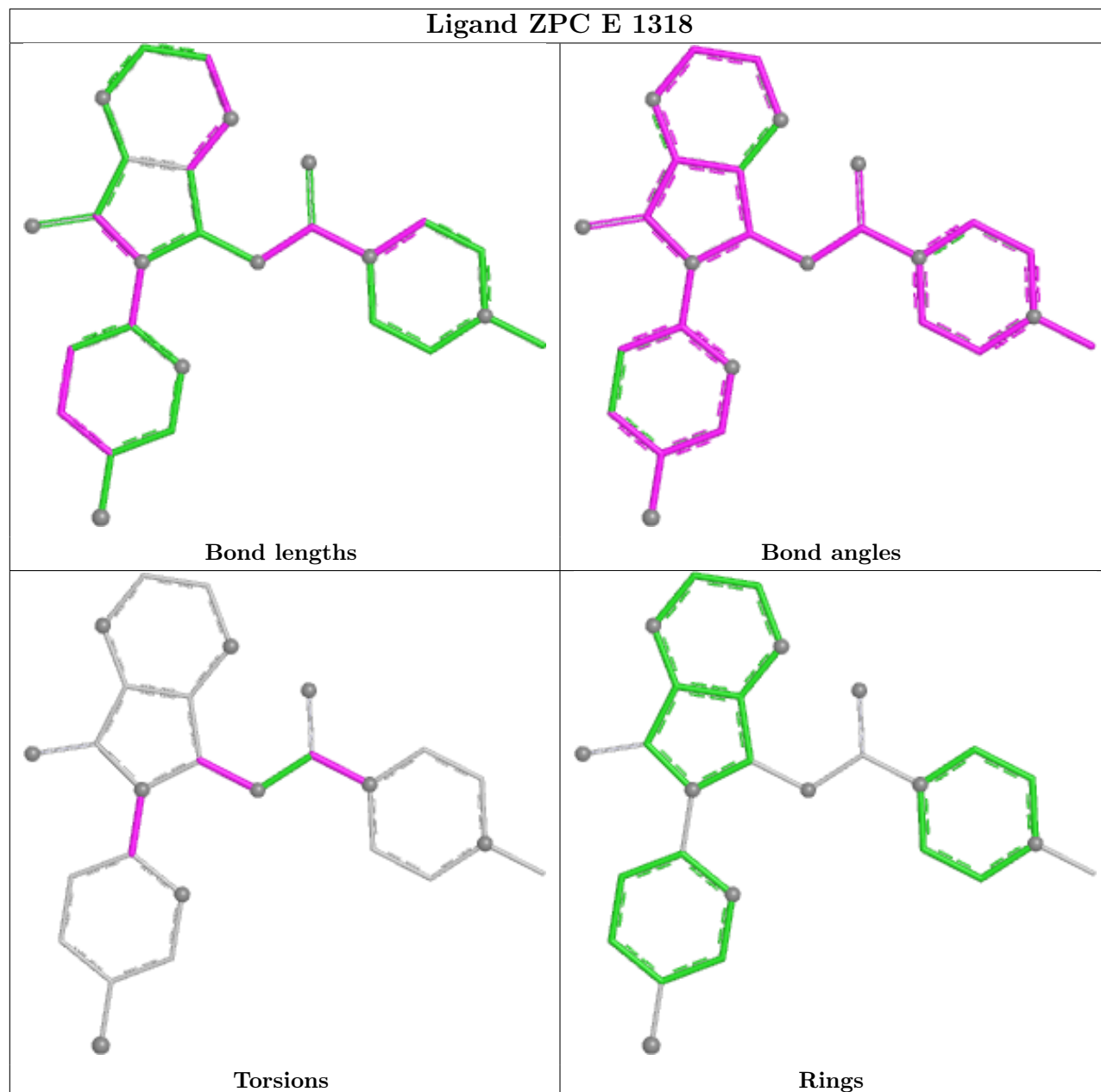
There are no ring outliers.

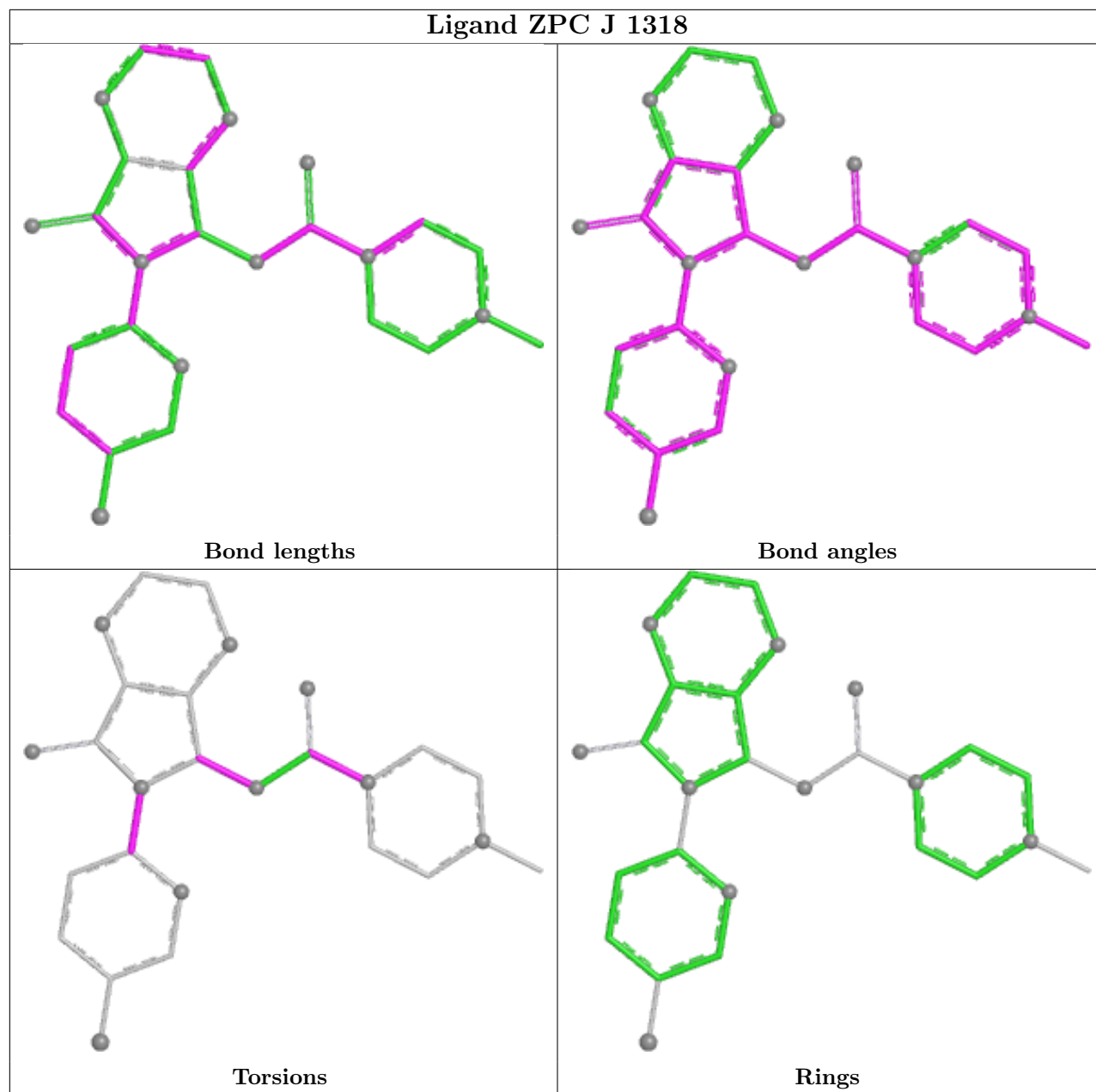
10 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1318	ZPC	7	0
2	J	1318	ZPC	4	0
2	H	1318	ZPC	7	0
2	B	1318	ZPC	3	0
2	I	1318	ZPC	8	0
2	F	1318	ZPC	11	0
2	G	1318	ZPC	6	0
2	A	1318	ZPC	9	0
2	D	1318	ZPC	12	0
2	C	1318	ZPC	8	0

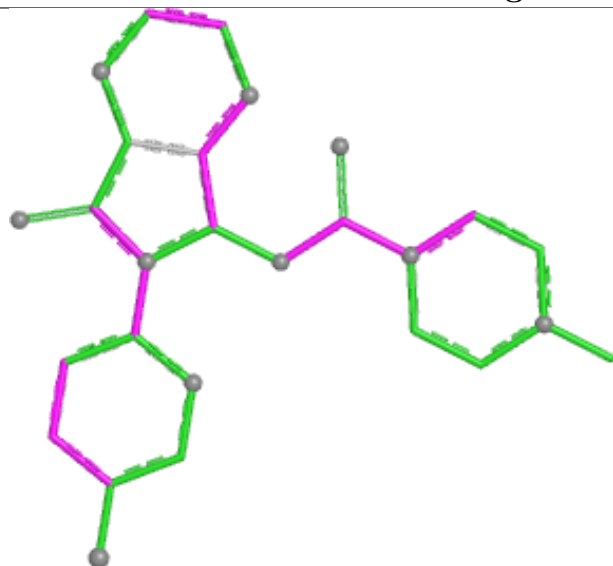
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

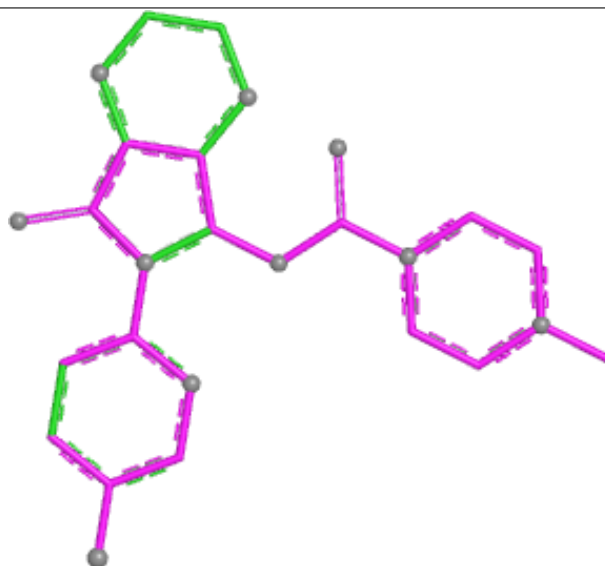




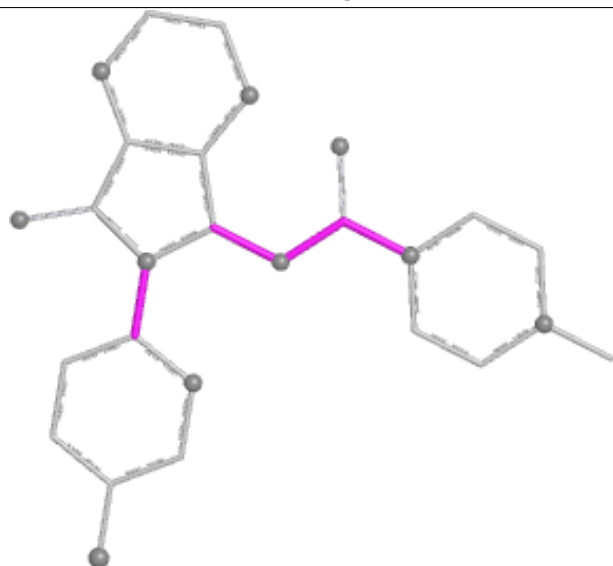
Ligand ZPC H 1318



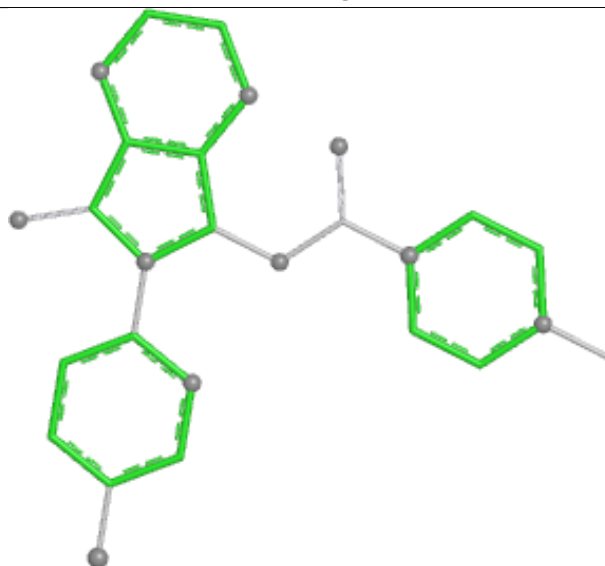
Bond lengths



Bond angles

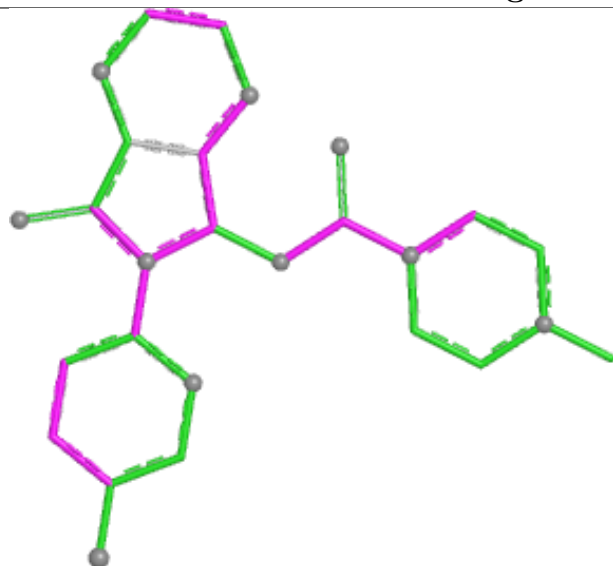


Torsions

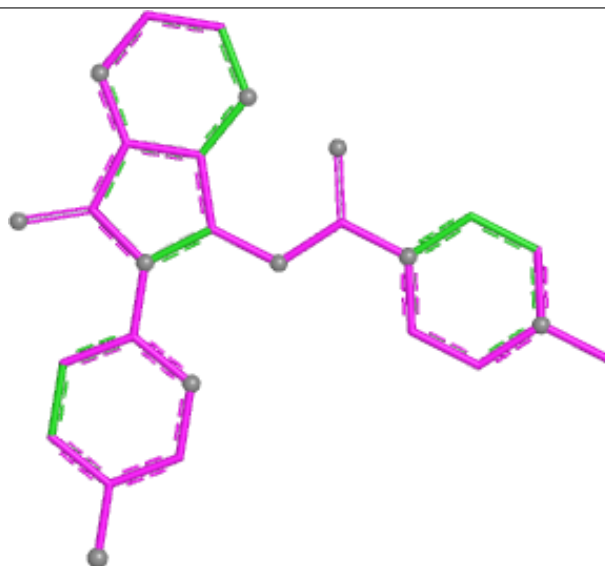


Rings

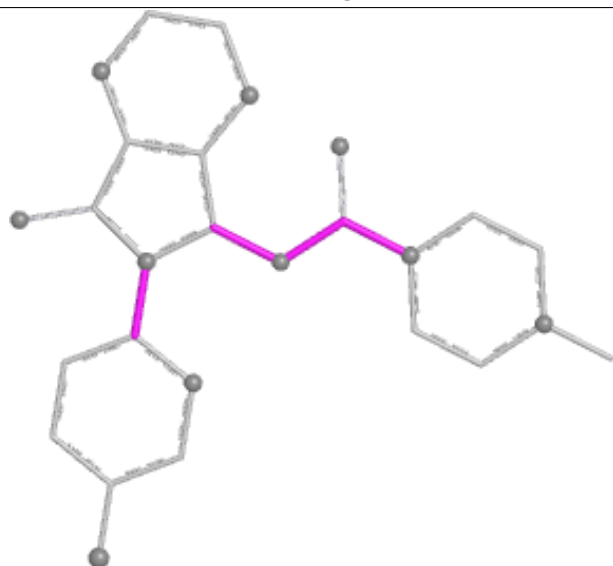
Ligand ZPC B 1318



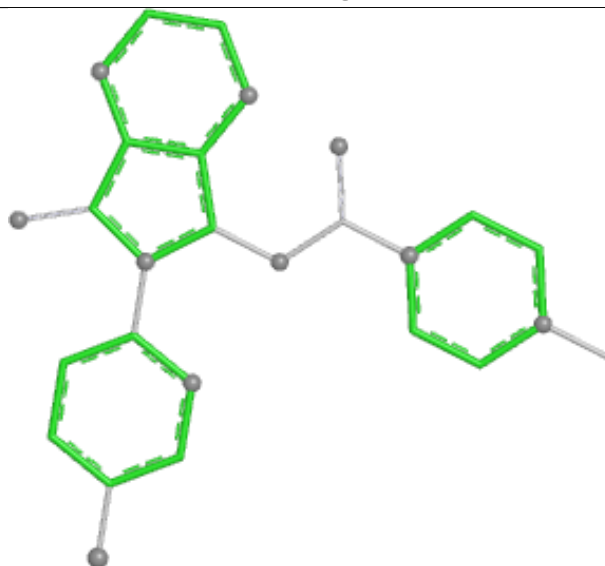
Bond lengths



Bond angles

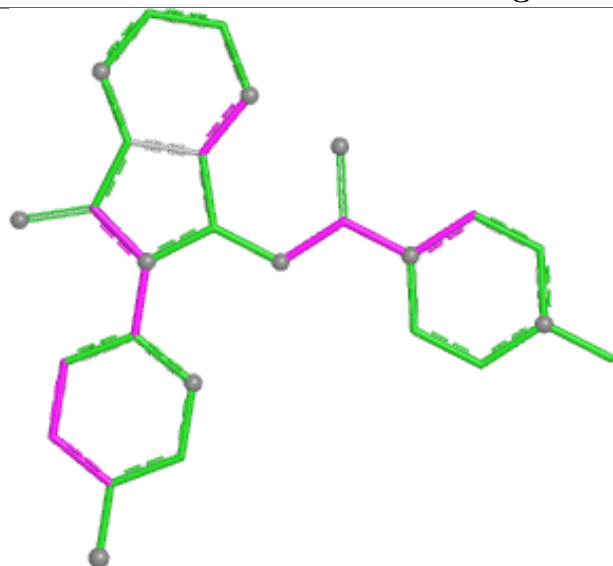


Torsions

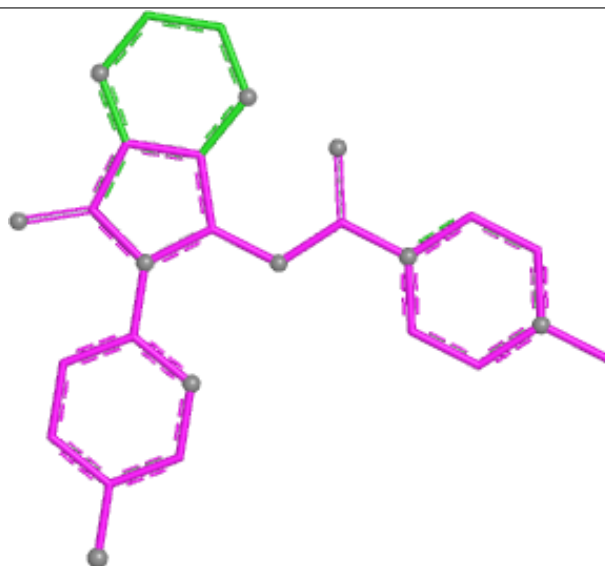


Rings

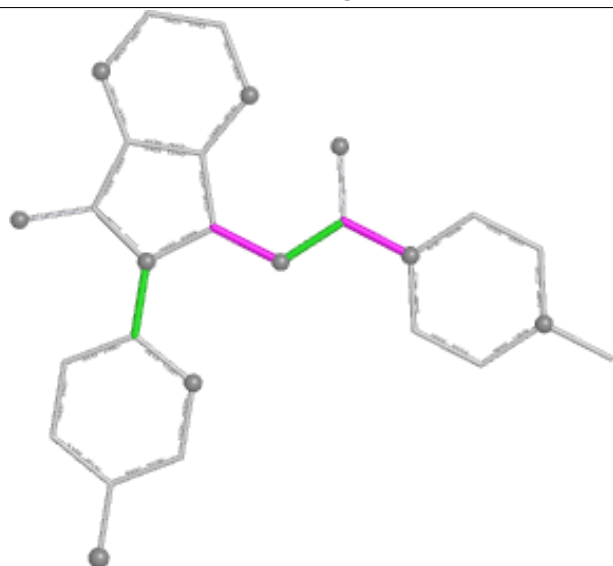
Ligand ZPC I 1318



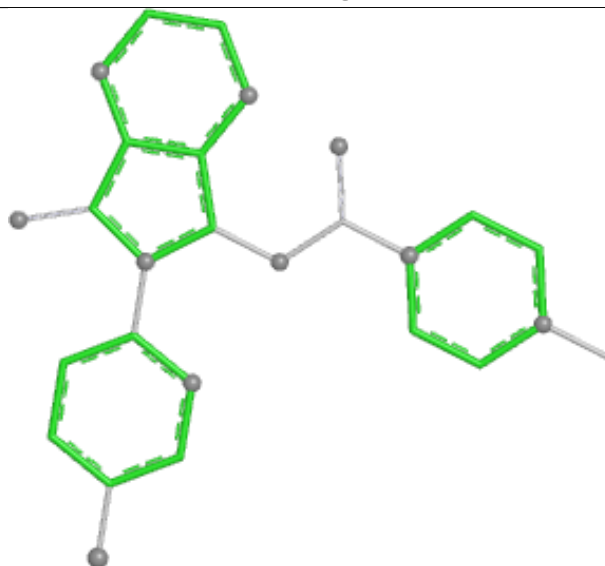
Bond lengths



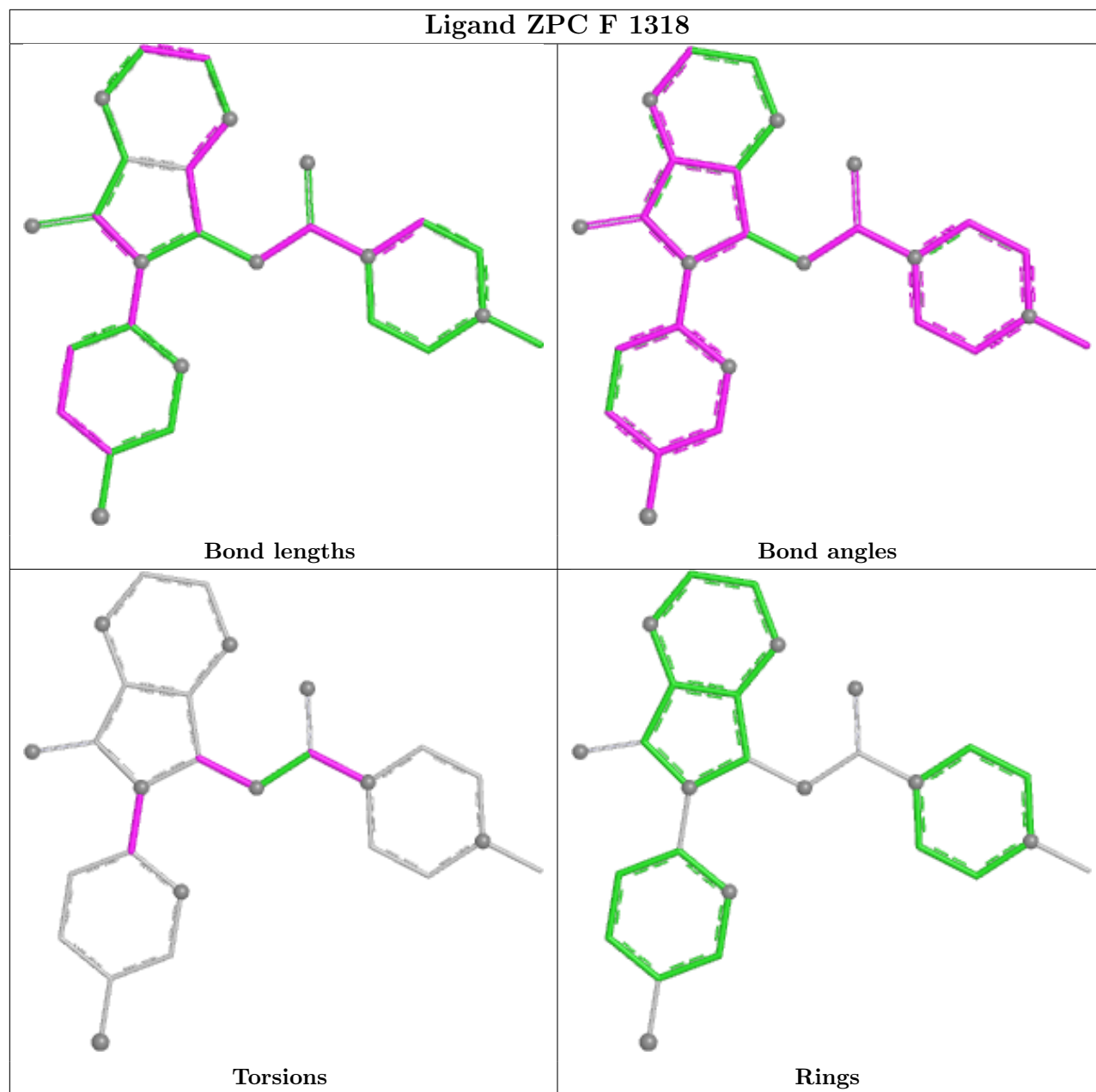
Bond angles



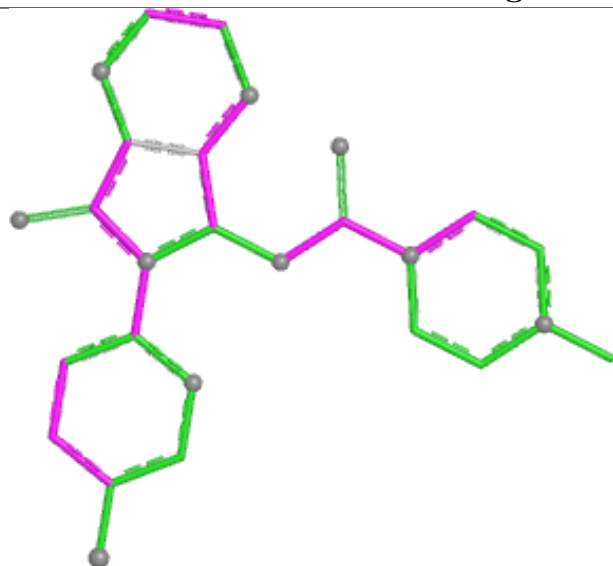
Torsions



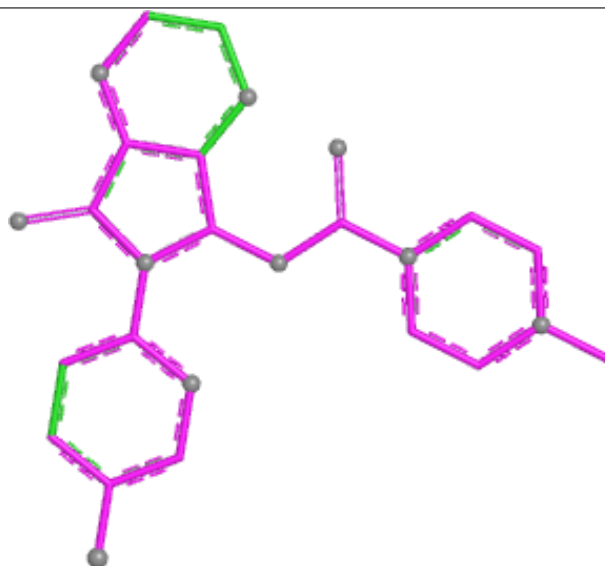
Rings



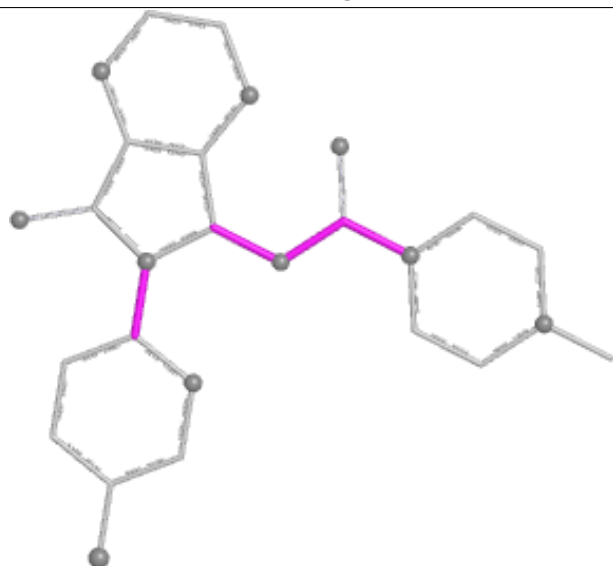
Ligand ZPC G 1318



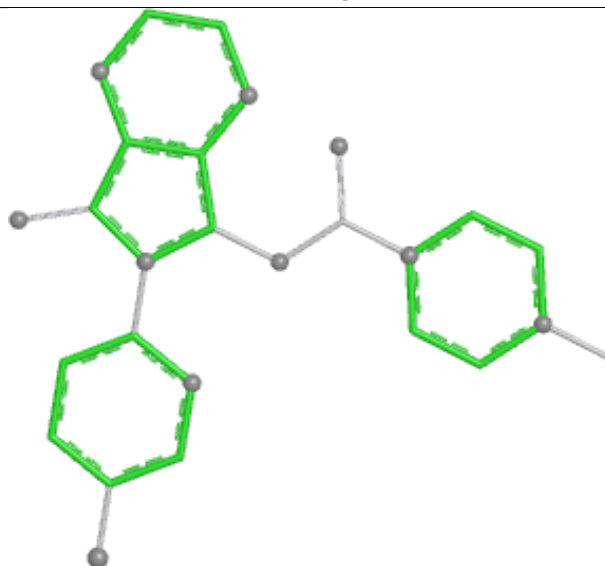
Bond lengths



Bond angles

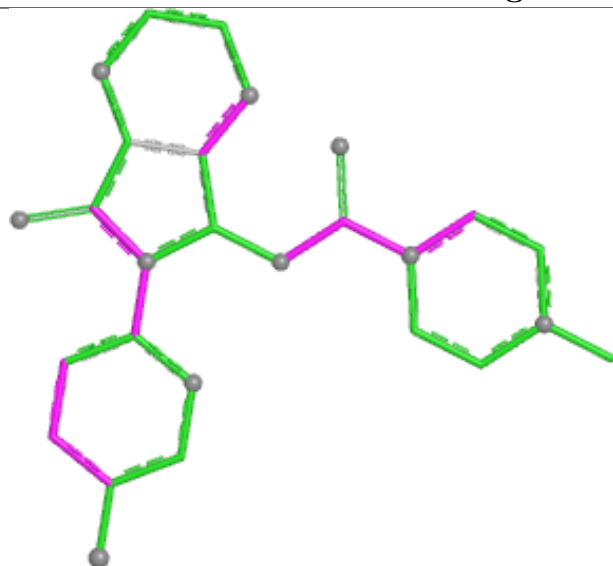


Torsions

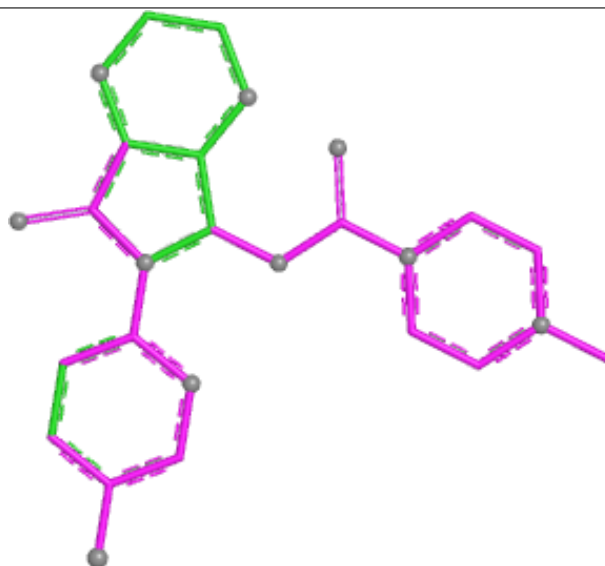


Rings

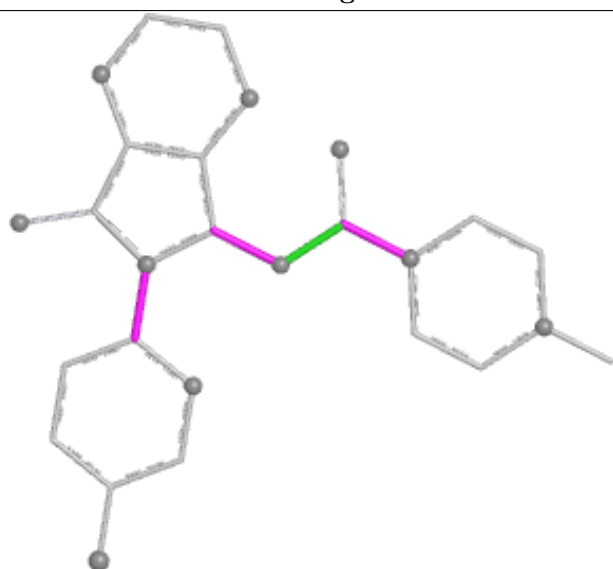
Ligand ZPC A 1318



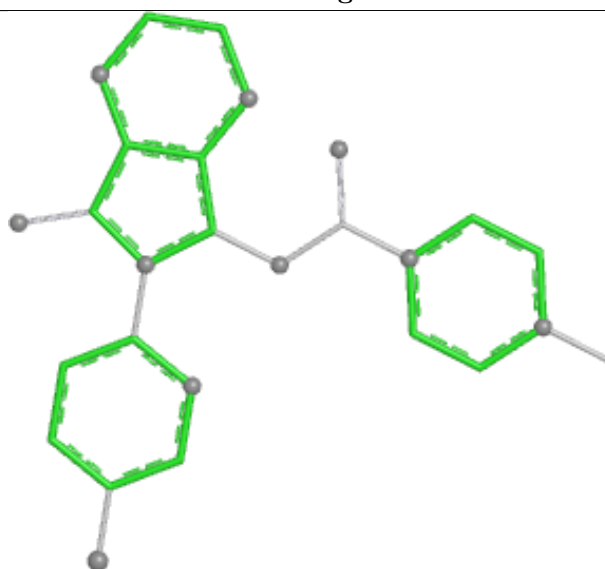
Bond lengths



Bond angles

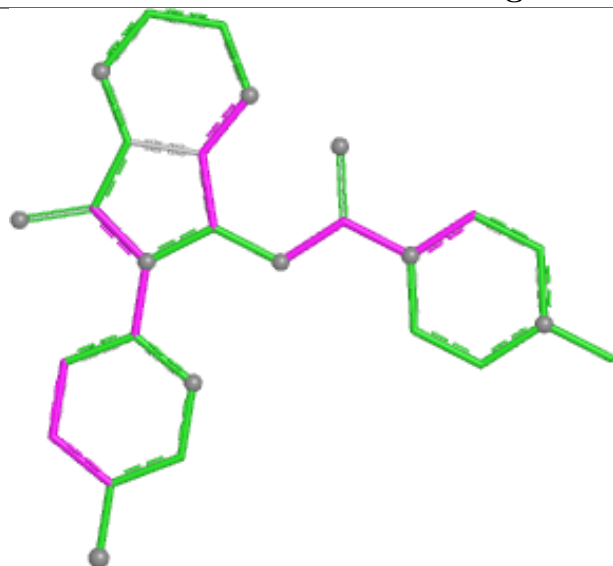


Torsions

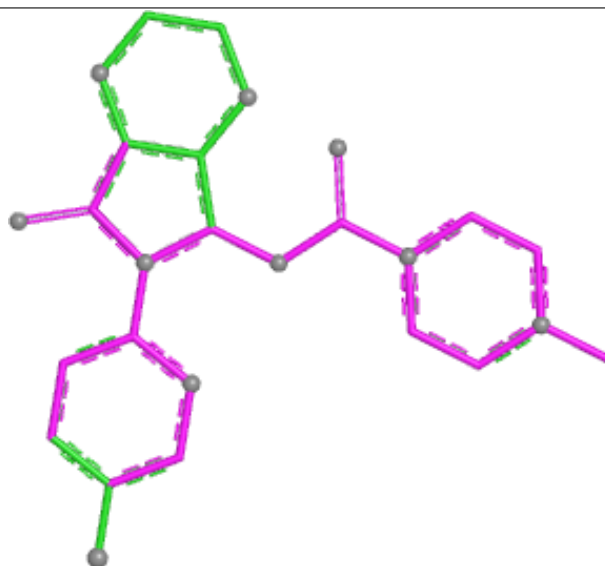


Rings

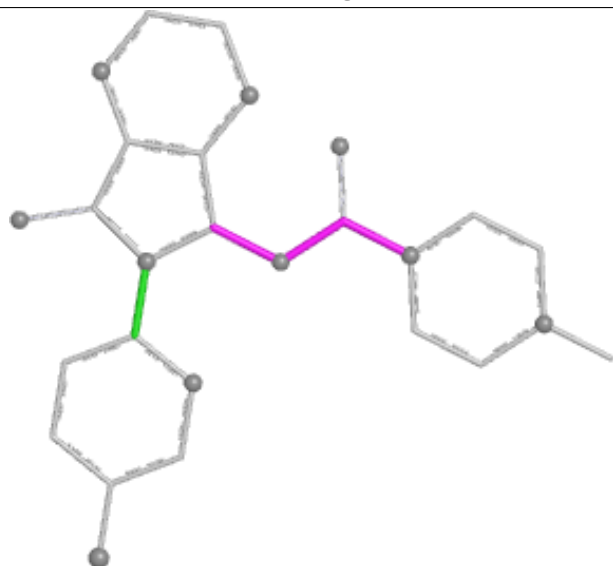
Ligand ZPC D 1318



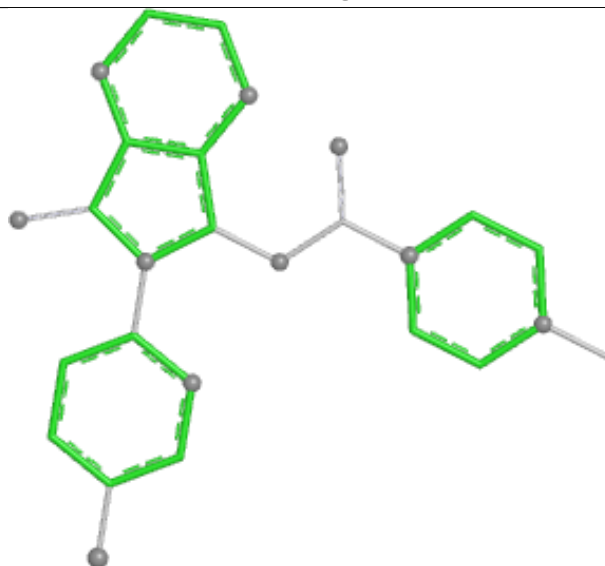
Bond lengths



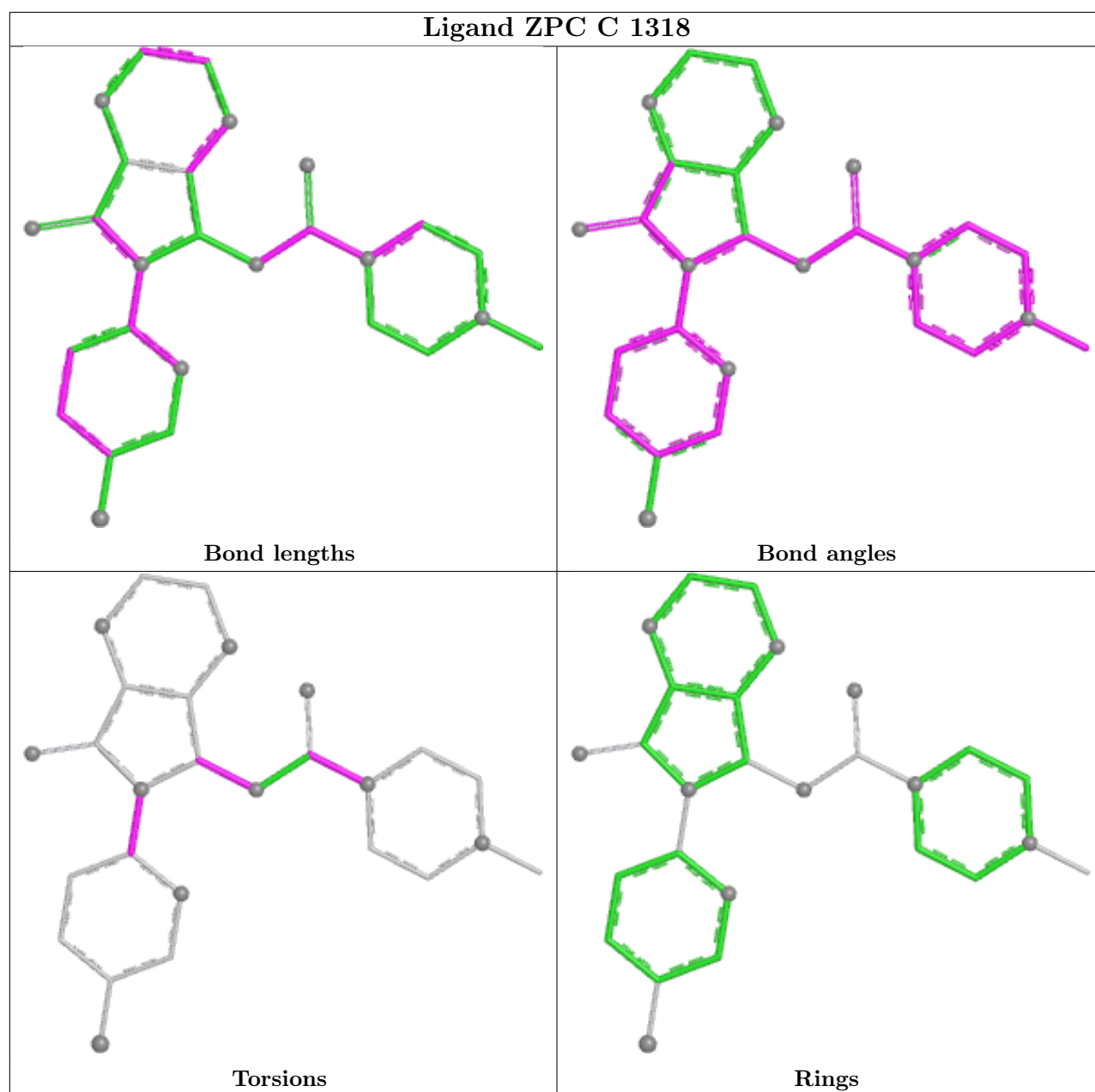
Bond angles



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%)	0.25	12 (3%)	43	29	74, 118, 187, 217	0
1	B	307/307 (100%)	0.49	20 (6%)	25	17	71, 108, 171, 263	0
1	C	307/307 (100%)	0.49	20 (6%)	25	17	71, 107, 186, 232	0
1	D	307/307 (100%)	0.25	8 (2%)	57	39	74, 104, 186, 263	0
1	E	307/307 (100%)	0.37	18 (5%)	28	19	73, 113, 188, 233	0
1	F	307/307 (100%)	0.18	12 (3%)	43	29	78, 118, 190, 276	0
1	G	307/307 (100%)	0.42	30 (9%)	13	11	75, 108, 171, 236	0
1	H	307/307 (100%)	0.51	29 (9%)	14	12	75, 111, 187, 279	0
1	I	307/307 (100%)	0.28	19 (6%)	26	18	76, 106, 192, 274	0
1	J	307/307 (100%)	0.49	30 (9%)	13	11	77, 115, 203, 261	0
All	All	3070/3070 (100%)	0.37	198 (6%)	25	17	71, 111, 189, 279	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	GLY	8.3
1	H	311	ILE	8.2
1	C	289	ASN	8.0
1	B	291	VAL	7.8
1	C	314	VAL	7.4
1	E	291	VAL	6.9
1	C	311	ILE	6.2
1	J	178	LEU	6.2
1	H	314	VAL	6.0
1	G	291	VAL	6.0
1	H	150	GLU	5.7
1	H	291	VAL	5.5
1	B	289	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	I	248	TYR	5.4
1	J	52	GLY	5.0
1	C	315	LEU	4.9
1	I	208	PHE	4.9
1	G	169	HIS	4.9
1	F	176	ASP	4.9
1	G	126	PHE	4.7
1	H	315	LEU	4.6
1	G	295	LEU	4.5
1	H	66	TRP	4.5
1	B	295	LEU	4.4
1	E	178	LEU	4.4
1	B	290	GLY	4.4
1	C	312	GLY	4.3
1	C	317	ILE	4.3
1	C	291	VAL	4.3
1	D	226	GLU	4.3
1	E	295	LEU	4.1
1	B	113	ASP	4.1
1	B	31	GLN	4.1
1	D	317	ILE	4.1
1	H	182	GLN	4.1
1	B	169	HIS	4.1
1	J	291	VAL	4.0
1	E	167	SER	4.0
1	F	285	HIS	4.0
1	G	290	GLY	4.0
1	I	157	ILE	4.0
1	J	304	PHE	4.0
1	D	11	PRO	3.9
1	I	52	GLY	3.9
1	E	296	LEU	3.9
1	J	49	LYS	3.9
1	C	11	PRO	3.8
1	J	308	PHE	3.8
1	H	138	GLN	3.8
1	B	288	ALA	3.7
1	I	251	ASN	3.7
1	E	166	ALA	3.7
1	C	288	ALA	3.7
1	J	11	PRO	3.7
1	H	137	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	288	ALA	3.6
1	H	312	GLY	3.6
1	C	49	LYS	3.6
1	J	167	SER	3.6
1	G	285	HIS	3.4
1	J	305	PRO	3.4
1	H	288	ALA	3.4
1	F	11	PRO	3.4
1	E	289	ASN	3.4
1	B	11	PRO	3.4
1	J	250	SER	3.3
1	B	102	TYR	3.3
1	J	80	ASN	3.3
1	F	317	ILE	3.3
1	G	196	ASP	3.3
1	H	289	ASN	3.3
1	B	178	LEU	3.2
1	E	288	ALA	3.2
1	H	65	ARG	3.2
1	D	178	LEU	3.2
1	H	153	ASP	3.2
1	G	157	ILE	3.1
1	I	178	LEU	3.1
1	G	289	ASN	3.0
1	F	178	LEU	3.0
1	B	33	TYR	3.0
1	J	196	ASP	3.0
1	A	188	PHE	3.0
1	A	152	ILE	3.0
1	J	301	ARG	2.9
1	H	164	GLY	2.9
1	H	62	GLN	2.9
1	G	141	ARG	2.9
1	G	298	GLN	2.9
1	G	292	GLU	2.9
1	J	315	LEU	2.9
1	A	137	ASN	2.9
1	G	57	ILE	2.8
1	G	151	ASN	2.8
1	E	152	ILE	2.8
1	A	175	TYR	2.8
1	B	293	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	112	ASN	2.8
1	G	287	GLN	2.8
1	I	64	GLU	2.8
1	I	252	ILE	2.8
1	H	185	GLN	2.8
1	G	178	LEU	2.8
1	B	150	GLU	2.8
1	H	69	ASN	2.7
1	G	317	ILE	2.7
1	I	207	SER	2.7
1	I	72	TRP	2.7
1	J	125	GLN	2.7
1	I	70	GLY	2.7
1	H	59	GLU	2.7
1	A	291	VAL	2.7
1	E	315	LEU	2.7
1	D	171	SER	2.6
1	D	181	VAL	2.6
1	C	51	PRO	2.6
1	C	178	LEU	2.6
1	H	309	LEU	2.6
1	C	303	ALA	2.6
1	D	157	ILE	2.6
1	H	165	LYS	2.6
1	J	157	ILE	2.6
1	C	121	PHE	2.6
1	E	47	PRO	2.6
1	J	298	GLN	2.5
1	J	194	ARG	2.5
1	C	316	VAL	2.5
1	G	11	PRO	2.5
1	G	255	ARG	2.5
1	I	250	SER	2.5
1	J	246	ALA	2.5
1	I	245	TYR	2.5
1	B	182	GLN	2.5
1	G	161	TRP	2.4
1	H	293	ASP	2.4
1	E	11	PRO	2.4
1	G	316	VAL	2.4
1	G	152	ILE	2.4
1	F	315	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	293	ASP	2.4
1	F	306	LEU	2.4
1	I	315	LEU	2.4
1	E	151	ASN	2.4
1	I	151	ASN	2.4
1	F	291	VAL	2.4
1	C	52	GLY	2.4
1	J	289	ASN	2.4
1	J	247	PHE	2.4
1	A	178	LEU	2.4
1	J	220	TRP	2.4
1	A	288	ALA	2.3
1	J	129	GLU	2.3
1	A	154	ASN	2.3
1	C	172	ASP	2.3
1	J	69	ASN	2.3
1	H	176	ASP	2.3
1	A	176	ASP	2.3
1	I	304	PHE	2.3
1	A	183	PRO	2.2
1	B	180	SER	2.2
1	D	150	GLU	2.2
1	G	294	ASP	2.2
1	G	284	HIS	2.2
1	C	302	LEU	2.2
1	G	160	TRP	2.2
1	F	143	SER	2.2
1	H	178	LEU	2.2
1	B	153	ASP	2.2
1	J	303	ALA	2.2
1	E	194	ARG	2.2
1	I	24	TYR	2.1
1	E	287	GLN	2.1
1	J	159	GLU	2.1
1	G	156	GLU	2.1
1	G	315	LEU	2.1
1	I	296	LEU	2.1
1	J	79	ILE	2.1
1	B	97	ASP	2.1
1	H	308	PHE	2.1
1	J	81	VAL	2.1
1	E	161	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	56	LEU	2.1
1	J	153	ASP	2.1
1	C	290	GLY	2.1
1	I	155	GLU	2.1
1	A	54	LYS	2.0
1	F	54	LYS	2.0
1	C	152	ILE	2.0
1	F	89	ASN	2.0
1	H	152	ILE	2.0
1	J	112	ASN	2.0
1	E	206	TRP	2.0
1	H	294	ASP	2.0
1	B	47	PRO	2.0
1	A	156	GLU	2.0
1	F	287	GLN	2.0
1	G	198	VAL	2.0
1	H	296	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

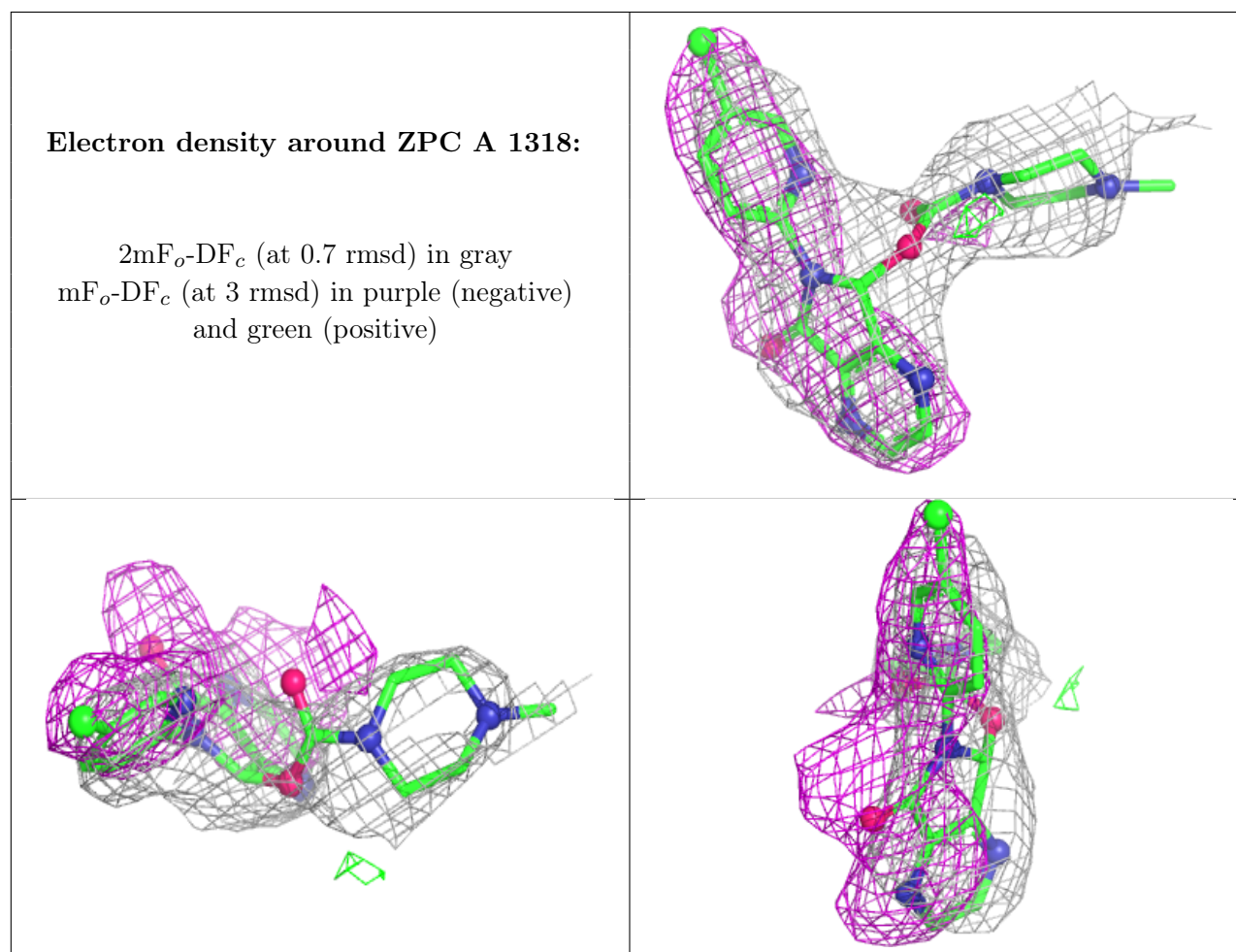
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZPC	A	1318	27/27	0.80	0.18	73,96,144,160	0
2	ZPC	D	1318	27/27	0.83	0.18	49,74,112,136	0
2	ZPC	I	1318	27/27	0.85	0.16	51,84,125,167	0
2	ZPC	H	1318	27/27	0.86	0.18	52,91,138,212	0
2	ZPC	E	1318	27/27	0.90	0.14	54,79,132,152	0
2	ZPC	G	1318	27/27	0.90	0.13	55,91,123,138	0

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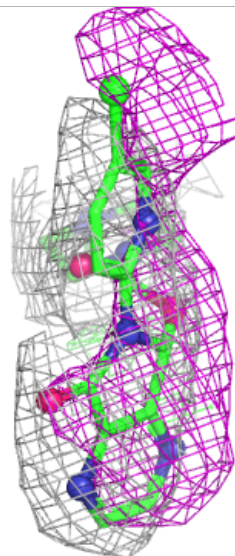
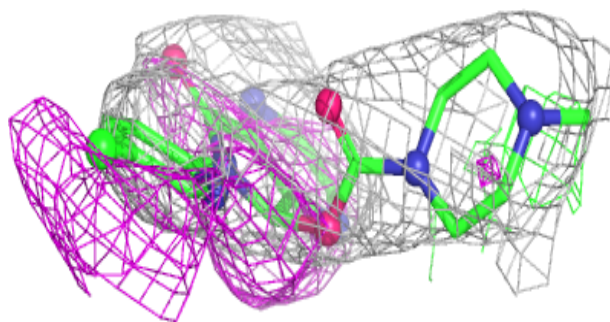
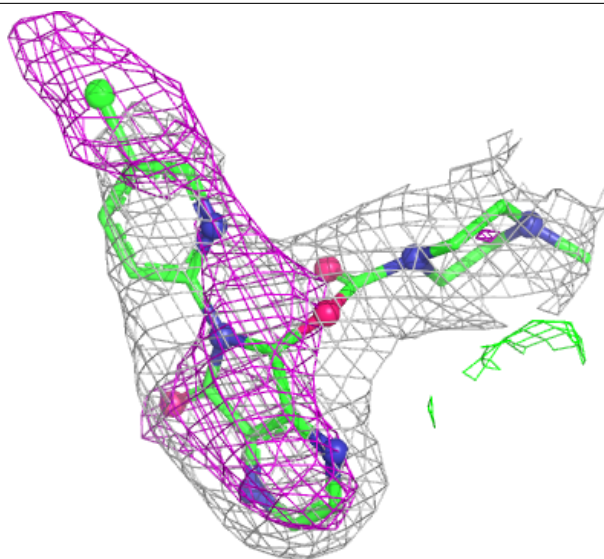
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZPC	C	1318	27/27	0.90	0.15	29,69,126,170	0
2	ZPC	B	1318	27/27	0.90	0.15	55,84,115,171	0
2	ZPC	F	1318	27/27	0.93	0.13	33,81,133,160	0
2	ZPC	J	1318	27/27	0.93	0.13	30,62,129,167	0

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.



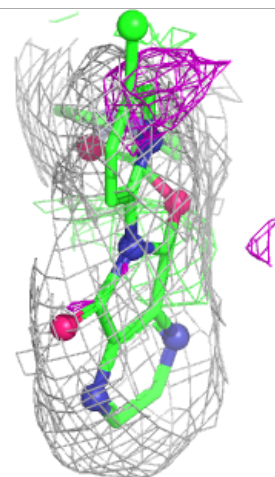
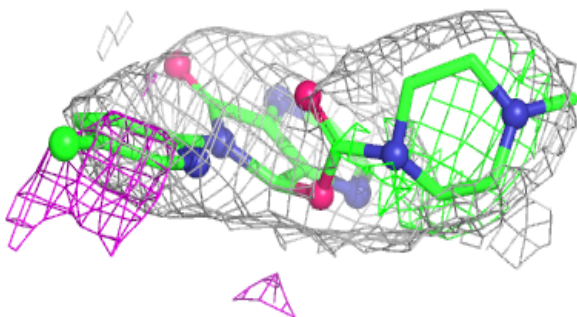
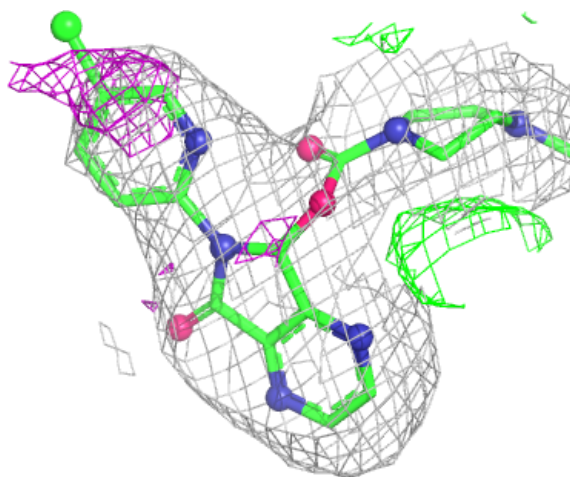
Electron density around ZPC D 1318:

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



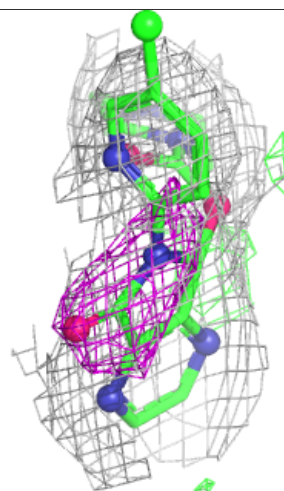
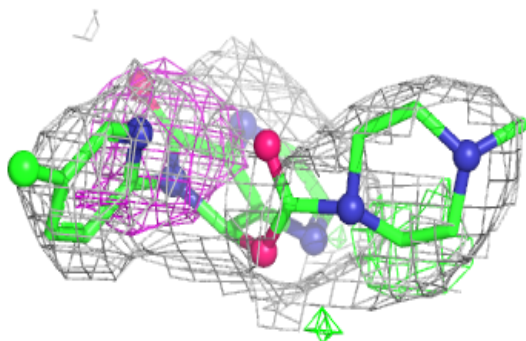
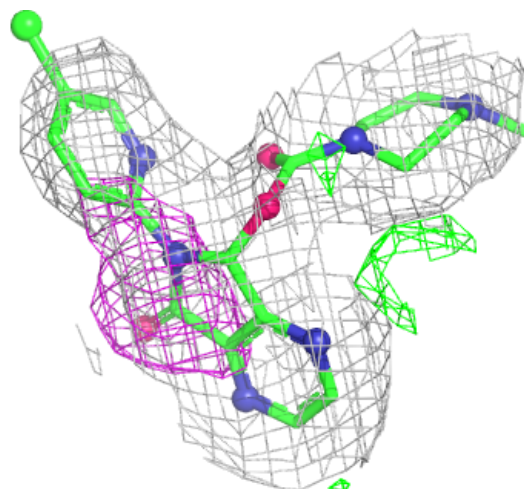
Electron density around ZPC I 1318:

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



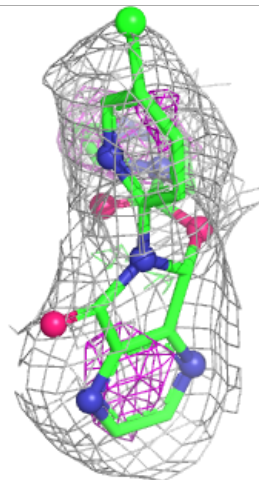
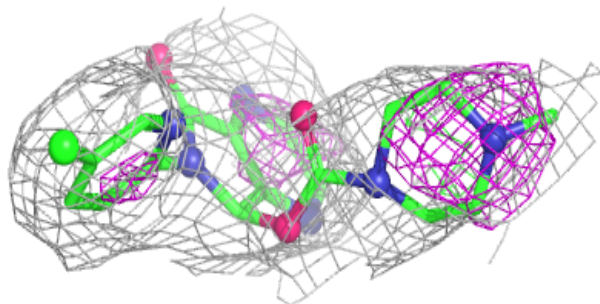
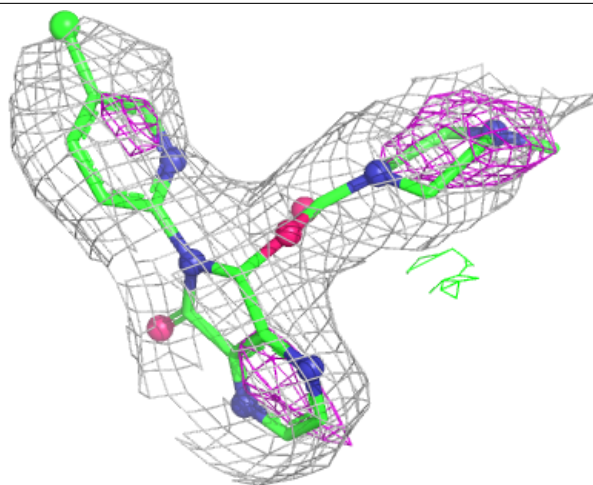
Electron density around ZPC H 1318:

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



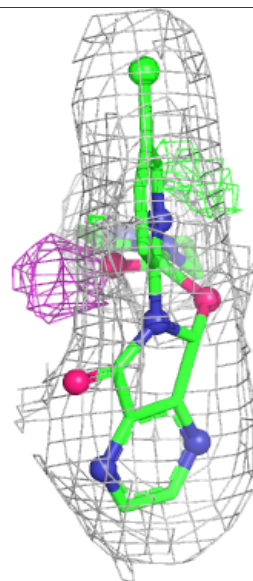
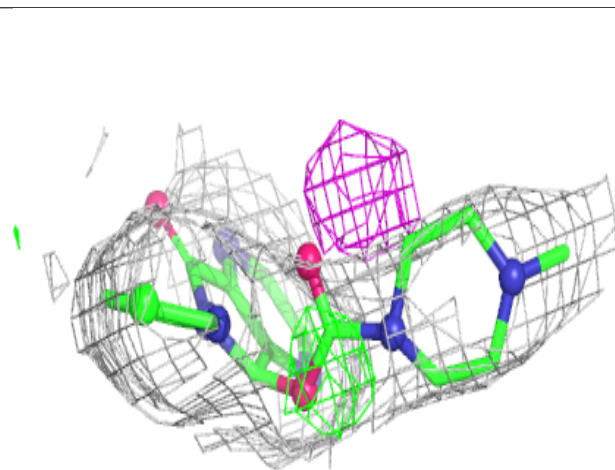
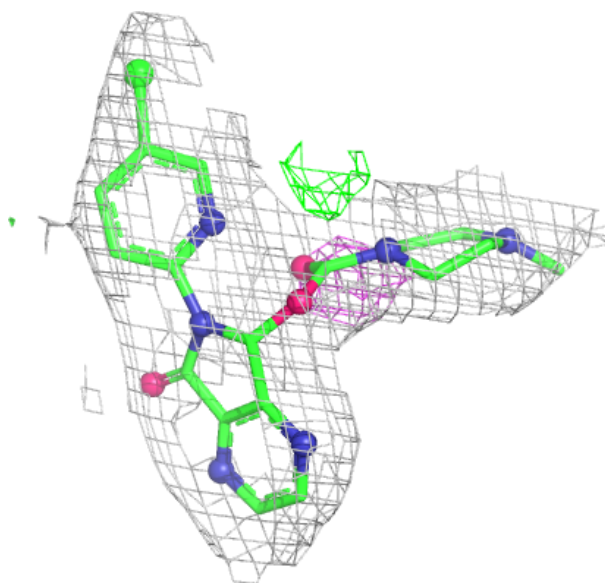
Electron density around ZPC E 1318:

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



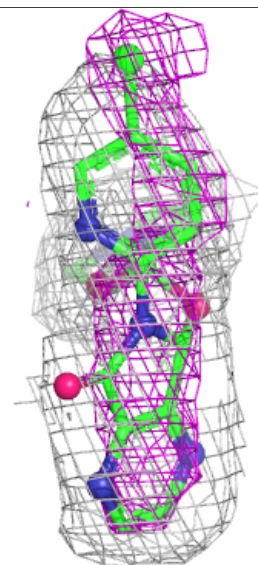
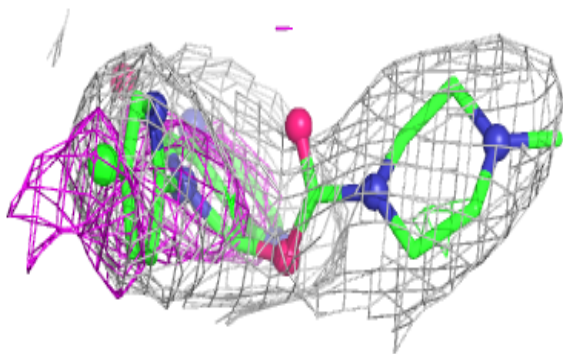
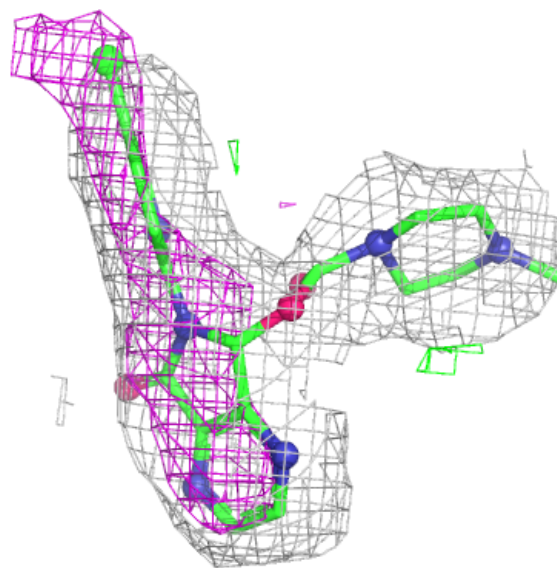
Electron density around ZPC G 1318:

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



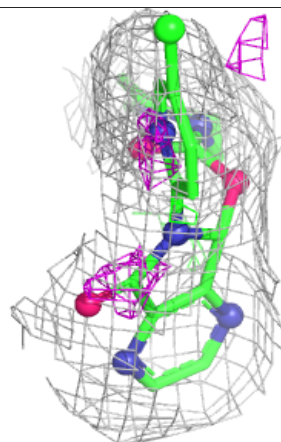
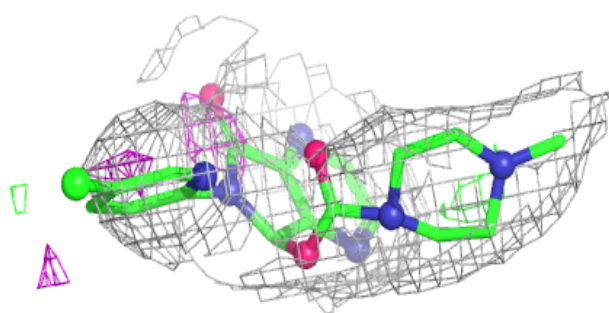
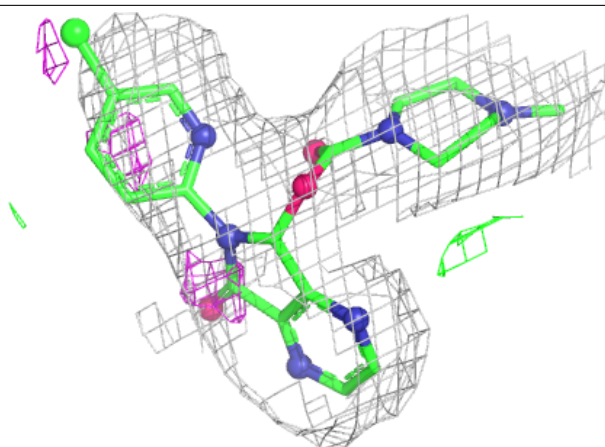
Electron density around ZPC C 1318:

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



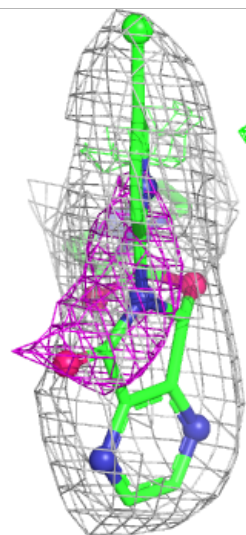
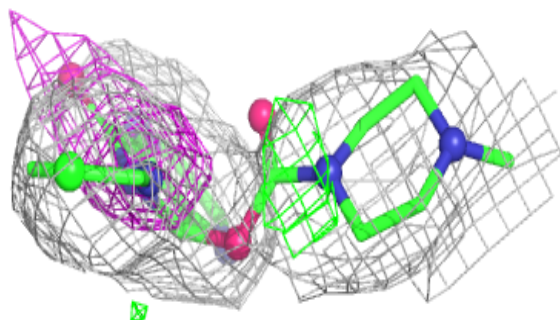
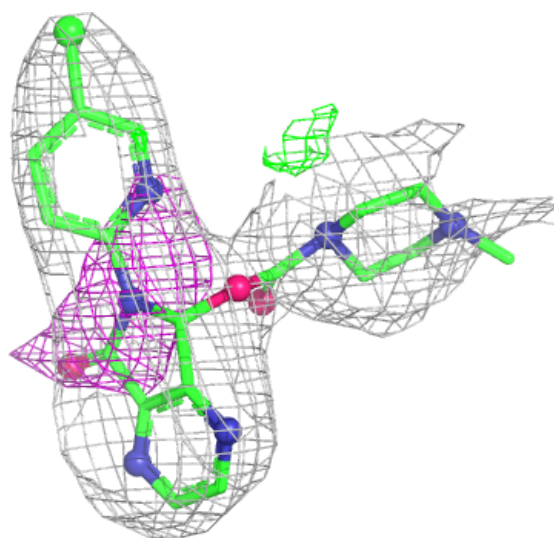
Electron density around ZPC B 1318:

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



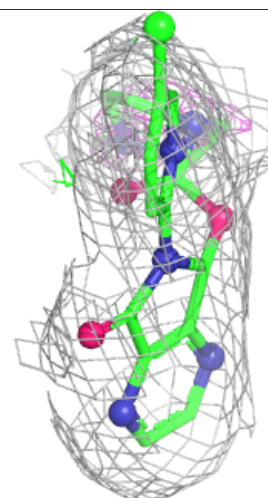
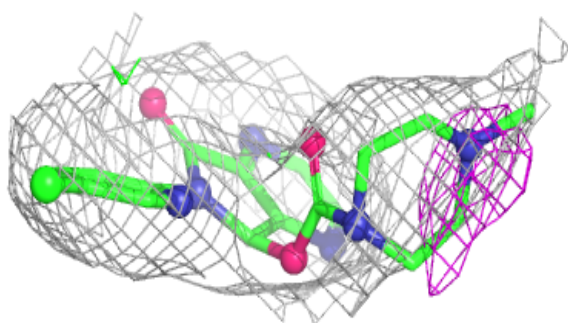
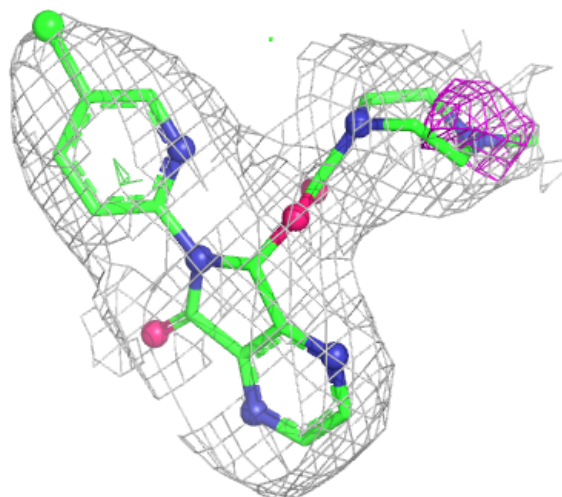
Electron density around ZPC F 1318:

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



Electron density around ZPC J 1318:

$2mF_o-DF_c$ (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.