



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:40 AM UTC

PDB ID : 5XO8 / pdb_00005xo8
Title : Crystal structure of a novel ZEN lactonase mutant with ligand Z
Authors : Zheng, Y.Y.; Liu, W.T.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on : 2017-05-27
Resolution : 1.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

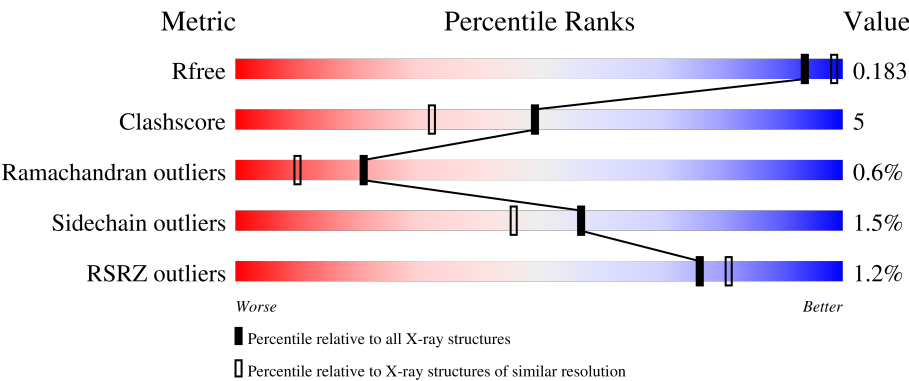
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	266	65%31%..
1	B	266	63%32%..
1	C	266	71%26%..
1	D	266	%71%24%..
1	E	266	75%22%..

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Mol	Chain	Length	Quality of chain
1	F	266	
1	G	266	
1	H	266	

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	ZER	A	301	-	-	X	-
2	ZER	B	301	-	-	X	-
2	ZER	G	301	-	-	X	-
2	ZER	H	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19224 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.

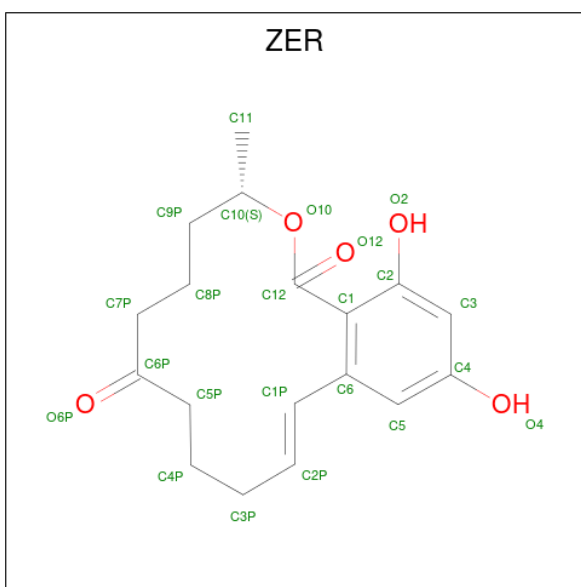
- Molecule 1 is a protein called Lactonase for protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	B	263	Total	C	N	O	S	0	1	0
			2063	1310	349	395	9			
1	C	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	D	264	Total	C	N	O	S	0	0	0
			2060	1309	348	394	9			
1	E	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	F	263	Total	C	N	O	S	0	0	0
			2055	1306	347	393	9			
1	G	262	Total	C	N	O	S	0	0	0
			2045	1300	345	391	9			
1	H	263	Total	C	N	O	S	0	1	0
			2058	1307	348	394	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
B	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
C	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
D	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
E	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
F	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
G	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1
H	105	ALA	SER	engineered mutation	UNP A0A0D2ILK1

- Molecule 2 is (3S,11E)-14,16-dihydroxy-3-methyl-3,4,5,6,9,10-hexahydro-1H-2-benzoxacyclo tetradecine-1,7(8H)-dione (CCD ID: ZER) (formula: C₁₈H₂₂O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 18 5	0	0
2	B	1	Total C O 23 18 5	0	0
2	C	1	Total C O 23 18 5	0	0
2	D	1	Total C O 23 18 5	0	0
2	E	1	Total C O 23 18 5	0	0
2	F	1	Total C O 23 18 5	0	0
2	G	1	Total C O 23 18 5	0	0
2	H	1	Total C O 23 18 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	397	Total O 397 397	0	0
3	B	390	Total O 390 390	0	0
3	C	324	Total O 324 324	0	0
3	D	316	Total O 316 316	0	0

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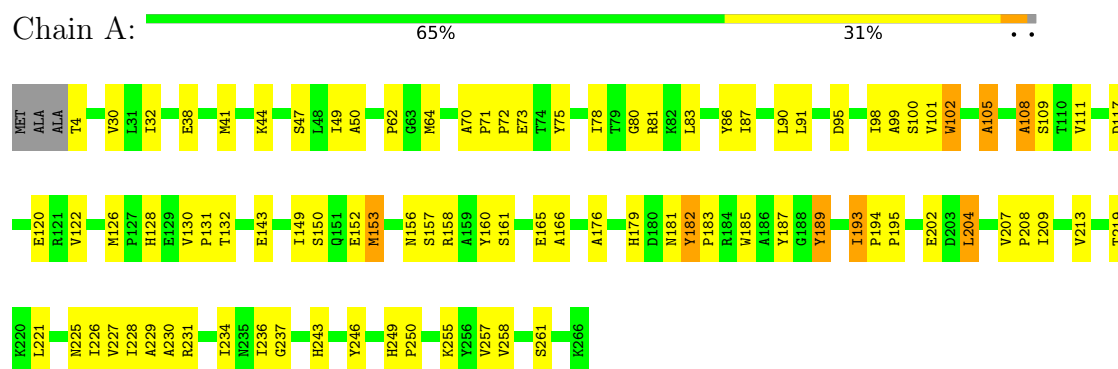
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	292	Total 292	O 292	0	0
3	F	209	Total 209	O 209	0	0
3	G	311	Total 311	O 311	0	0
3	H	355	Total 355	O 355	0	0

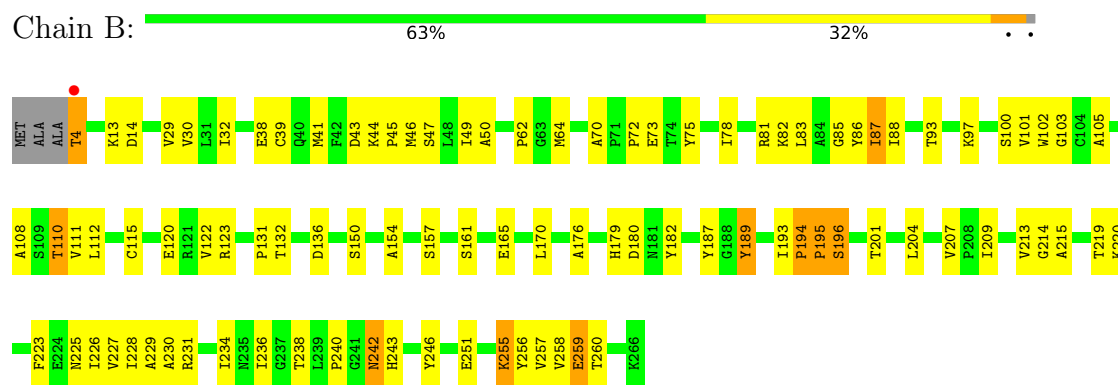
3 Residue-property plots [i](#)

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.

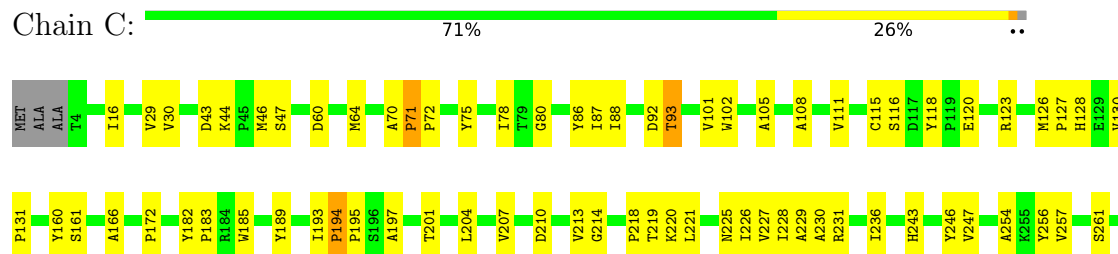
• Molecule 1: Lactonase for protein



• Molecule 1: Lactonase for protein

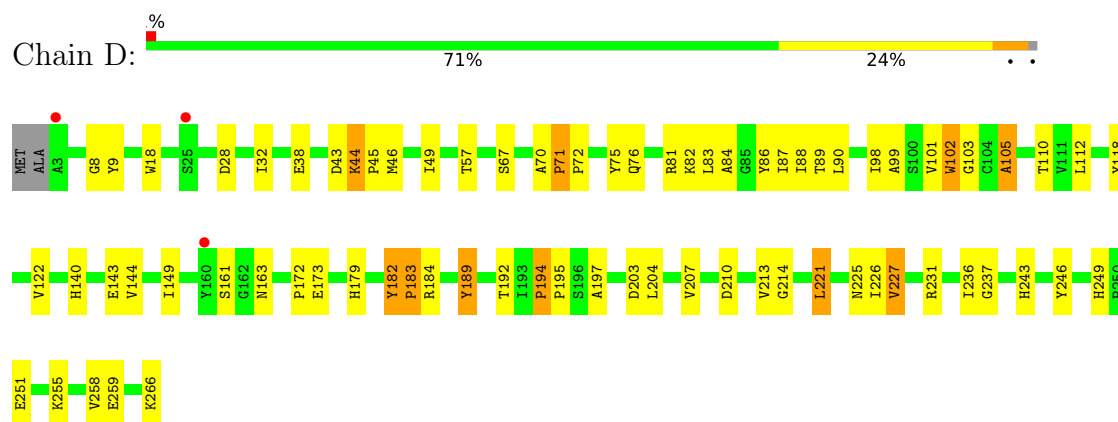


• Molecule 1: Lactonase for protein

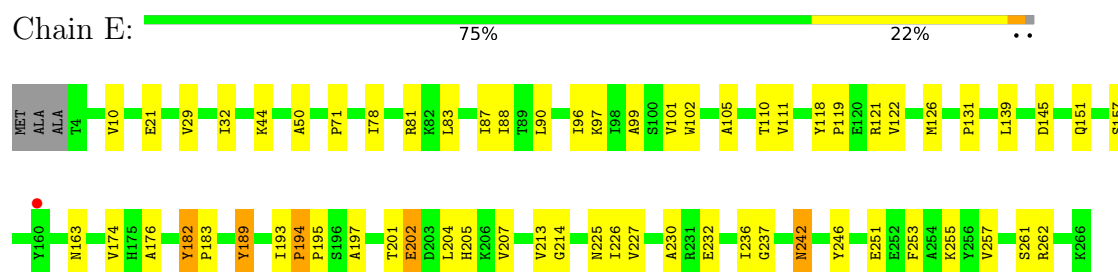


K266

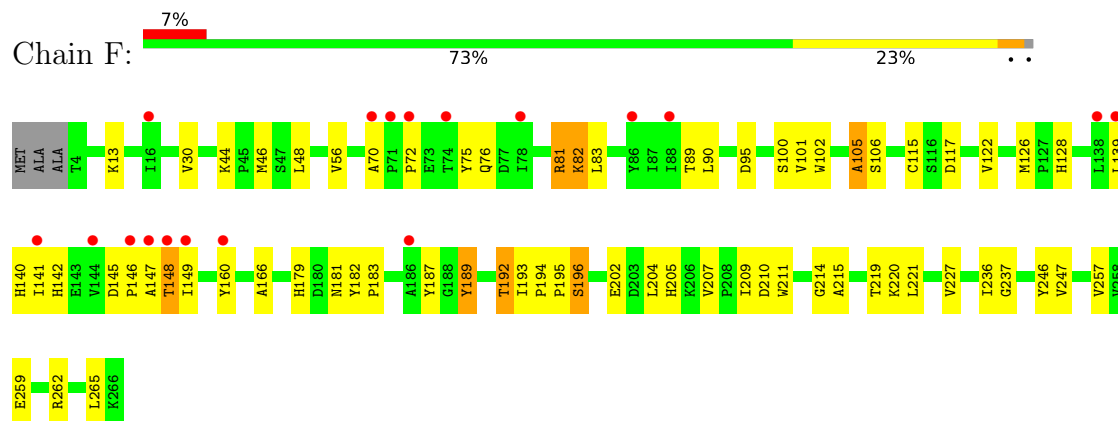
- Molecule 1: Lactonase for protein



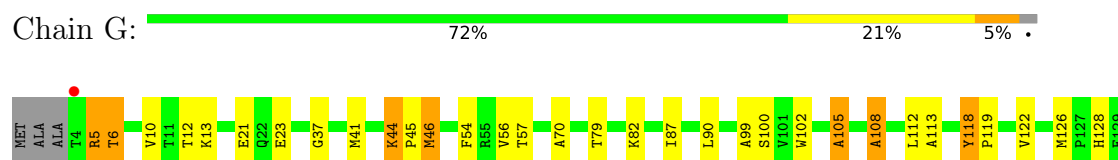
- Molecule 1: Lactonase for protein

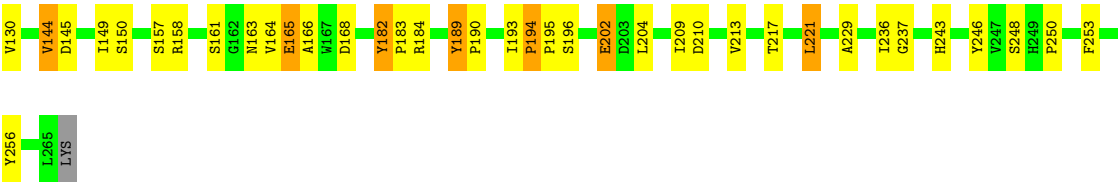


- Molecule 1: Lactonase for protein

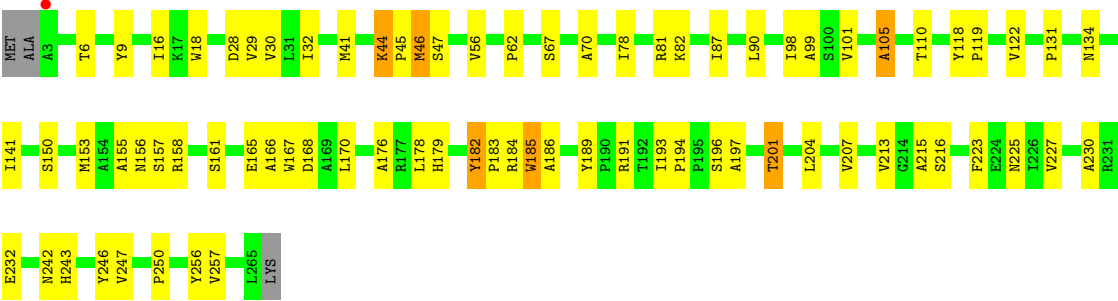


- Molecule 1: Lactonase for protein





• Molecule 1: Lactonase for protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.47Å 95.20Å 101.66Å 90.21° 92.34° 91.48°	Depositor
Resolution (Å)	24.95 – 1.88 24.95 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.7 (24.95-1.88) 97.7 (24.95-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.145 , 0.181 0.158 , 0.183	Depositor DCC
R_{free} test set	2000 reflections (0.87%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l 0.010 for -h,k,-l 0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19224	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: ZER

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.95	72/2114 (3.4%)	1.09	7/2886 (0.2%)
1	B	1.93	80/2122 (3.8%)	1.08	9/2897 (0.3%)
1	C	1.86	51/2114 (2.4%)	1.06	5/2886 (0.2%)
1	D	1.85	51/2119 (2.4%)	1.09	9/2893 (0.3%)
1	E	1.79	38/2114 (1.8%)	1.07	13/2886 (0.5%)
1	F	1.74	31/2114 (1.5%)	1.15	11/2886 (0.4%)
1	G	1.85	46/2104 (2.2%)	1.10	13/2875 (0.5%)
1	H	1.89	60/2117 (2.8%)	1.06	8/2893 (0.3%)
All	All	1.86	429/16918 (2.5%)	1.09	75/23102 (0.3%)

All (429) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	207	VAL	C-O	-10.53	1.16	1.24
1	E	207	VAL	C-O	-9.83	1.16	1.24
1	B	207	VAL	C-O	-9.53	1.16	1.24
1	F	207	VAL	C-O	-9.44	1.16	1.24
1	G	105	ALA	C-O	-8.60	1.16	1.24
1	F	259	GLU	C-N	-7.91	1.23	1.33
1	B	70	ALA	C-O	-7.78	1.17	1.24
1	C	207	VAL	C-O	-7.49	1.18	1.24
1	B	44	LYS	C-O	-7.49	1.17	1.24
1	B	193	ILE	C-O	-7.38	1.18	1.24
1	A	120	GLU	C-N	-7.29	1.23	1.33
1	H	158	ARG	C-O	-7.24	1.15	1.24
1	E	213	VAL	C-O	-7.23	1.16	1.24
1	A	44	LYS	C-O	-7.15	1.17	1.24
1	A	236	ILE	C-O	-7.15	1.16	1.24
1	D	214	GLY	C-O	-7.10	1.17	1.24
1	B	39	CYS	C-O	-7.03	1.14	1.24
1	D	194	PRO	C-O	-7.03	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	VAL	C-O	-7.02	1.16	1.24
1	F	83	LEU	C-O	-6.96	1.15	1.24
1	A	207	VAL	C-O	-6.92	1.18	1.24
1	D	44	LYS	C-O	-6.89	1.18	1.24
1	D	118	TYR	C-O	-6.88	1.16	1.23
1	A	71	PRO	C-O	-6.88	1.19	1.25
1	A	209	ILE	C-O	-6.88	1.17	1.24
1	A	73	GLU	C-O	-6.87	1.15	1.24
1	C	229	ALA	C-O	-6.84	1.16	1.24
1	B	179	HIS	C-O	-6.81	1.16	1.24
1	B	176	ALA	C-O	-6.81	1.16	1.24
1	H	70	ALA	C-O	-6.78	1.16	1.24
1	C	236	ILE	C-O	-6.74	1.17	1.24
1	F	181	ASN	C-O	-6.74	1.16	1.24
1	H	193	ILE	C-O	-6.73	1.18	1.24
1	D	179	HIS	C-O	-6.72	1.16	1.24
1	A	122	VAL	C-O	-6.66	1.17	1.24
1	C	193	ILE	C-O	-6.65	1.19	1.24
1	A	126	MET	C-O	-6.64	1.16	1.24
1	G	44	LYS	C-O	-6.63	1.18	1.24
1	A	225	ASN	C-O	-6.58	1.16	1.24
1	D	182	TYR	C-O	-6.57	1.18	1.24
1	G	157	SER	C-O	-6.57	1.16	1.24
1	A	105	ALA	C-O	-6.56	1.18	1.24
1	C	126	MET	C-O	-6.48	1.16	1.24
1	A	157	SER	C-O	-6.42	1.16	1.24
1	F	128	HIS	C-O	-6.41	1.16	1.24
1	C	194	PRO	C-O	-6.41	1.17	1.24
1	A	166	ALA	C-O	-6.39	1.16	1.24
1	A	179	HIS	C-O	-6.38	1.16	1.24
1	A	193	ILE	C-O	-6.37	1.19	1.24
1	B	122	VAL	C-O	-6.36	1.17	1.24
1	H	197	ALA	C-O	-6.36	1.16	1.24
1	A	255	LYS	C-O	-6.36	1.16	1.24
1	A	128	HIS	C-O	-6.34	1.16	1.24
1	H	176	ALA	C-O	-6.29	1.16	1.24
1	D	105	ALA	C-O	-6.29	1.18	1.24
1	D	207	VAL	C-O	-6.28	1.16	1.24
1	C	230	ALA	C-O	-6.28	1.16	1.24
1	H	105	ALA	C-O	-6.27	1.18	1.24
1	A	70	ALA	C-O	-6.26	1.17	1.24
1	D	227	VAL	C-O	-6.26	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	30	VAL	C-O	-6.24	1.17	1.24
1	G	165	GLU	C-O	-6.24	1.16	1.24
1	C	111	VAL	C-O	-6.22	1.17	1.24
1	A	229	ALA	C-O	-6.21	1.17	1.24
1	E	197	ALA	C-O	-6.21	1.16	1.24
1	E	237	GLY	C-O	-6.21	1.16	1.23
1	B	230	ALA	C-O	-6.21	1.16	1.24
1	H	44	LYS	C-O	-6.20	1.18	1.24
1	E	101	VAL	C-O	-6.20	1.17	1.24
1	B	123	ARG	C-O	-6.19	1.17	1.24
1	B	115	CYS	C-O	-6.17	1.16	1.24
1	A	228	ILE	C-O	-6.16	1.17	1.24
1	G	184	ARG	C-O	-6.13	1.17	1.24
1	F	105	ALA	C-O	-6.13	1.19	1.24
1	A	38	GLU	C-O	-6.12	1.16	1.24
1	F	193	ILE	C-O	-6.11	1.19	1.24
1	C	228	ILE	C-O	-6.11	1.17	1.24
1	H	161	SER	C-O	-6.11	1.16	1.24
1	F	166	ALA	C-O	-6.11	1.17	1.24
1	F	48	LEU	C-O	-6.10	1.17	1.24
1	H	201	THR	C-O	-6.10	1.17	1.24
1	A	161	SER	C-O	-6.10	1.16	1.24
1	D	70	ALA	C-O	-6.09	1.17	1.24
1	C	185	TRP	C-O	-6.06	1.17	1.24
1	G	237	GLY	C-O	-6.06	1.17	1.23
1	E	10	VAL	C-O	-6.06	1.17	1.23
1	G	70	ALA	C-O	-6.06	1.17	1.24
1	D	213	VAL	C-O	-6.05	1.18	1.24
1	C	166	ALA	C-O	-6.05	1.17	1.24
1	E	44	LYS	C-O	-6.04	1.18	1.24
1	D	84	ALA	C-O	-6.04	1.17	1.24
1	B	103	GLY	C-O	-6.03	1.15	1.23
1	A	62	PRO	C-O	-6.03	1.15	1.23
1	C	225	ASN	C-O	-6.02	1.17	1.24
1	A	258	VAL	C-O	-6.01	1.17	1.24
1	A	149	ILE	C-O	-6.00	1.17	1.24
1	A	249	HIS	C-O	-6.00	1.17	1.24
1	G	182	TYR	C-O	-5.99	1.18	1.24
1	B	255	LYS	C-O	-5.97	1.17	1.24
1	F	214	GLY	C-O	-5.96	1.17	1.23
1	B	220	LYS	C-O	-5.96	1.17	1.24
1	D	210	ASP	C-O	-5.96	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	96	ILE	C-O	-5.96	1.17	1.24
1	B	150	SER	C-O	-5.95	1.17	1.24
1	D	49	ILE	C-O	-5.94	1.17	1.24
1	C	256	TYR	C-O	-5.91	1.17	1.24
1	C	86	TYR	C-O	-5.90	1.17	1.24
1	H	247	VAL	C-O	-5.90	1.17	1.23
1	B	214	GLY	C-O	-5.89	1.17	1.23
1	A	49	ILE	C-O	-5.89	1.17	1.24
1	A	87	ILE	C-O	-5.88	1.17	1.24
1	D	161	SER	C-O	-5.85	1.17	1.24
1	B	85	GLY	C-O	-5.85	1.16	1.23
1	A	257	VAL	C-O	-5.85	1.17	1.24
1	B	236	ILE	C-O	-5.85	1.18	1.24
1	H	257	VAL	C-O	-5.84	1.17	1.24
1	B	258	VAL	C-O	-5.84	1.17	1.24
1	B	88	ILE	C-O	-5.83	1.17	1.24
1	E	83	LEU	C-O	-5.83	1.17	1.24
1	G	210	ASP	C-O	-5.83	1.17	1.24
1	B	47	SER	C-O	-5.82	1.17	1.24
1	B	182	TYR	C-O	-5.82	1.18	1.24
1	H	99	ALA	C-O	-5.81	1.16	1.23
1	A	213	VAL	C-O	-5.80	1.18	1.23
1	H	186	ALA	C-O	-5.80	1.17	1.24
1	G	57	THR	C-O	-5.80	1.17	1.24
1	A	30	VAL	C-O	-5.79	1.18	1.24
1	A	101	VAL	C-O	-5.79	1.18	1.24
1	B	112	LEU	C-O	-5.79	1.17	1.24
1	G	256	TYR	C-O	-5.79	1.17	1.24
1	C	115	CYS	C-O	-5.78	1.16	1.24
1	H	194	PRO	C-O	-5.78	1.18	1.24
1	E	111	VAL	C-O	-5.78	1.17	1.24
1	G	128	HIS	C-O	-5.78	1.17	1.24
1	H	167	TRP	C-O	-5.77	1.17	1.24
1	G	126	MET	C-O	-5.77	1.17	1.24
1	C	161	SER	C-O	-5.76	1.17	1.24
1	A	108	ALA	C-O	-5.75	1.17	1.24
1	E	126	MET	C-O	-5.75	1.17	1.24
1	F	210	ASP	C-O	-5.75	1.17	1.24
1	F	220	LYS	C-O	-5.74	1.17	1.24
1	E	226	ILE	C-O	-5.73	1.17	1.24
1	E	230	ALA	C-O	-5.71	1.17	1.24
1	E	90	LEU	C-O	-5.71	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	TYR	C-O	-5.70	1.17	1.24
1	D	258	VAL	C-N	5.70	1.40	1.33
1	B	228	ILE	C-O	-5.70	1.17	1.24
1	H	182	TYR	C-O	-5.69	1.19	1.24
1	B	81	ARG	C-O	-5.68	1.17	1.24
1	F	106	SER	C-O	-5.67	1.17	1.24
1	F	115	CYS	C-O	-5.67	1.17	1.24
1	D	87	ILE	C-O	-5.67	1.17	1.24
1	H	82	LYS	C-O	-5.67	1.17	1.24
1	F	46	MET	C-O	-5.66	1.17	1.24
1	E	193	ILE	C-O	-5.66	1.17	1.24
1	B	86	TYR	C-O	-5.65	1.17	1.24
1	B	229	ALA	C-O	-5.65	1.17	1.24
1	B	260	THR	C-O	-5.65	1.17	1.24
1	H	213	VAL	C-O	-5.65	1.18	1.23
1	A	261	SER	C-O	-5.64	1.17	1.24
1	C	60	ASP	C-O	-5.64	1.17	1.23
1	A	91	LEU	C-O	-5.63	1.17	1.24
1	G	150	SER	C-O	-5.63	1.17	1.24
1	A	80	GLY	C-O	-5.62	1.17	1.23
1	A	86	TYR	C-O	-5.62	1.17	1.24
1	H	170	LEU	C-O	-5.62	1.17	1.24
1	B	201	THR	C-O	-5.62	1.17	1.24
1	B	170	LEU	C-O	-5.61	1.17	1.24
1	C	47	SER	C-O	-5.61	1.17	1.24
1	D	122	VAL	C-O	-5.61	1.18	1.24
1	B	73	GLU	C-O	-5.61	1.17	1.24
1	H	230	ALA	C-O	-5.61	1.17	1.24
1	B	259	GLU	C-O	-5.61	1.17	1.24
1	B	105	ALA	C-O	-5.61	1.19	1.24
1	C	87	ILE	C-O	-5.61	1.17	1.24
1	C	261	SER	C-O	-5.61	1.17	1.24
1	H	184	ARG	C-O	-5.61	1.17	1.24
1	B	64	MET	C-O	-5.60	1.17	1.23
1	C	70	ALA	C-O	-5.59	1.18	1.24
1	B	161	SER	C-O	-5.59	1.17	1.24
1	B	256	TYR	C-O	-5.59	1.17	1.24
1	E	236	ILE	C-O	-5.59	1.18	1.24
1	E	182	TYR	C-O	-5.59	1.19	1.24
1	B	97	LYS	C-O	-5.58	1.17	1.24
1	H	134	ASN	C-O	-5.58	1.16	1.23
1	H	30	VAL	C-O	-5.57	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	213	VAL	C-O	-5.57	1.18	1.24
1	H	168	ASP	C-O	-5.57	1.17	1.24
1	B	82	LYS	C-O	-5.57	1.17	1.24
1	E	255	LYS	C-O	-5.56	1.17	1.24
1	H	215	ALA	C-O	-5.56	1.17	1.24
1	B	187	TYR	C-O	-5.56	1.17	1.24
1	H	141	ILE	C-O	-5.55	1.17	1.24
1	A	219	THR	C-O	-5.55	1.17	1.24
1	B	87	ILE	C-O	-5.55	1.17	1.24
1	G	250	PRO	C-O	-5.55	1.17	1.24
1	A	98	ILE	C-O	-5.54	1.17	1.23
1	C	128	HIS	C-O	-5.53	1.17	1.24
1	C	120	GLU	C-O	-5.53	1.16	1.24
1	B	110	THR	C-O	-5.53	1.17	1.24
1	B	111	VAL	C-O	-5.53	1.17	1.24
1	E	261	SER	C-O	-5.53	1.17	1.24
1	D	112	LEU	C-O	-5.52	1.17	1.24
1	H	165	GLU	C-O	-5.52	1.17	1.24
1	B	154	ALA	C-O	-5.52	1.17	1.24
1	C	214	GLY	C-O	-5.52	1.18	1.23
1	G	10	VAL	C-O	-5.52	1.18	1.23
1	H	98	ILE	C-O	-5.52	1.17	1.23
1	H	227	VAL	C-O	-5.51	1.18	1.24
1	C	226	ILE	C-O	-5.51	1.18	1.24
1	B	108	ALA	C-O	-5.51	1.17	1.24
1	C	210	ASP	C-O	-5.50	1.17	1.24
1	G	79	THR	C-O	-5.50	1.17	1.23
1	G	236	ILE	C-O	-5.48	1.18	1.24
1	G	248	SER	C-O	-5.48	1.17	1.24
1	C	213	VAL	C-O	-5.47	1.18	1.24
1	E	214	GLY	C-O	-5.47	1.18	1.23
1	A	117	ASP	C-O	-5.46	1.17	1.24
1	F	44	LYS	C-O	-5.46	1.19	1.24
1	H	131	PRO	C-O	-5.45	1.18	1.23
1	H	16	ILE	C-O	-5.45	1.18	1.24
1	H	185	TRP	C-O	-5.45	1.17	1.24
1	G	209	ILE	C-O	-5.45	1.18	1.24
1	A	131	PRO	C-O	-5.44	1.18	1.23
1	D	237	GLY	C-O	-5.44	1.17	1.23
1	F	219	THR	C-O	-5.44	1.17	1.24
1	H	47	SER	C-O	-5.43	1.17	1.24
1	G	5	ARG	C-O	-5.43	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	29	VAL	C-O	-5.43	1.18	1.24
1	D	110	THR	C-O	-5.43	1.17	1.24
1	H	67	SER	C-O	-5.43	1.17	1.24
1	D	43	ASP	C-O	-5.42	1.17	1.24
1	E	194	PRO	C-O	-5.42	1.18	1.24
1	F	126	MET	C-O	-5.42	1.18	1.24
1	C	201	THR	C-O	-5.42	1.17	1.24
1	C	219	THR	C-O	-5.42	1.17	1.24
1	D	88	ILE	C-O	-5.41	1.18	1.24
1	C	92	ASP	C-O	-5.41	1.17	1.24
1	C	197	ALA	C-O	-5.41	1.17	1.24
1	H	46	MET	C-O	-5.41	1.17	1.24
1	B	195	PRO	C-O	-5.40	1.17	1.24
1	E	174	VAL	C-O	-5.40	1.18	1.24
1	H	250	PRO	C-O	-5.40	1.17	1.24
1	D	249	HIS	C-O	-5.40	1.17	1.24
1	A	83	LEU	C-O	-5.40	1.17	1.24
1	A	90	LEU	C-O	-5.40	1.17	1.24
1	F	237	GLY	C-O	-5.39	1.17	1.23
1	D	225	ASN	C-O	-5.39	1.18	1.24
1	E	257	VAL	C-O	-5.38	1.17	1.24
1	D	172	PRO	C-O	-5.38	1.17	1.24
1	B	238	THR	C-O	-5.38	1.17	1.23
1	G	87	ILE	C-O	-5.38	1.17	1.24
1	H	157	SER	C-O	-5.38	1.18	1.24
1	H	225	ASN	C-O	-5.37	1.18	1.24
1	E	88	ILE	C-O	-5.37	1.17	1.24
1	H	56	VAL	C-O	-5.37	1.18	1.24
1	B	45	PRO	C-O	-5.37	1.17	1.24
1	D	184	ARG	C-O	-5.37	1.18	1.24
1	D	183	PRO	C-O	-5.36	1.17	1.24
1	A	156	ASN	C-O	-5.35	1.18	1.24
1	D	8	GLY	C-O	-5.35	1.18	1.23
1	F	227	VAL	C-O	-5.34	1.18	1.24
1	B	180	ASP	C-O	-5.34	1.17	1.24
1	G	243	HIS	C-O	-5.33	1.17	1.24
1	C	88	ILE	C-O	-5.33	1.18	1.24
1	F	81	ARG	C-O	-5.33	1.17	1.24
1	C	78	ILE	C-O	-5.32	1.17	1.24
1	D	89	THR	C-O	-5.32	1.17	1.24
1	A	78	ILE	C-O	-5.32	1.17	1.24
1	B	223	PHE	C-O	-5.32	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	256	TYR	C-O	-5.32	1.18	1.24
1	G	41	MET	C-O	-5.31	1.17	1.24
1	B	213	VAL	C-O	-5.31	1.18	1.23
1	A	109	SER	C-O	-5.30	1.18	1.24
1	C	118	TYR	C-O	-5.30	1.18	1.23
1	D	173	GLU	C-O	-5.30	1.18	1.24
1	A	208	PRO	C-O	-5.30	1.17	1.23
1	D	86	TYR	C-O	-5.30	1.18	1.24
1	B	49	ILE	C-O	-5.30	1.18	1.24
1	B	157	SER	C-O	-5.30	1.18	1.24
1	B	209	ILE	C-O	-5.29	1.18	1.24
1	B	251	GLU	C-O	-5.29	1.18	1.24
1	F	90	LEU	C-O	-5.29	1.18	1.24
1	C	220	LYS	C-O	-5.29	1.17	1.24
1	H	29	VAL	C-O	-5.29	1.18	1.24
1	F	247	VAL	C-O	-5.29	1.17	1.23
1	G	112	LEU	C-O	-5.28	1.17	1.24
1	D	101	VAL	C-O	-5.28	1.18	1.24
1	E	122	VAL	C-O	-5.28	1.18	1.24
1	H	166	ALA	C-O	-5.28	1.18	1.24
1	A	187	TYR	C-O	-5.28	1.17	1.24
1	E	50	ALA	C-O	-5.28	1.17	1.24
1	B	234	ILE	C-O	-5.27	1.17	1.24
1	H	223	PHE	C-O	-5.27	1.18	1.24
1	B	240	PRO	C-O	-5.27	1.17	1.23
1	F	257	VAL	C-O	-5.27	1.18	1.24
1	E	21	GLU	C-O	-5.27	1.17	1.23
1	C	44	LYS	C-O	-5.27	1.19	1.24
1	D	81	ARG	C-O	-5.27	1.18	1.24
1	E	99	ALA	C-O	-5.26	1.17	1.23
1	E	251	GLU	C-O	-5.26	1.18	1.24
1	B	246	TYR	C-O	-5.26	1.17	1.24
1	H	6	THR	C-O	-5.26	1.17	1.24
1	G	108	ALA	C-O	-5.26	1.17	1.24
1	A	182	TYR	C-O	-5.25	1.19	1.24
1	G	113	ALA	C-O	-5.25	1.18	1.24
1	H	28	ASP	C-O	-5.25	1.17	1.23
1	E	262	ARG	C-O	-5.24	1.18	1.24
1	C	16	ILE	C-O	-5.24	1.18	1.24
1	D	258	VAL	C-O	-5.24	1.18	1.24
1	G	23	GLU	C-O	-5.24	1.17	1.23
1	D	251	GLU	C-O	-5.24	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	81	ARG	C-O	-5.24	1.18	1.24
1	B	136	ASP	C-O	-5.23	1.18	1.24
1	G	56	VAL	C-O	-5.23	1.17	1.24
1	B	131	PRO	C-O	-5.23	1.17	1.23
1	A	81	ARG	C-O	-5.23	1.17	1.24
1	B	29	VAL	C-O	-5.23	1.18	1.24
1	H	155	ALA	C-O	-5.23	1.17	1.24
1	A	226	ILE	C-O	-5.22	1.18	1.24
1	D	203	ASP	C-O	-5.22	1.17	1.24
1	C	80	GLY	C-O	-5.22	1.17	1.23
1	A	237	GLY	C-O	-5.22	1.18	1.23
1	C	64	MET	C-O	-5.22	1.17	1.23
1	A	132	THR	C-O	-5.21	1.17	1.24
1	B	226	ILE	C-O	-5.21	1.18	1.24
1	F	215	ALA	C-O	-5.21	1.17	1.24
1	A	202	GLU	C-O	-5.21	1.17	1.24
1	A	176	ALA	C-O	-5.20	1.18	1.24
1	D	57	THR	C-O	-5.20	1.17	1.23
1	F	209	ILE	C-O	-5.20	1.19	1.24
1	G	217	THR	C-O	-5.20	1.17	1.24
1	G	168	ASP	C-O	-5.20	1.18	1.24
1	H	191	ARG	C-O	-5.20	1.17	1.24
1	G	161	SER	C-O	-5.20	1.17	1.24
1	A	153	MET	C-O	-5.20	1.17	1.24
1	C	254	ALA	C-O	-5.19	1.18	1.24
1	B	50	ALA	C-O	-5.19	1.18	1.24
1	H	178	LEU	C-O	-5.19	1.18	1.24
1	A	102	TRP	C-O	-5.18	1.17	1.23
1	B	219	THR	C-O	-5.18	1.17	1.24
1	D	38	GLU	C-O	-5.18	1.17	1.23
1	D	67	SER	C-O	-5.17	1.17	1.24
1	A	111	VAL	C-O	-5.17	1.18	1.24
1	F	30	VAL	C-O	-5.17	1.18	1.24
1	B	62	PRO	C-O	-5.17	1.17	1.23
1	H	90	LEU	C-O	-5.17	1.18	1.24
1	F	189	TYR	C-O	-5.16	1.17	1.24
1	G	253	PHE	C-O	-5.16	1.18	1.24
1	G	21	GLU	C-O	-5.16	1.17	1.23
1	F	262	ARG	C-O	-5.16	1.17	1.24
1	G	194	PRO	C-O	-5.16	1.18	1.24
1	A	41	MET	C-O	-5.16	1.17	1.24
1	D	82	LYS	C-O	-5.15	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	226	ILE	C-O	-5.15	1.18	1.24
1	C	123	ARG	C-O	-5.15	1.18	1.24
1	D	90	LEU	C-O	-5.15	1.18	1.24
1	D	197	ALA	C-O	-5.15	1.17	1.24
1	H	216	SER	C-O	-5.15	1.17	1.24
1	G	221	LEU	C-O	-5.15	1.18	1.24
1	H	81	ARG	C-O	-5.15	1.18	1.24
1	E	242	ASN	C-O	-5.14	1.17	1.24
1	B	257	VAL	C-O	-5.14	1.18	1.24
1	H	62	PRO	C-O	-5.14	1.16	1.23
1	E	225	ASN	C-O	-5.14	1.18	1.24
1	G	166	ALA	C-O	-5.13	1.18	1.24
1	A	250	PRO	C-O	-5.13	1.17	1.24
1	A	221	LEU	C-O	-5.12	1.18	1.24
1	B	14	ASP	C-O	-5.12	1.17	1.24
1	C	247	VAL	C-O	-5.12	1.18	1.23
1	F	56	VAL	C-O	-5.12	1.18	1.24
1	A	152	GLU	C-O	-5.12	1.18	1.24
1	B	43	ASP	C-O	-5.12	1.18	1.24
1	G	193	ILE	C-O	-5.12	1.18	1.24
1	D	103	GLY	C-O	-5.11	1.17	1.23
1	G	54	PHE	C-O	-5.11	1.17	1.23
1	F	211	TRP	C-O	-5.11	1.17	1.23
1	A	47	SER	C-O	-5.11	1.18	1.24
1	A	64	MET	C-O	-5.11	1.17	1.24
1	E	227	VAL	C-O	-5.11	1.18	1.24
1	C	46	MET	C-O	-5.10	1.18	1.24
1	G	90	LEU	C-O	-5.10	1.18	1.24
1	B	83	LEU	C-O	-5.10	1.18	1.24
1	D	102	TRP	C-O	-5.10	1.17	1.23
1	B	41	MET	C-O	-5.09	1.17	1.24
1	E	29	VAL	C-O	-5.09	1.18	1.24
1	H	196	SER	C-O	-5.09	1.17	1.24
1	E	176	ALA	C-O	-5.08	1.18	1.24
1	H	101	VAL	C-O	-5.08	1.18	1.24
1	A	99	ALA	C-O	-5.08	1.17	1.23
1	A	230	ALA	C-O	-5.08	1.18	1.24
1	C	43	ASP	C-O	-5.08	1.18	1.24
1	B	132	THR	C-O	-5.08	1.17	1.24
1	A	32	ILE	C-O	-5.08	1.18	1.24
1	H	179	HIS	C-O	-5.08	1.18	1.24
1	E	157	SER	C-O	-5.07	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	156	ASN	C-O	-5.07	1.18	1.24
1	B	120	GLU	C-O	-5.07	1.17	1.24
1	C	172	PRO	C-O	-5.06	1.18	1.24
1	B	78	ILE	C-O	-5.06	1.18	1.24
1	G	229	ALA	C-O	-5.06	1.18	1.24
1	B	196	SER	C-O	-5.05	1.17	1.24
1	B	242[A]	ASN	C-O	-5.05	1.17	1.24
1	B	242[B]	ASN	C-O	-5.05	1.17	1.24
1	D	98	ILE	C-O	-5.05	1.18	1.23
1	B	30	VAL	C-O	-5.05	1.18	1.24
1	H	243	HIS	C-O	-5.05	1.17	1.24
1	D	83	LEU	C-O	-5.05	1.18	1.24
1	G	190	PRO	C-O	-5.04	1.18	1.24
1	A	181	ASN	C-O	-5.04	1.18	1.24
1	C	116	SER	C-O	-5.04	1.18	1.24
1	C	257	VAL	C-O	-5.04	1.18	1.24
1	E	253	PHE	C-O	-5.03	1.18	1.24
1	G	144	VAL	C-O	-5.03	1.18	1.24
1	A	158	ARG	C-O	-5.03	1.18	1.24
1	A	150	SER	C-O	-5.03	1.18	1.24
1	G	82	LYS	C-O	-5.03	1.18	1.24
1	A	165	GLU	C-O	-5.02	1.18	1.24
1	C	127	PRO	C-O	-5.02	1.18	1.23
1	B	215	ALA	C-O	-5.02	1.18	1.24
1	D	99	ALA	C-O	-5.02	1.17	1.23
1	H	41	MET	C-O	-5.02	1.17	1.24
1	A	50	ALA	C-O	-5.01	1.18	1.24
1	B	243	HIS	C-O	-5.01	1.17	1.24
1	B	38	GLU	C-O	-5.01	1.18	1.23
1	D	236	ILE	C-O	-5.01	1.18	1.23
1	B	46	MET	C-O	-5.00	1.18	1.24
1	G	46	MET	C-O	-5.00	1.18	1.24
1	H	150	SER	C-O	-5.00	1.18	1.24

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	204	LEU	N-CA-C	8.93	124.42	113.17
1	B	204	LEU	N-CA-C	8.72	124.13	112.88
1	F	148	THR	N-CA-C	-8.65	101.80	111.14
1	A	204	LEU	N-CA-C	7.91	123.08	112.88
1	F	204	LEU	N-CA-C	7.88	123.09	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	LEU	N-CA-C	7.82	122.97	112.88
1	C	123	ARG	O-C-N	7.74	130.08	122.03
1	H	204	LEU	N-CA-C	7.50	122.62	113.17
1	E	204	LEU	N-CA-C	7.47	122.58	113.17
1	H	122	VAL	N-CA-C	7.15	118.17	107.80
1	C	204	LEU	N-CA-C	7.08	122.78	113.30
1	E	101	VAL	N-CA-C	6.67	117.49	107.75
1	D	32	ILE	CA-C-N	-6.60	113.87	120.21
1	D	32	ILE	C-N-CA	-6.60	113.87	120.21
1	G	5	ARG	N-CA-C	6.56	119.93	109.24
1	D	71	PRO	CA-C-N	6.39	126.88	119.47
1	D	71	PRO	C-N-CA	6.39	126.88	119.47
1	E	32	ILE	CA-C-N	-6.25	114.21	120.21
1	E	32	ILE	C-N-CA	-6.25	114.21	120.21
1	F	141	ILE	N-CA-C	6.01	116.75	110.62
1	F	149	ILE	CB-CA-C	-5.94	104.27	111.88
1	D	122	VAL	N-CA-C	5.92	116.38	107.80
1	G	189	TYR	N-CA-C	5.90	122.85	109.81
1	H	99	ALA	N-CA-C	5.90	118.04	109.07
1	G	100	SER	N-CA-C	-5.88	99.61	108.96
1	E	205	HIS	N-CA-C	5.87	120.03	112.41
1	B	122	VAL	N-CA-C	5.86	116.31	107.75
1	C	101	VAL	N-CA-C	5.86	116.31	108.11
1	H	101	VAL	N-CA-C	5.83	116.27	108.11
1	F	101	VAL	N-CA-C	5.79	116.21	107.75
1	B	101	VAL	N-CA-C	5.77	116.17	107.75
1	B	194	PRO	N-CA-C	5.71	117.67	110.70
1	F	221	LEU	N-CA-C	5.71	117.17	111.07
1	G	122	VAL	N-CA-C	5.70	116.07	107.80
1	C	71	PRO	CA-C-N	5.61	125.72	119.32
1	C	71	PRO	C-N-CA	5.61	125.72	119.32
1	F	89	THR	N-CA-C	-5.57	105.11	111.07
1	F	192	THR	N-CA-C	5.55	121.08	113.97
1	E	122	VAL	N-CA-C	5.55	115.85	107.75
1	A	101	VAL	N-CA-C	5.54	115.87	108.11
1	E	71	PRO	CA-C-N	5.54	125.64	119.32
1	E	71	PRO	C-N-CA	5.54	125.64	119.32
1	B	32	ILE	CA-C-N	-5.53	114.91	120.21
1	B	32	ILE	C-N-CA	-5.53	114.91	120.21
1	B	220	LYS	N-CA-C	5.51	117.29	111.28
1	A	32	ILE	CA-C-N	-5.48	114.95	120.21
1	A	32	ILE	C-N-CA	-5.48	114.95	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	78	ILE	N-CA-C	5.46	116.62	109.58
1	G	118	TYR	CA-C-N	5.45	125.28	119.28
1	G	118	TYR	C-N-CA	5.45	125.28	119.28
1	G	145	ASP	CA-C-N	5.43	124.89	119.24
1	G	145	ASP	C-N-CA	5.43	124.89	119.24
1	D	28	ASP	N-CA-C	5.42	118.77	110.20
1	E	189	TYR	N-CA-C	5.41	121.77	109.81
1	E	194	PRO	N-CA-C	5.39	117.28	110.70
1	G	37	GLY	N-CA-C	5.36	122.19	114.10
1	B	100	SER	N-CA-C	-5.34	100.59	109.46
1	H	28	ASP	N-CA-C	5.32	118.61	110.20
1	A	143	GLU	N-CA-C	5.31	119.86	113.17
1	D	101	VAL	N-CA-C	5.26	115.43	107.75
1	F	70	ALA	N-CA-C	5.21	114.30	108.25
1	D	192	THR	N-CA-C	5.20	119.90	113.50
1	F	122	VAL	N-CA-C	5.20	115.34	107.75
1	B	189	TYR	N-CA-C	5.18	121.26	109.81
1	F	100	SER	N-CA-C	-5.17	100.87	109.46
1	H	32	ILE	CA-C-N	-5.15	115.27	120.21
1	H	32	ILE	C-N-CA	-5.15	115.27	120.21
1	G	99	ALA	N-CA-C	5.10	116.83	109.07
1	E	145	ASP	CA-C-N	5.10	124.55	119.24
1	E	145	ASP	C-N-CA	5.10	124.55	119.24
1	A	189	TYR	N-CA-C	5.03	120.93	109.81
1	G	126	MET	CA-C-N	5.03	125.42	119.99
1	G	126	MET	C-N-CA	5.03	125.42	119.99
1	A	100	SER	N-CA-C	-5.01	100.99	108.96
1	E	78	ILE	N-CA-C	5.01	116.04	109.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2055	0	1993	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2063	0	1998	14	0
1	C	2055	0	1993	12	0
1	D	2060	0	1998	19	0
1	E	2055	0	1993	12	0
1	F	2055	0	1993	25	0
1	G	2045	0	1980	17	0
1	H	2058	0	1990	10	0
2	A	23	0	21	13	0
2	B	23	0	20	9	0
2	C	23	0	21	5	0
2	D	23	0	21	5	0
2	E	23	0	21	3	0
2	F	23	0	21	8	0
2	G	23	0	21	11	0
2	H	23	0	20	10	0
3	A	397	0	0	2	0
3	B	390	0	0	6	1
3	C	324	0	0	1	0
3	D	316	0	0	2	1
3	E	292	0	0	4	1
3	F	209	0	0	4	0
3	G	311	0	0	6	0
3	H	355	0	0	1	1
All	All	19224	0	16104	176	2

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 5.

All (176) 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)
2:H:301:ZER:C10	2:H:301:ZER:C9P	1.76	1.58
2:A:301:ZER:C8P	2:A:301:ZER:C9P	1.87	1.53
2:B:301:ZER:C10	2:B:301:ZER:C9P	1.84	1.52
2:G:301:ZER:C9P	2:G:301:ZER:C10	1.90	1.48
2:D:301:ZER:O10	2:D:301:ZER:C10	1.64	1.44
2:E:301:ZER:C10	2:E:301:ZER:O10	1.65	1.43
2:F:301:ZER:C10	2:F:301:ZER:O10	1.64	1.41
1:E:242:ASN:HB3	3:E:444:HOH:O	1.30	1.30
2:H:301:ZER:C10	2:H:301:ZER:O10	1.80	1.27
2:G:301:ZER:C10	2:G:301:ZER:O10	1.84	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:ZER:C10	2:A:301:ZER:O10	1.83	1.25
1:F:95:ASP:HB2	3:F:544:HOH:O	1.32	1.25
2:C:301:ZER:O10	2:C:301:ZER:C10	1.83	1.25
1:A:95:ASP:HB2	3:A:663:HOH:O	1.28	1.22
2:B:301:ZER:C10	2:B:301:ZER:O10	1.89	1.20
1:F:146:PRO:HD3	1:F:187:TYR:OH	1.53	1.08
1:F:76:GLN:O	1:F:82:LYS:NZ	1.99	0.95
2:H:301:ZER:C9P	2:H:301:ZER:H1	2.03	0.83
1:H:242[B]:ASN:OD1	3:H:401:HOH:O	1.95	0.83
2:H:301:ZER:C10	2:H:301:ZER:C8P	2.58	0.82
2:G:301:ZER:C9P	2:G:301:ZER:H1	2.09	0.81
2:H:301:ZER:C9P	2:H:301:ZER:C11	2.58	0.80
2:B:301:ZER:C9P	2:B:301:ZER:H1	2.08	0.80
1:F:265:LEU:O	3:F:401:HOH:O	2.03	0.77
2:B:301:ZER:C9P	2:B:301:ZER:C11	2.63	0.76
2:A:301:ZER:C10	2:A:301:ZER:C12	2.62	0.76
1:D:255:LYS:NZ	1:D:259:GLU:OE2	2.19	0.75
1:F:72:PRO:HA	1:F:75:TYR:CZ	2.22	0.75
2:A:301:ZER:C8P	2:A:301:ZER:C10	2.65	0.74
2:B:301:ZER:C10	2:B:301:ZER:C8P	2.66	0.74
1:F:72:PRO:HA	1:F:75:TYR:CE1	2.23	0.74
1:F:145:ASP:OD1	1:F:148:THR:OG1	2.05	0.73
1:F:81:ARG:NE	1:F:117:ASP:OD2	2.20	0.71
1:B:4:THR:HA	3:B:642:HOH:O	1.92	0.69
1:F:146:PRO:HD3	1:F:187:TYR:HH	1.54	0.69
2:D:301:ZER:C10	2:D:301:ZER:C12	2.70	0.69
1:G:165:GLU:HG3	3:G:546:HOH:O	1.92	0.69
1:F:202:GLU:O	3:F:402:HOH:O	2.12	0.68
1:G:6:THR:CG2	3:G:532:HOH:O	2.42	0.67
2:D:301:ZER:O10	2:D:301:ZER:H1	1.85	0.67
1:B:165:GLU:HG3	3:B:626:HOH:O	1.95	0.66
2:G:301:ZER:C10	2:G:301:ZER:C8P	2.72	0.65
2:E:301:ZER:C10	2:E:301:ZER:C12	2.72	0.65
1:G:6:THR:HG22	3:G:532:HOH:O	1.96	0.65
2:G:301:ZER:C9P	2:G:301:ZER:C11	2.73	0.64
1:F:194:PRO:HB2	1:F:195:PRO:HD3	1.80	0.64
2:H:301:ZER:O10	2:H:301:ZER:H1	1.92	0.63
1:H:201:THR:HG23	1:H:232:GLU:OE2	1.99	0.63
2:E:301:ZER:O10	2:E:301:ZER:H11	1.97	0.62
1:F:146:PRO:CD	1:F:187:TYR:OH	2.39	0.62
1:A:194:PRO:HB2	1:A:195:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:TYR:CE2	2:F:301:ZER:H15	2.35	0.61
1:G:6:THR:HG21	3:G:471:HOH:O	1.99	0.61
1:E:182:TYR:HB2	1:E:183:PRO:HD3	1.82	0.61
1:F:160:TYR:CD2	2:F:301:ZER:H18	2.36	0.60
2:F:301:ZER:O10	2:F:301:ZER:H11	2.00	0.60
2:A:301:ZER:C8P	2:A:301:ZER:C11	2.80	0.60
2:B:301:ZER:H1	2:B:301:ZER:C8P	2.30	0.59
2:G:301:ZER:H1	2:G:301:ZER:C8P	2.33	0.59
1:E:121:ARG:HD3	3:E:497:HOH:O	2.00	0.59
1:B:196:SER:OG	3:B:401:HOH:O	2.01	0.58
2:H:301:ZER:C10	2:H:301:ZER:H22	2.32	0.58
1:F:182:TYR:HB2	1:F:183:PRO:HD3	1.85	0.58
2:C:301:ZER:C10	2:C:301:ZER:C12	2.81	0.58
2:D:301:ZER:O10	2:D:301:ZER:H11	2.03	0.58
2:H:301:ZER:O10	2:H:301:ZER:H11	2.05	0.57
2:G:301:ZER:O10	2:G:301:ZER:H11	2.05	0.57
1:D:144:VAL:HG23	1:D:149:ILE:HG13	1.88	0.56
1:A:160:TYR:CD2	2:A:301:ZER:H18	2.40	0.56
2:C:301:ZER:O10	2:C:301:ZER:H11	2.05	0.56
1:F:146:PRO:HB3	1:F:183:PRO:HB3	1.87	0.56
1:A:227:VAL:CG1	1:A:231:ARG:CZ	2.85	0.55
1:E:201:THR:HG23	1:E:232:GLU:OE2	2.07	0.54
2:H:301:ZER:C10	2:H:301:ZER:C12	2.81	0.54
1:G:118:TYR:N	1:G:119:PRO:CD	2.71	0.54
2:F:301:ZER:C10	2:F:301:ZER:C12	2.77	0.53
1:B:93:THR:HG21	3:B:593:HOH:O	2.07	0.53
1:B:227:VAL:CG1	1:B:231:ARG:NH2	2.72	0.53
1:B:242[B]:ASN:OD1	3:B:402:HOH:O	2.19	0.53
2:B:301:ZER:O10	2:B:301:ZER:H11	2.08	0.52
1:G:158:ARG:CZ	1:G:164:VAL:CG1	2.88	0.52
1:G:196:SER:OG	3:G:401:HOH:O	1.94	0.52
1:C:194:PRO:HB2	1:C:195:PRO:HD3	1.91	0.52
1:G:158:ARG:CZ	1:G:164:VAL:HG11	2.40	0.52
1:G:194:PRO:HB2	1:G:195:PRO:HD3	1.92	0.51
2:A:301:ZER:H3	2:A:301:ZER:H21	1.93	0.51
2:A:301:ZER:O10	2:A:301:ZER:H11	2.11	0.50
1:D:243:HIS:CD2	2:D:301:ZER:H4	2.46	0.50
1:B:87:ILE:HD12	1:B:110:THR:HG21	1.94	0.49
1:F:105:ALA:HB1	2:F:301:ZER:C12	2.41	0.49
1:D:227:VAL:CG1	1:D:231:ARG:CZ	2.90	0.49
1:H:105:ALA:HB1	2:H:301:ZER:C12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:ARG:HD3	1:G:46:MET:HE2	1.94	0.49
1:A:105:ALA:HB1	2:A:301:ZER:C12	2.43	0.49
1:A:227:VAL:CG1	1:A:231:ARG:NH2	2.75	0.49
1:D:72:PRO:HA	1:D:75:TYR:CZ	2.47	0.49
1:A:4:THR:N	3:A:409:HOH:O	2.46	0.49
1:D:140:HIS:HD1	1:D:143:GLU:CD	2.21	0.48
1:D:44:LYS:HB2	1:D:45:PRO:HD3	1.95	0.48
1:B:102:TRP:CD1	1:B:102:TRP:C	2.91	0.48
2:B:301:ZER:H1	2:B:301:ZER:H21	1.94	0.48
2:G:301:ZER:H1	2:G:301:ZER:H21	1.95	0.48
1:D:182:TYR:HB2	1:D:183:PRO:HD3	1.96	0.48
1:F:205:HIS:ND1	3:F:406:HOH:O	2.35	0.48
1:B:227:VAL:HG13	1:B:231:ARG:CZ	2.44	0.47
1:D:9:TYR:OH	3:D:401:HOH:O	2.19	0.47
1:A:182:TYR:HB2	1:A:183:PRO:HD3	1.96	0.47
2:A:301:ZER:C8P	2:A:301:ZER:H3	2.44	0.47
1:F:142:HIS:CD2	1:F:142:HIS:C	2.92	0.47
1:C:243:HIS:CD2	2:C:301:ZER:H6	2.48	0.47
1:B:227:VAL:CG1	1:B:231:ARG:CZ	2.92	0.47
1:F:139:LEU:HD23	1:F:140:HIS:NE2	2.29	0.47
1:D:140:HIS:HB3	1:D:143:GLU:OE1	2.15	0.47
2:G:301:ZER:O10	2:G:301:ZER:H1	2.03	0.46
1:F:160:TYR:CE2	2:F:301:ZER:C4P	2.98	0.46
1:G:182:TYR:HB2	1:G:183:PRO:HD3	1.96	0.46
1:D:72:PRO:HA	1:D:75:TYR:CE2	2.50	0.46
1:D:194:PRO:HB2	1:D:195:PRO:HD3	1.97	0.46
2:A:301:ZER:O2	2:A:301:ZER:O12	2.33	0.46
1:E:87:ILE:HD12	1:E:110:THR:HG21	1.98	0.46
1:C:108:ALA:HB1	1:C:130:VAL:HG22	1.97	0.46
1:E:102:TRP:CD1	1:E:102:TRP:C	2.92	0.46
1:B:13:LYS:NZ	3:B:408:HOH:O	2.49	0.45
1:D:76:GLN:NE2	3:D:405:HOH:O	2.41	0.45
1:B:194:PRO:HB2	1:B:195:PRO:HD3	1.97	0.45
1:C:72:PRO:HA	1:C:75:TYR:CZ	2.51	0.45
1:E:105:ALA:HA	1:E:131:PRO:HD3	1.97	0.45
1:C:71:PRO:HA	1:C:72:PRO:HD3	1.82	0.45
1:F:102:TRP:CD1	1:F:102:TRP:C	2.95	0.45
1:H:87:ILE:HD12	1:H:110:THR:HG21	1.98	0.44
1:A:153:MET:HE2	1:A:185:TRP:CZ3	2.53	0.44
1:A:108:ALA:HB1	1:A:130:VAL:HG22	1.99	0.44
1:G:44:LYS:N	1:G:45:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ALA:HA	1:C:131:PRO:HD3	1.99	0.44
1:H:153:MET:HE2	1:H:185:TRP:CZ3	2.54	0.43
1:B:72:PRO:HA	1:B:75:TYR:CZ	2.53	0.43
1:D:102:TRP:CD1	1:D:102:TRP:C	2.96	0.43
1:F:179:HIS:ND1	1:F:179:HIS:C	2.76	0.43
1:G:102:TRP:CD1	1:G:102:TRP:C	2.96	0.43
1:A:204:LEU:HB3	1:A:234:ILE:HD11	2.00	0.43
1:H:182:TYR:HB2	1:H:183:PRO:HD3	2.00	0.43
1:E:97:LYS:HG3	3:E:564:HOH:O	2.19	0.43
1:B:255:LYS:HE2	1:B:259:GLU:OE2	2.19	0.43
1:C:102:TRP:CD1	1:C:102:TRP:C	2.96	0.43
1:D:9:TYR:HA	1:D:18:TRP:O	2.19	0.43
1:H:44:LYS:HB2	1:H:45:PRO:HD3	2.01	0.43
1:D:105:ALA:HB2	1:D:243:HIS:CE1	2.54	0.42
1:F:145:ASP:OD1	1:F:148:THR:CB	2.67	0.42
2:F:301:ZER:H17	2:F:301:ZER:H1	2.01	0.42
1:G:202:GLU:HG2	3:G:538:HOH:O	2.19	0.42
1:A:102:TRP:CD1	1:A:102:TRP:C	2.97	0.42
1:G:144:VAL:HG23	1:G:149:ILE:HG13	2.02	0.42
1:A:160:TYR:CE2	2:A:301:ZER:H18	2.55	0.42
1:E:202:GLU:CD	1:E:202:GLU:H	2.26	0.42
1:D:71:PRO:HA	1:D:72:PRO:HD3	1.87	0.42
1:C:93:THR:HG22	3:C:539:HOH:O	2.19	0.42
1:C:182:TYR:HB2	1:C:183:PRO:HD3	2.02	0.42
1:C:227:VAL:CG1	1:C:231:ARG:CZ	2.98	0.42
2:G:301:ZER:O2	2:G:301:ZER:O12	2.36	0.42
1:E:151:GLN:NE2	3:E:404:HOH:O	2.42	0.41
1:D:221:LEU:HD12	1:D:221:LEU:HA	1.85	0.41
1:C:160:TYR:CD2	2:C:301:ZER:H18	2.55	0.41
1:D:227:VAL:HG13	1:D:231:ARG:CZ	2.50	0.41
1:H:118:TYR:N	1:H:119:PRO:CD	2.84	0.41
2:B:301:ZER:O12	2:B:301:ZER:O2	2.39	0.41
1:C:218:PRO:HD2	1:C:221:LEU:HD12	2.02	0.41
1:A:72:PRO:HA	1:A:75:TYR:CZ	2.56	0.41
1:E:194:PRO:HB2	1:E:195:PRO:HD3	2.02	0.41
1:H:9:TYR:HA	1:H:18:TRP:O	2.21	0.41
1:A:243:HIS:CD2	2:A:301:ZER:H6	2.56	0.41
1:E:118:TYR:N	1:E:119:PRO:CD	2.84	0.41
1:F:192:THR:O	1:F:196:SER:OG	2.39	0.41
1:G:105:ALA:HB1	2:G:301:ZER:C12	2.51	0.41
1:A:193:ILE:HB	1:A:194:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:ALA:HB1	1:G:130:VAL:HG22	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:572:HOH:O	3:E:611:HOH:O[1_455]	2.11	0.09
3:D:466:HOH:O	3:H:559:HOH:O[1_464]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/266 (98%)	254 (97%)	6 (2%)	1 (0%)	30	18
1	B	262/266 (98%)	254 (97%)	7 (3%)	1 (0%)	30	18
1	C	261/266 (98%)	253 (97%)	7 (3%)	1 (0%)	30	18
1	D	262/266 (98%)	254 (97%)	6 (2%)	2 (1%)	16	5
1	E	261/266 (98%)	254 (97%)	5 (2%)	2 (1%)	16	5
1	F	261/266 (98%)	250 (96%)	9 (3%)	2 (1%)	16	5
1	G	260/266 (98%)	252 (97%)	6 (2%)	2 (1%)	16	5
1	H	262/266 (98%)	254 (97%)	7 (3%)	1 (0%)	30	18
All	All	2090/2128 (98%)	2025 (97%)	53 (2%)	12 (1%)	21	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	147	ALA
1	D	163	ASN
1	G	163	ASN

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Mol	Chain	Res	Type
1	A	189	TYR
1	D	189	TYR
1	E	189	TYR
1	H	189	TYR
1	B	189	TYR
1	C	189	TYR
1	E	163	ASN
1	F	189	TYR
1	G	189	TYR

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	223/224 (100%)	222 (100%)	1 (0%)	84	79
1	B	224/224 (100%)	222 (99%)	2 (1%)	70	63
1	C	223/224 (100%)	220 (99%)	3 (1%)	61	50
1	D	223/224 (100%)	219 (98%)	4 (2%)	51	38
1	E	223/224 (100%)	220 (99%)	3 (1%)	61	50
1	F	223/224 (100%)	218 (98%)	5 (2%)	45	30
1	G	222/224 (99%)	216 (97%)	6 (3%)	39	23
1	H	223/224 (100%)	221 (99%)	2 (1%)	70	63
All	All	1784/1792 (100%)	1758 (98%)	26 (2%)	57	46

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	TYR
1	B	4	THR
1	B	225	ASN
1	C	93	THR
1	C	246	TYR
1	C	266	LYS

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Mol	Chain	Res	Type
1	D	46	MET
1	D	221	LEU
1	D	246	TYR
1	D	266	LYS
1	E	139	LEU
1	E	202	GLU
1	E	246	TYR
1	F	13	LYS
1	F	82	LYS
1	F	196	SER
1	F	236	ILE
1	F	246	TYR
1	G	6	THR
1	G	12	THR
1	G	13	LYS
1	G	202	GLU
1	G	221	LEU
1	G	246	TYR
1	H	46	MET
1	H	246	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	B	22	GLN
1	B	134	ASN
1	C	179	HIS
1	D	76	GLN
1	D	151	GLN
1	D	179	HIS
1	F	22	GLN
1	G	22	GLN
1	G	124	ASN
1	G	134	ASN
1	H	52	ASN
1	H	124	ASN
1	H	134	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	ZER	A	301	-	24,24,24	5.08	9 (37%)	32,32,32	2.59	13 (40%)
2	ZER	H	301	-	24,24,24	4.60	8 (33%)	32,32,32	3.43	7 (21%)
2	ZER	D	301	-	24,24,24	2.62	7 (29%)	32,32,32	2.76	7 (21%)
2	ZER	F	301	-	24,24,24	2.67	6 (25%)	32,32,32	2.60	7 (21%)
2	ZER	B	301	-	24,24,24	5.65	9 (37%)	32,32,32	3.45	12 (37%)
2	ZER	G	301	-	24,24,24	5.30	8 (33%)	32,32,32	3.88	10 (31%)
2	ZER	E	301	-	24,24,24	2.86	8 (33%)	32,32,32	3.71	11 (34%)
2	ZER	C	301	-	24,24,24	4.59	6 (25%)	32,32,32	2.14	11 (34%)

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	ZER	A	301	-	-	9/22/22/22	0/1/2/2
2	ZER	H	301	-	-	7/22/22/22	0/1/2/2
2	ZER	D	301	-	-	12/22/22/22	0/1/2/2
2	ZER	F	301	-	-	8/22/22/22	0/1/2/2
2	ZER	B	301	-	-	9/22/22/22	0/1/2/2
2	ZER	G	301	-	-	8/22/22/22	0/1/2/2
2	ZER	E	301	-	-	8/22/22/22	0/1/2/2
2	ZER	C	301	-	-	9/22/22/22	0/1/2/2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ZER	O10-C10	24.79	1.89	1.47
2	G	301	ZER	O10-C10	21.77	1.84	1.47
2	A	301	ZER	O10-C10	21.11	1.83	1.47
2	C	301	ZER	O10-C10	20.93	1.83	1.47
2	H	301	ZER	O10-C10	19.32	1.80	1.47
2	G	301	ZER	C9P-C10	11.26	1.90	1.52
2	E	301	ZER	O10-C10	10.57	1.65	1.47
2	F	301	ZER	O10-C10	10.15	1.64	1.47
2	D	301	ZER	O10-C10	9.82	1.64	1.47
2	B	301	ZER	C9P-C10	9.52	1.84	1.52
2	A	301	ZER	C8P-C9P	8.41	1.87	1.52
2	H	301	ZER	C9P-C10	7.01	1.76	1.52
2	A	301	ZER	C8P-C7P	5.05	1.70	1.52
2	A	301	ZER	C9P-C10	-4.61	1.36	1.52
2	E	301	ZER	C9P-C10	4.26	1.66	1.52
2	H	301	ZER	C5P-C6P	-4.24	1.38	1.51
2	G	301	ZER	C8P-C7P	4.20	1.67	1.52
2	G	301	ZER	C4P-C5P	4.08	1.67	1.52
2	F	301	ZER	C9P-C10	3.90	1.65	1.52
2	C	301	ZER	C8P-C7P	3.77	1.66	1.52
2	A	301	ZER	C11-C10	3.56	1.64	1.51
2	D	301	ZER	C8P-C7P	3.56	1.65	1.52
2	E	301	ZER	C1P-C2P	3.54	1.42	1.31
2	H	301	ZER	C3-C4	-3.50	1.34	1.39
2	A	301	ZER	O6P-C6P	3.49	1.27	1.21
2	E	301	ZER	C6-C1P	-3.42	1.41	1.47
2	D	301	ZER	C8P-C9P	3.39	1.66	1.52
2	F	301	ZER	C5P-C6P	-3.36	1.41	1.51
2	D	301	ZER	C1-C12	-3.32	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	ZER	C1P-C2P	3.24	1.41	1.31
2	H	301	ZER	C8P-C7P	3.14	1.63	1.52
2	C	301	ZER	C1-C12	-3.11	1.43	1.50
2	F	301	ZER	C1P-C2P	3.09	1.41	1.31
2	D	301	ZER	C1P-C2P	3.01	1.40	1.31
2	E	301	ZER	C1-C12	-2.84	1.44	1.50
2	B	301	ZER	O6P-C6P	2.84	1.26	1.21
2	A	301	ZER	C5P-C6P	-2.78	1.43	1.51
2	C	301	ZER	C1P-C2P	2.70	1.40	1.31
2	G	301	ZER	O6P-C6P	2.67	1.26	1.21
2	B	301	ZER	C4P-C5P	2.62	1.61	1.52
2	H	301	ZER	C1-C2	-2.59	1.37	1.41
2	A	301	ZER	C1P-C2P	2.59	1.39	1.31
2	G	301	ZER	C6-C1P	-2.57	1.43	1.47
2	C	301	ZER	C5P-C6P	-2.55	1.43	1.51
2	G	301	ZER	C1-C12	-2.55	1.44	1.50
2	E	301	ZER	C5P-C6P	-2.46	1.43	1.51
2	B	301	ZER	C5P-C6P	-2.44	1.44	1.51
2	C	301	ZER	O6P-C6P	2.42	1.26	1.21
2	F	301	ZER	C7P-C6P	-2.33	1.44	1.51
2	A	301	ZER	C4P-C5P	2.31	1.60	1.52
2	D	301	ZER	O6P-C6P	2.28	1.25	1.21
2	B	301	ZER	O4-C4	-2.27	1.31	1.37
2	E	301	ZER	C1-C6	2.27	1.45	1.42
2	D	301	ZER	C4P-C5P	2.26	1.60	1.52
2	B	301	ZER	C1P-C2P	2.26	1.38	1.31
2	B	301	ZER	C1-C12	-2.25	1.45	1.50
2	F	301	ZER	C6-C1P	-2.17	1.43	1.47
2	E	301	ZER	O2-C2	2.16	1.40	1.36
2	H	301	ZER	C1P-C2P	2.13	1.38	1.31
2	B	301	ZER	C3-C2	-2.09	1.36	1.38
2	H	301	ZER	C7P-C6P	-2.08	1.45	1.51

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	ZER	O10-C10-C9P	14.45	137.18	106.75
2	G	301	ZER	O10-C10-C9P	14.03	136.29	106.75
2	B	301	ZER	O10-C10-C9P	13.98	136.19	106.75
2	E	301	ZER	C6-C1P-C2P	12.55	152.02	125.55
2	G	301	ZER	C10-O10-C12	11.67	139.40	117.67
2	E	301	ZER	C3P-C2P-C1P	10.58	148.95	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	ZER	C10-O10-C12	9.94	136.18	117.67
2	B	301	ZER	C10-O10-C12	8.83	134.11	117.67
2	D	301	ZER	O10-C10-C9P	8.08	123.77	106.75
2	A	301	ZER	O10-C10-C9P	7.87	123.32	106.75
2	F	301	ZER	O10-C10-C9P	7.39	122.32	106.75
2	E	301	ZER	O10-C10-C9P	6.67	120.79	106.75
2	E	301	ZER	C10-O10-C12	6.56	129.89	117.67
2	H	301	ZER	C9P-C8P-C7P	6.53	130.66	113.26
2	D	301	ZER	C9P-C8P-C7P	6.38	130.27	113.26
2	C	301	ZER	O10-C10-C9P	6.18	119.76	106.75
2	H	301	ZER	C10-O10-C12	5.96	128.76	117.67
2	G	301	ZER	C7P-C6P-C5P	5.79	127.89	116.95
2	D	301	ZER	C11-C10-C9P	-5.51	99.62	113.90
2	D	301	ZER	C10-O10-C12	5.40	127.73	117.67
2	D	301	ZER	O10-C10-C11	5.21	119.63	107.96
2	H	301	ZER	C5P-C4P-C3P	-5.15	102.09	113.35
2	G	301	ZER	C8P-C7P-C6P	-5.10	101.67	114.59
2	G	301	ZER	C9P-C8P-C7P	4.87	126.25	113.26
2	E	301	ZER	O10-C12-O12	-4.76	115.80	123.55
2	A	301	ZER	C9P-C8P-C7P	4.58	125.46	113.26
2	B	301	ZER	C8P-C7P-C6P	-4.57	103.00	114.59
2	A	301	ZER	C11-C10-C9P	-4.31	102.74	113.90
2	C	301	ZER	C6-C5-C4	4.30	125.43	120.92
2	F	301	ZER	C5P-C4P-C3P	-4.20	104.17	113.35
2	B	301	ZER	C9P-C8P-C7P	4.17	124.37	113.26
2	A	301	ZER	C5P-C4P-C3P	-4.14	104.31	113.35
2	A	301	ZER	C2-C3-C4	-4.07	115.92	119.67
2	A	301	ZER	C10-O10-C12	-3.82	110.54	117.67
2	G	301	ZER	C6-C1P-C2P	3.78	133.53	125.55
2	H	301	ZER	C11-C10-C9P	-3.70	104.32	113.90
2	H	301	ZER	C8P-C9P-C10	-3.66	100.43	115.26
2	C	301	ZER	C5P-C4P-C3P	-3.48	105.74	113.35
2	F	301	ZER	C9P-C8P-C7P	3.38	122.27	113.26
2	A	301	ZER	C3-C2-C1	3.25	124.55	120.92
2	C	301	ZER	C11-C10-C9P	-3.23	105.53	113.90
2	C	301	ZER	C5-C6-C1	-3.10	116.04	119.94
2	A	301	ZER	C5-C6-C1	-3.09	116.06	119.94
2	D	301	ZER	C8P-C9P-C10	-3.07	102.85	115.26
2	B	301	ZER	C6-C1P-C2P	3.06	132.01	125.55
2	E	301	ZER	O10-C12-C1	3.01	121.10	113.53
2	B	301	ZER	C11-C10-C9P	-2.99	106.15	113.90
2	C	301	ZER	C6-C1P-C2P	2.91	131.69	125.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	ZER	C8P-C7P-C6P	-2.88	107.30	114.59
2	D	301	ZER	C6-C1P-C2P	2.84	131.53	125.55
2	E	301	ZER	C9P-C8P-C7P	2.82	120.79	113.26
2	G	301	ZER	O6P-C6P-C5P	-2.80	114.04	121.40
2	C	301	ZER	C3-C2-C1	2.77	124.02	120.92
2	A	301	ZER	C6-C1P-C2P	2.69	131.23	125.55
2	G	301	ZER	C8P-C9P-C10	-2.67	104.47	115.26
2	C	301	ZER	O10-C12-C1	2.62	120.12	113.53
2	B	301	ZER	C7P-C6P-C5P	2.56	121.79	116.95
2	B	301	ZER	O10-C12-O12	-2.52	119.45	123.55
2	C	301	ZER	O2-C2-C1	-2.46	116.59	121.14
2	G	301	ZER	C5P-C4P-C3P	-2.45	108.01	113.35
2	F	301	ZER	C6-C1P-C2P	2.42	130.65	125.55
2	G	301	ZER	C11-C10-C9P	-2.38	107.74	113.90
2	E	301	ZER	O10-C10-C11	2.37	113.27	107.96
2	B	301	ZER	C8P-C9P-C10	-2.37	105.69	115.26
2	H	301	ZER	C3-C2-C1	2.34	123.54	120.92
2	F	301	ZER	C4P-C3P-C2P	-2.33	99.56	112.60
2	A	301	ZER	C3P-C2P-C1P	2.31	130.61	125.48
2	E	301	ZER	C8P-C7P-C6P	2.31	120.45	114.59
2	C	301	ZER	C10-O10-C12	2.31	121.97	117.67
2	A	301	ZER	O2-C2-C1	-2.26	116.96	121.14
2	E	301	ZER	C8P-C9P-C10	-2.25	106.14	115.26
2	B	301	ZER	C4P-C3P-C2P	2.21	125.00	112.60
2	E	301	ZER	C4P-C5P-C6P	-2.19	109.03	114.59
2	A	301	ZER	C6-C5-C4	2.15	123.17	120.92
2	A	301	ZER	O10-C10-C11	2.13	112.74	107.96
2	B	301	ZER	C6-C1-C2	-2.11	116.58	118.73
2	B	301	ZER	C6-C5-C4	2.06	123.08	120.92
2	F	301	ZER	C8P-C9P-C10	-2.04	106.98	115.26

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ZER	C1-C12-O10-C10
2	A	301	ZER	C11-C10-O10-C12
2	B	301	ZER	O12-C12-O10-C10
2	B	301	ZER	C1-C12-O10-C10
2	C	301	ZER	C1-C12-O10-C10
2	C	301	ZER	C11-C10-O10-C12
2	D	301	ZER	O12-C12-O10-C10

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Mol	Chain	Res	Type	Atoms
2	D	301	ZER	C1-C12-O10-C10
2	D	301	ZER	C9P-C10-O10-C12
2	D	301	ZER	O10-C10-C9P-C8P
2	D	301	ZER	C7P-C8P-C9P-C10
2	E	301	ZER	O12-C12-O10-C10
2	E	301	ZER	C1-C12-O10-C10
2	E	301	ZER	C9P-C10-O10-C12
2	E	301	ZER	C6-C1P-C2P-C3P
2	F	301	ZER	O12-C12-O10-C10
2	F	301	ZER	C1-C12-O10-C10
2	G	301	ZER	O12-C12-O10-C10
2	G	301	ZER	C1-C12-O10-C10
2	H	301	ZER	O12-C12-O10-C10
2	H	301	ZER	C1-C12-O10-C10
2	C	301	ZER	O12-C12-O10-C10
2	A	301	ZER	O12-C12-O10-C10
2	H	301	ZER	C6P-C7P-C8P-C9P
2	F	301	ZER	C6P-C7P-C8P-C9P
2	H	301	ZER	C9P-C10-O10-C12
2	D	301	ZER	C11-C10-C9P-C8P
2	H	301	ZER	O10-C10-C9P-C8P
2	E	301	ZER	C3P-C4P-C5P-C6P
2	F	301	ZER	C9P-C10-O10-C12
2	C	301	ZER	C2P-C3P-C4P-C5P
2	D	301	ZER	C2P-C3P-C4P-C5P
2	E	301	ZER	C1P-C2P-C3P-C4P
2	A	301	ZER	C2P-C3P-C4P-C5P
2	B	301	ZER	C2P-C3P-C4P-C5P
2	F	301	ZER	C2P-C3P-C4P-C5P
2	E	301	ZER	O10-C10-C9P-C8P
2	F	301	ZER	O10-C10-C9P-C8P
2	G	301	ZER	C2P-C3P-C4P-C5P
2	A	301	ZER	C3P-C4P-C5P-C6P
2	A	301	ZER	C6P-C7P-C8P-C9P
2	B	301	ZER	C11-C10-C9P-C8P
2	B	301	ZER	C3P-C4P-C5P-C6P
2	C	301	ZER	C11-C10-C9P-C8P
2	C	301	ZER	C6P-C7P-C8P-C9P
2	B	301	ZER	C9P-C10-O10-C12
2	B	301	ZER	C5P-C6P-C7P-C8P
2	D	301	ZER	C6P-C7P-C8P-C9P
2	H	301	ZER	C2P-C3P-C4P-C5P

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Mol	Chain	Res	Type	Atoms
2	H	301	ZER	C7P-C8P-C9P-C10
2	D	301	ZER	C5P-C6P-C7P-C8P
2	A	301	ZER	C7P-C8P-C9P-C10
2	G	301	ZER	C11-C10-C9P-C8P
2	C	301	ZER	O10-C10-C9P-C8P
2	D	301	ZER	O6P-C6P-C7P-C8P
2	D	301	ZER	C3P-C4P-C5P-C6P
2	A	301	ZER	C5P-C6P-C7P-C8P
2	F	301	ZER	C5P-C6P-C7P-C8P
2	D	301	ZER	C1P-C2P-C3P-C4P
2	G	301	ZER	C3P-C4P-C5P-C6P
2	B	301	ZER	O6P-C6P-C7P-C8P
2	F	301	ZER	O6P-C6P-C7P-C8P
2	G	301	ZER	C7P-C8P-C9P-C10
2	A	301	ZER	O6P-C6P-C7P-C8P
2	C	301	ZER	O6P-C6P-C7P-C8P
2	G	301	ZER	C5P-C6P-C7P-C8P
2	E	301	ZER	C6P-C7P-C8P-C9P
2	G	301	ZER	O6P-C6P-C7P-C8P
2	B	301	ZER	C7P-C8P-C9P-C10
2	C	301	ZER	C1P-C2P-C3P-C4P

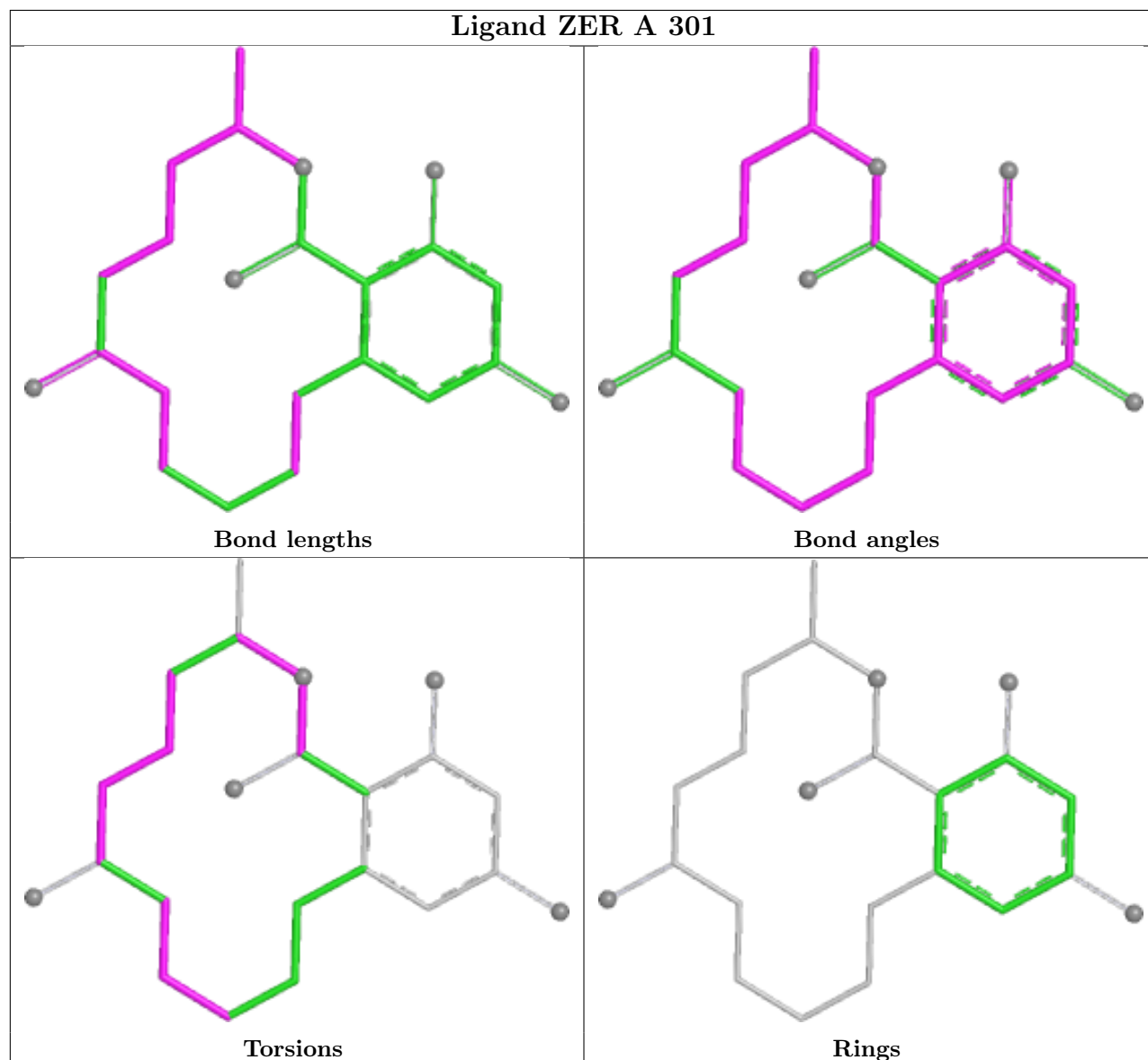
There are no ring outliers.

8 monomers are involved in 64 short contacts:

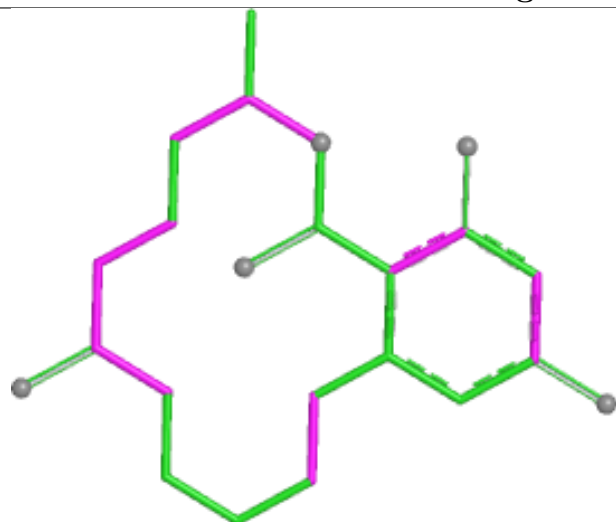
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ZER	13	0
2	H	301	ZER	10	0
2	D	301	ZER	5	0
2	F	301	ZER	8	0
2	B	301	ZER	9	0
2	G	301	ZER	11	0
2	E	301	ZER	3	0
2	C	301	ZER	5	0

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

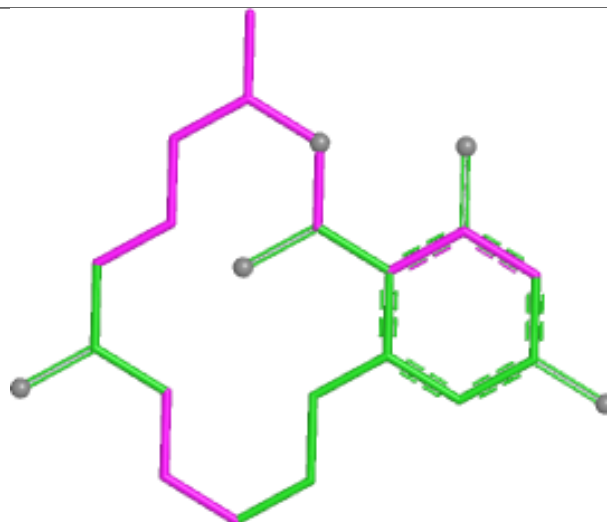
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



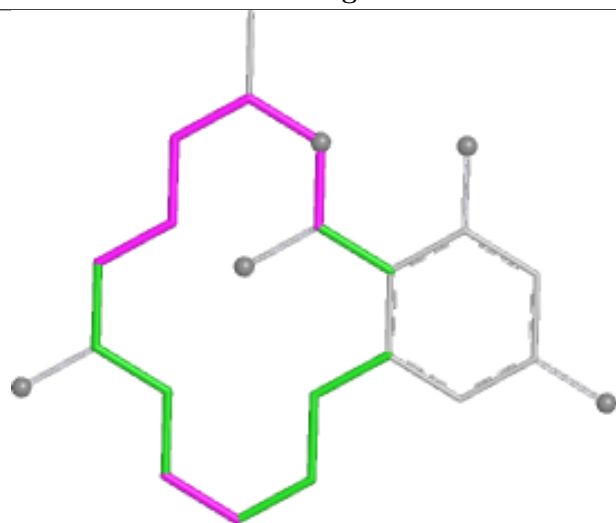
Ligand ZER H 301



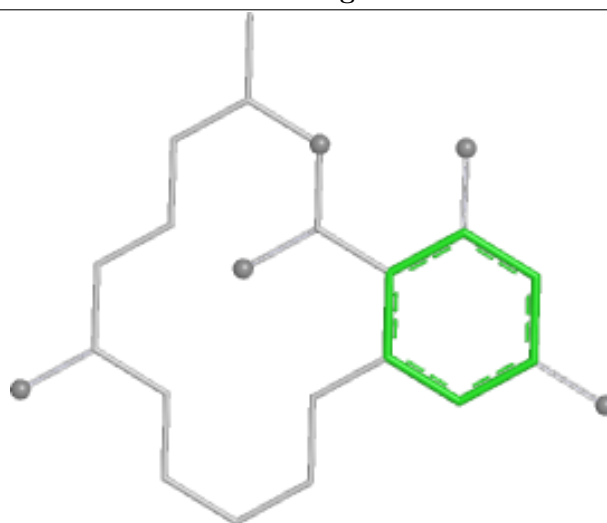
Bond lengths



Bond angles

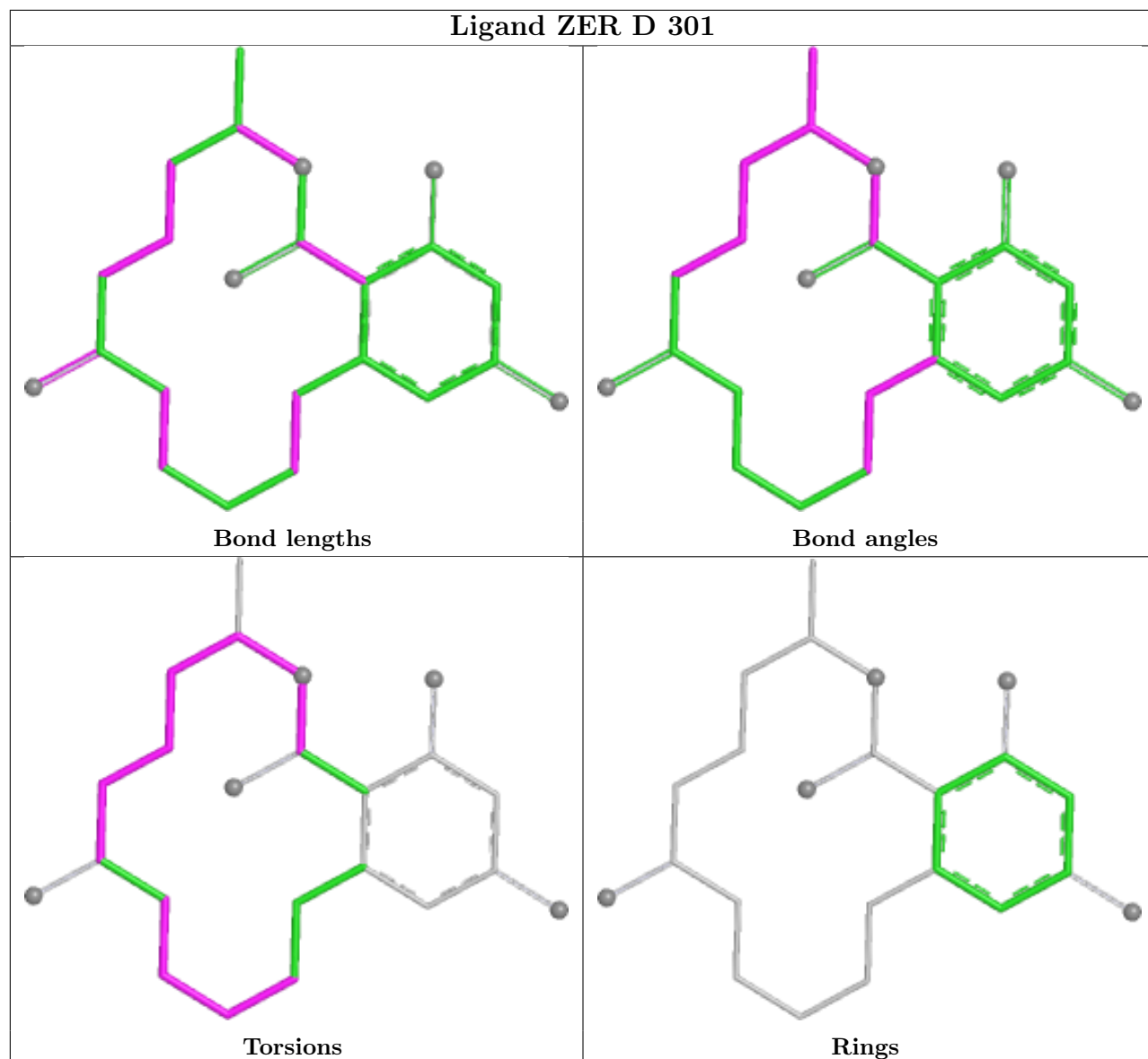


Torsions

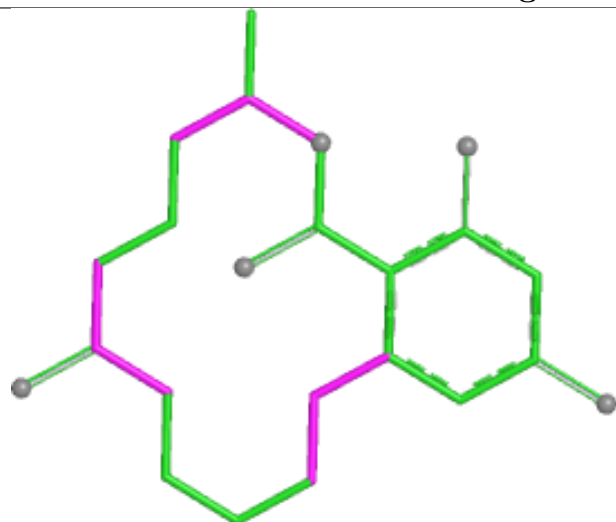


Rings

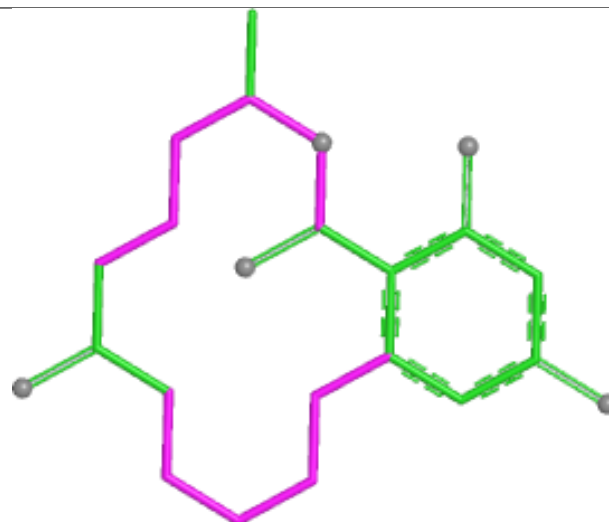
Ligand ZER D 301



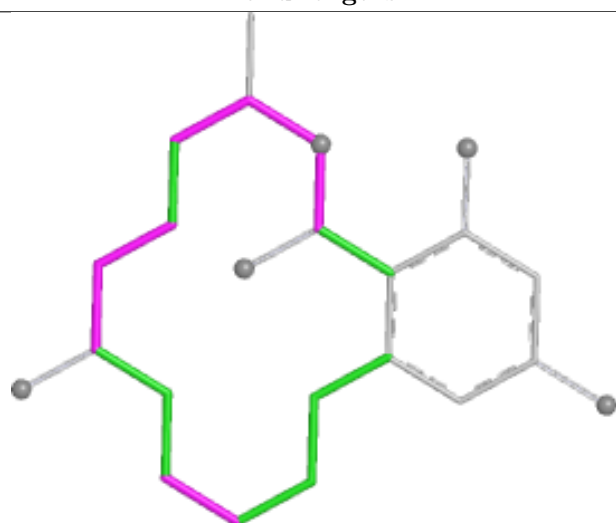
Ligand ZER F 301



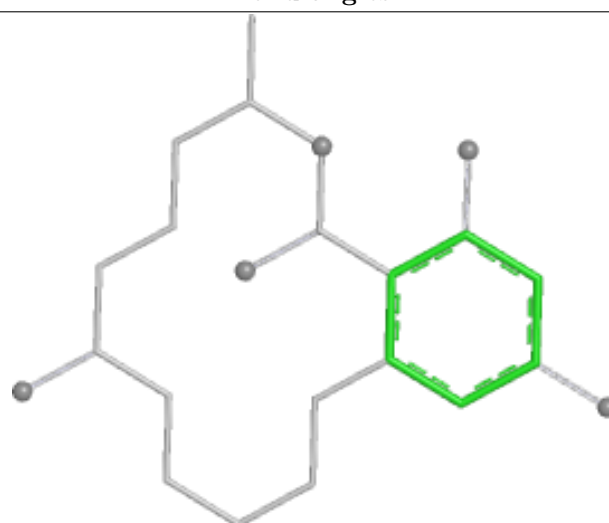
Bond lengths



Bond angles

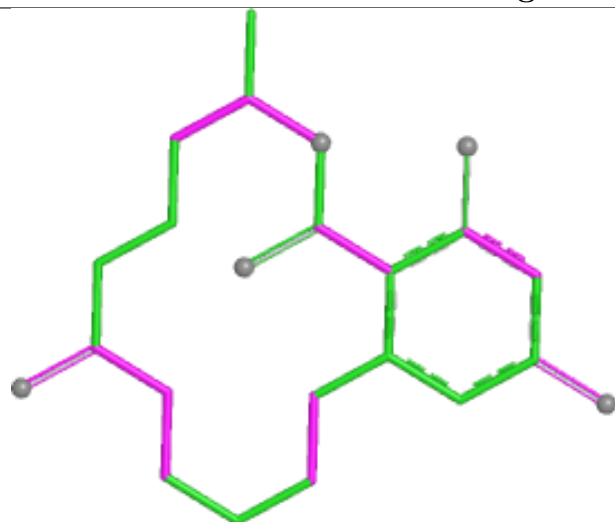


Torsions

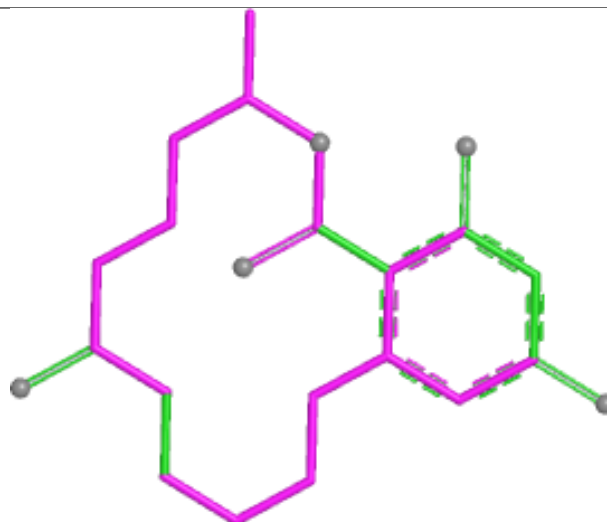


Rings

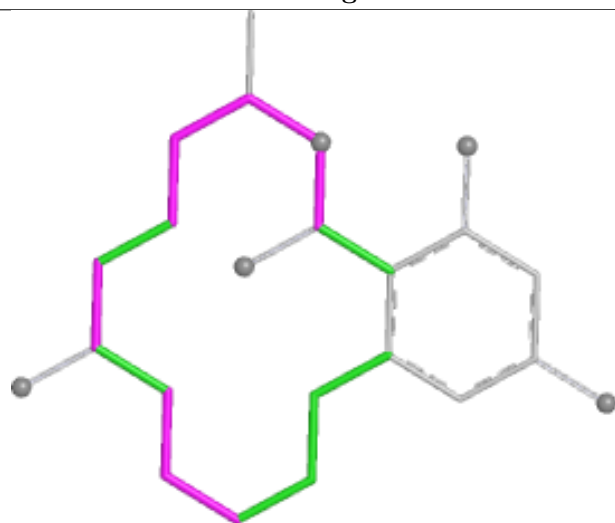
Ligand ZER B 301



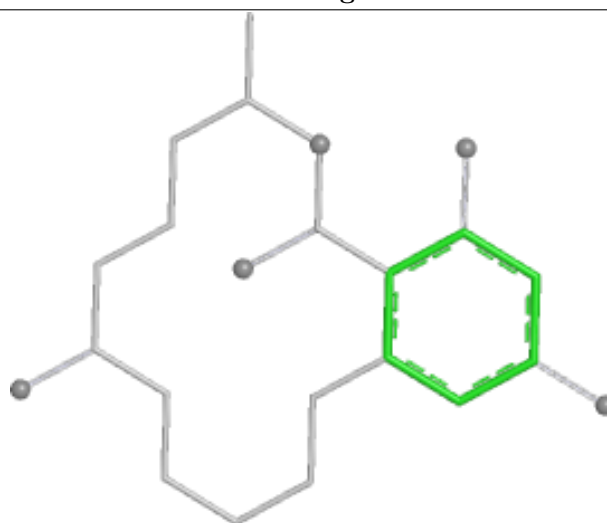
Bond lengths



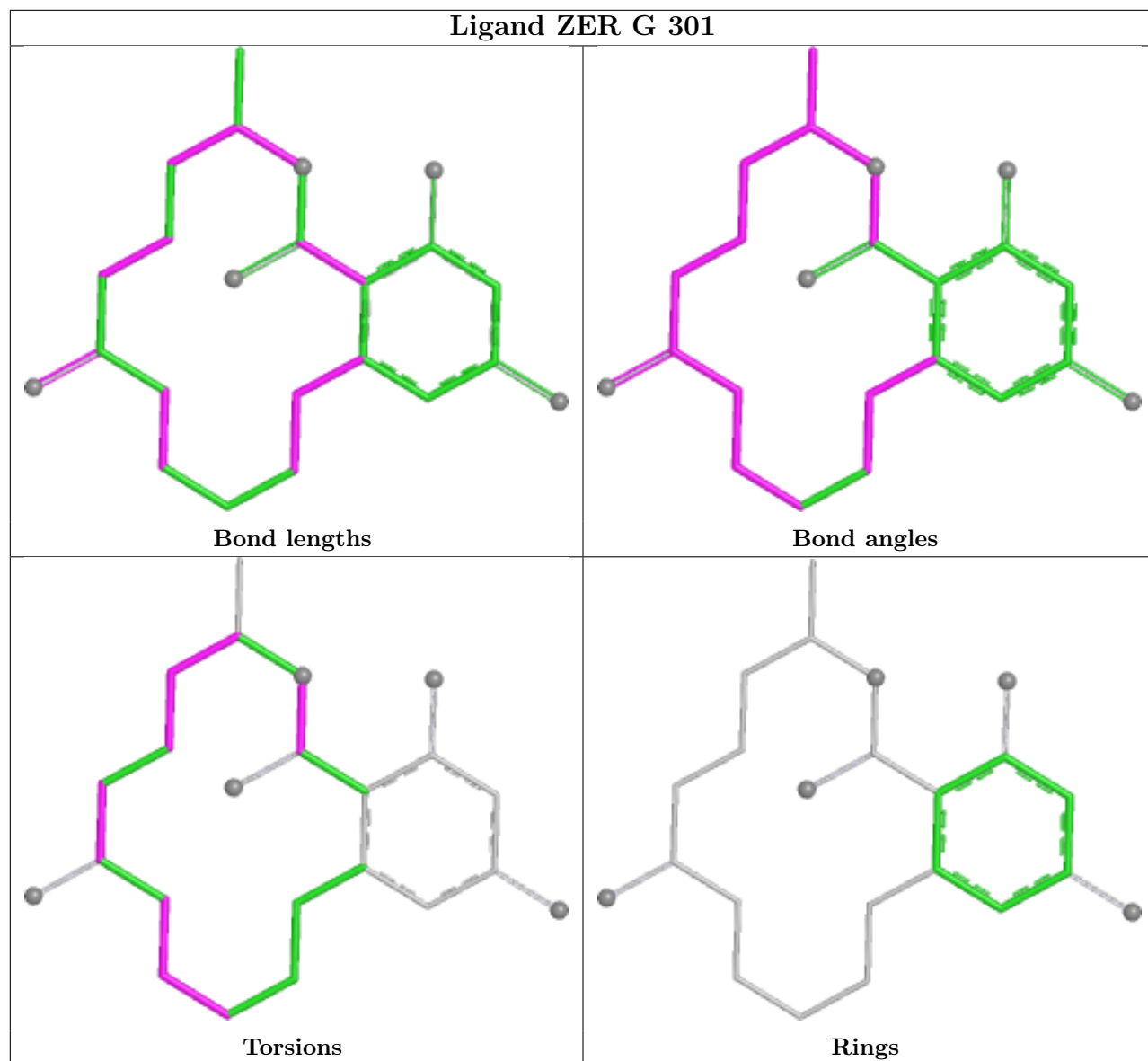
Bond angles



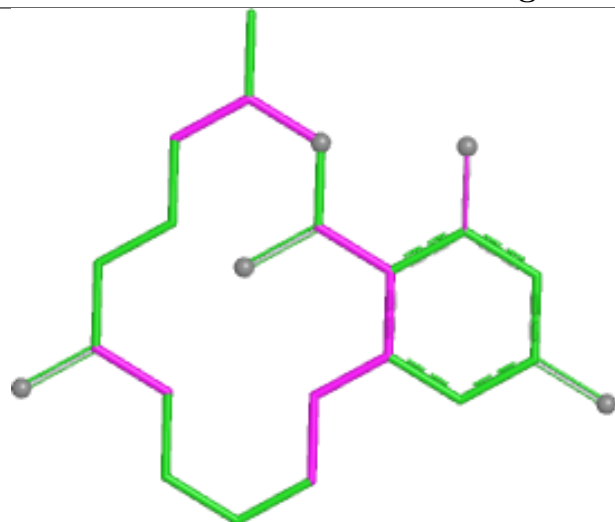
Torsions



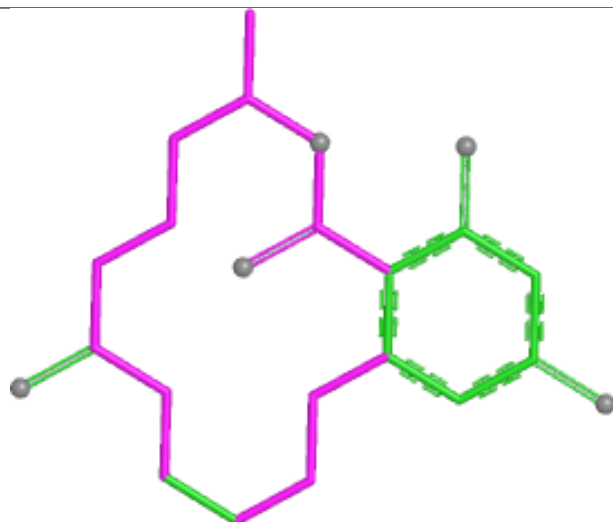
Rings



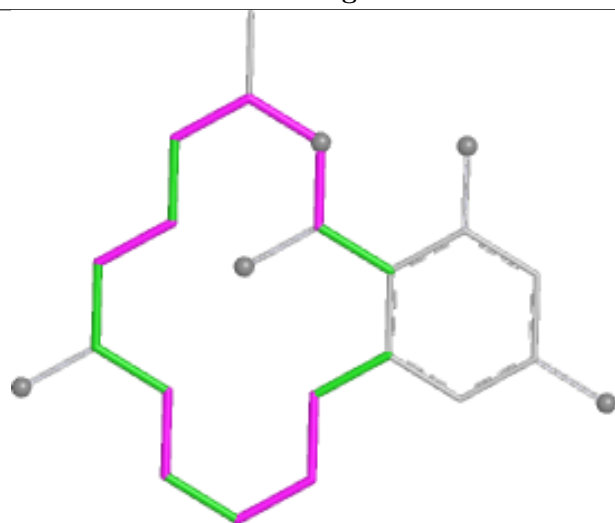
Ligand ZER E 301



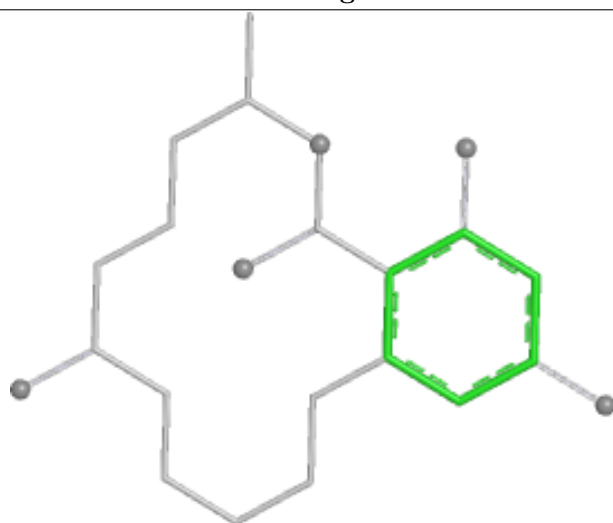
Bond lengths



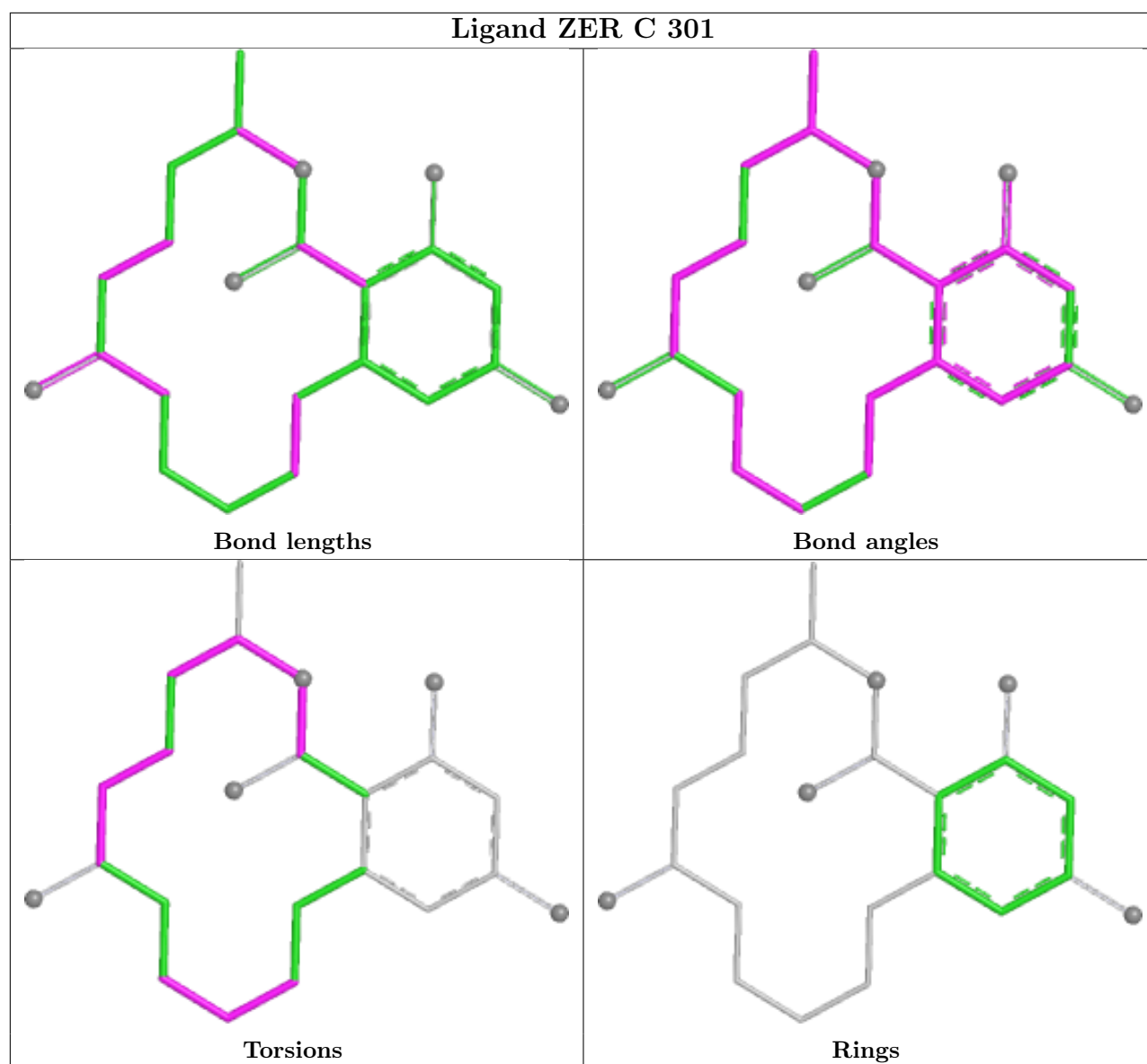
Bond angles



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	263/266 (98%)	-0.41	0 100 100	14, 20, 32, 49	0
1	B	263/266 (98%)	-0.38	1 (0%) 88 92	12, 21, 33, 48	1 (0%)
1	C	263/266 (98%)	-0.24	0 100 100	15, 24, 41, 73	0
1	D	264/266 (99%)	-0.10	3 (1%) 78 82	16, 24, 43, 62	0
1	E	263/266 (98%)	-0.02	1 (0%) 88 92	19, 27, 43, 57	0
1	F	263/266 (98%)	0.48	18 (6%) 23 26	19, 33, 59, 71	0
1	G	262/266 (98%)	-0.18	1 (0%) 88 92	18, 26, 37, 50	0
1	H	263/266 (98%)	-0.26	1 (0%) 88 92	12, 23, 35, 56	1 (0%)
All	All	2104/2128 (98%)	-0.14	25 (1%) 76 81	12, 24, 43, 73	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	ALA	4.2
1	F	147	ALA	3.5
1	D	160	TYR	3.4
1	E	160	TYR	3.1
1	F	139	LEU	3.0
1	F	146	PRO	3.0
1	F	16	ILE	2.9
1	F	148	THR	2.9
1	F	71	PRO	2.7
1	F	72	PRO	2.7
1	F	186	ALA	2.7
1	F	78	ILE	2.6
1	G	4	THR	2.5
1	F	141	ILE	2.4
1	F	149	ILE	2.4
1	F	74	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	160	TYR	2.3
1	H	3	ALA	2.2
1	F	138	LEU	2.2
1	D	25	SER	2.1
1	B	4	THR	2.1
1	F	144	VAL	2.1
1	F	86	TYR	2.1
1	F	88	ILE	2.1
1	F	70	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

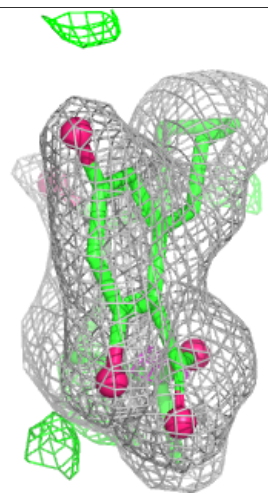
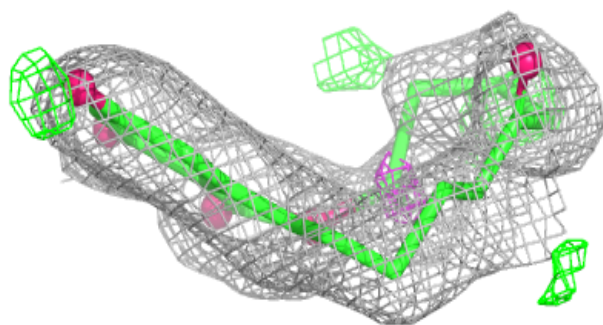
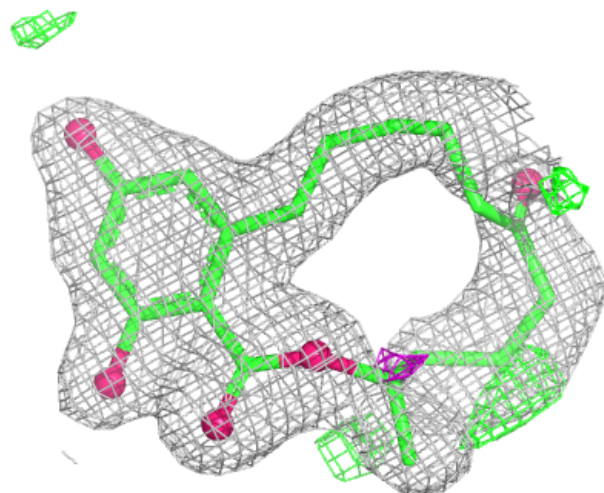
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZER	F	301	23/23	0.89	0.13	30,37,63,70	0
2	ZER	G	301	23/23	0.89	0.11	19,23,43,48	0
2	ZER	A	301	23/23	0.91	0.10	15,22,33,36	0
2	ZER	E	301	23/23	0.91	0.11	24,27,52,56	0
2	ZER	C	301	23/23	0.93	0.10	19,26,45,47	0
2	ZER	D	301	23/23	0.94	0.10	17,26,50,56	0
2	ZER	B	301	23/23	0.94	0.10	16,22,52,61	0
2	ZER	H	301	23/23	0.94	0.08	16,20,35,37	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.

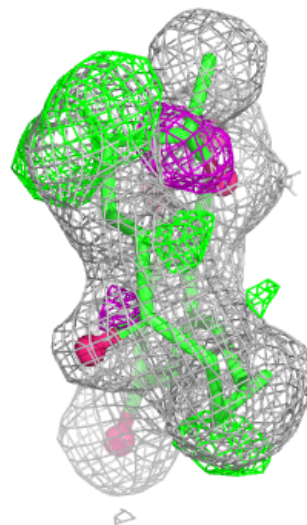
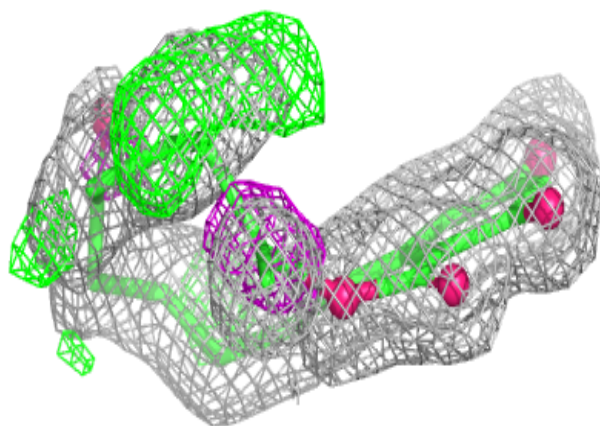
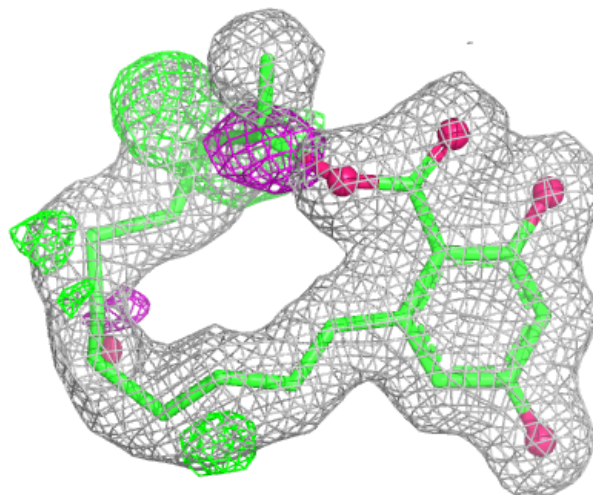
Electron density around ZER F 301:

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



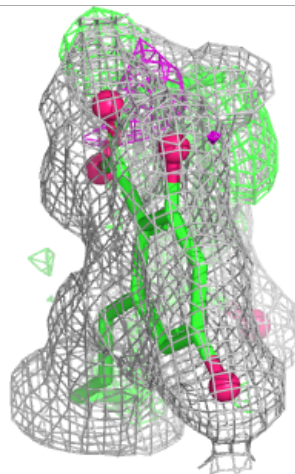
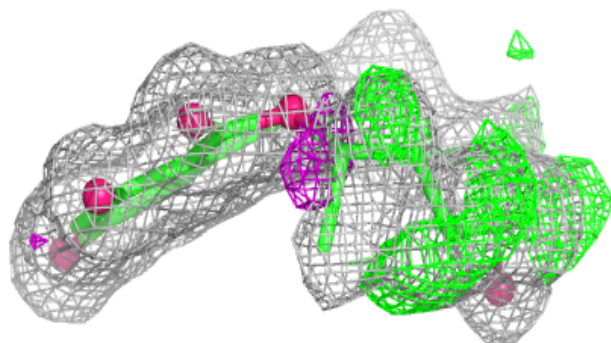
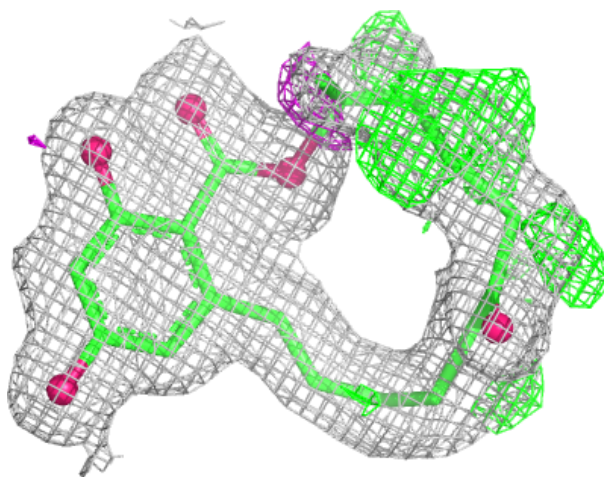
Electron density around ZER G 301:

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



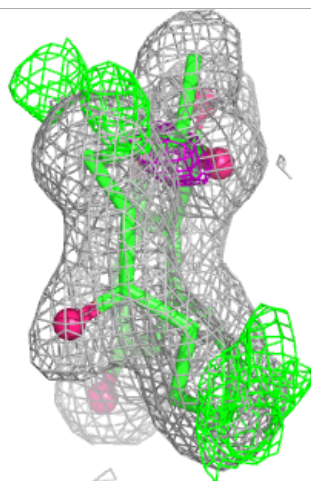
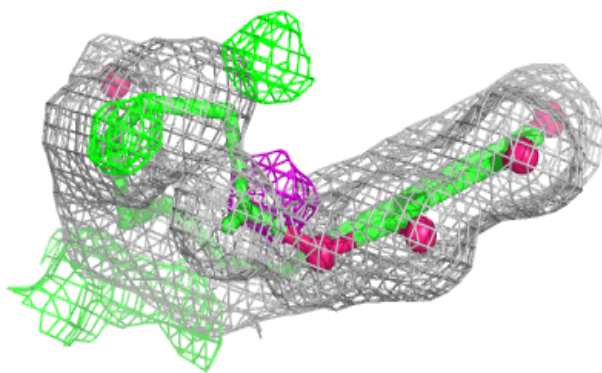
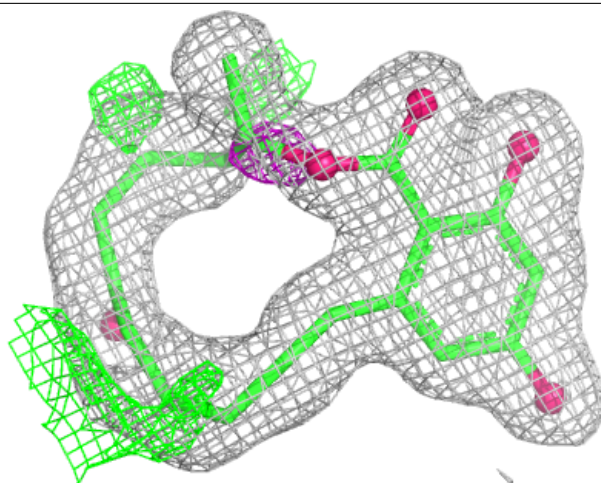
Electron density around ZER A 301:

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



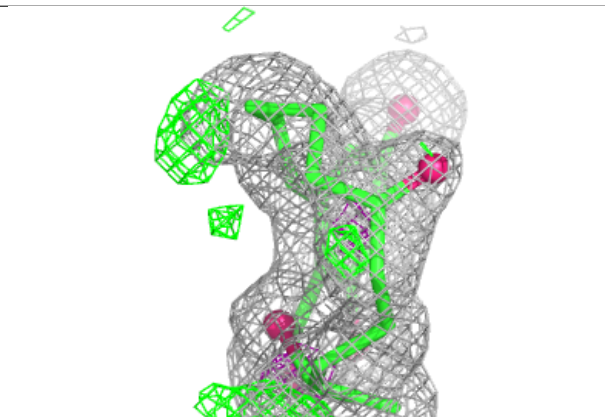
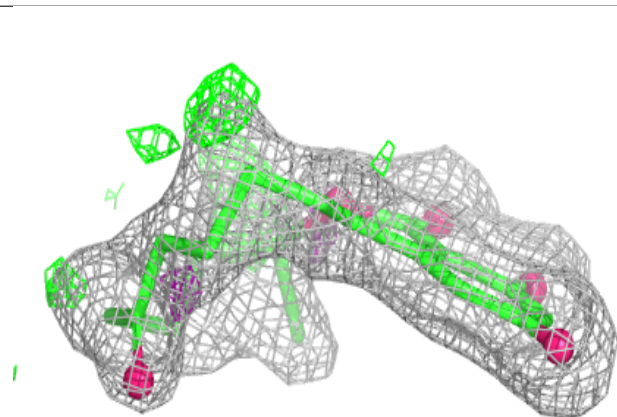
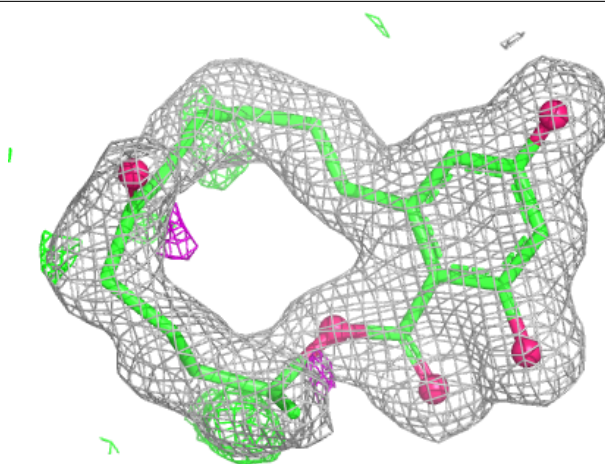
Electron density around ZER E 301:

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



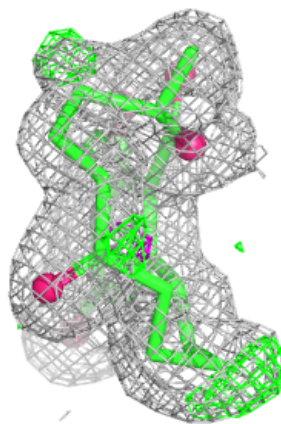
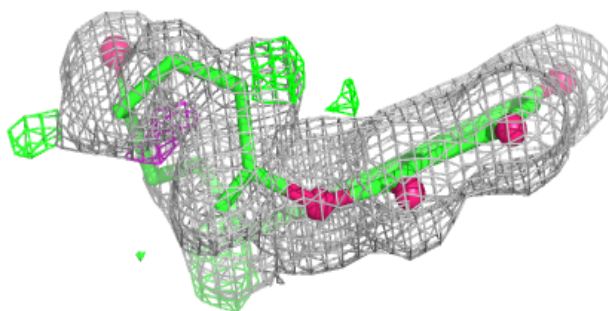
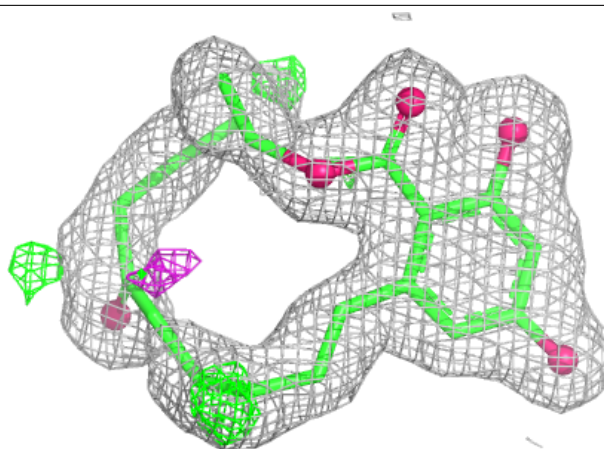
Electron density around ZER C 301:

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



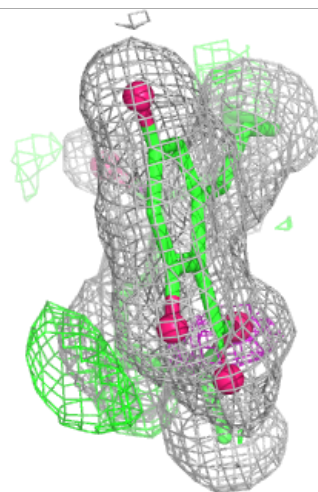
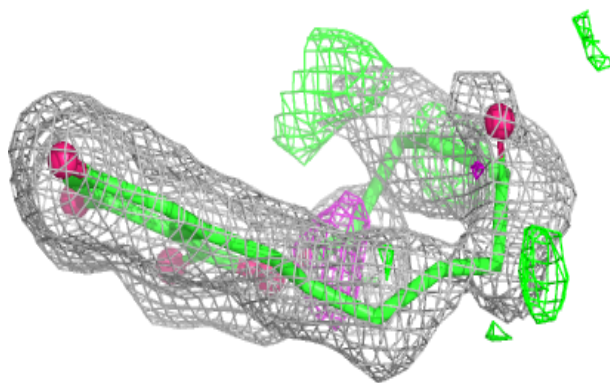
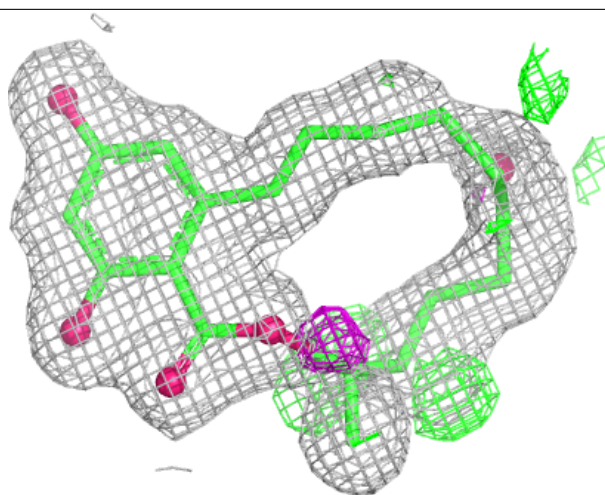
Electron density around ZER D 301:

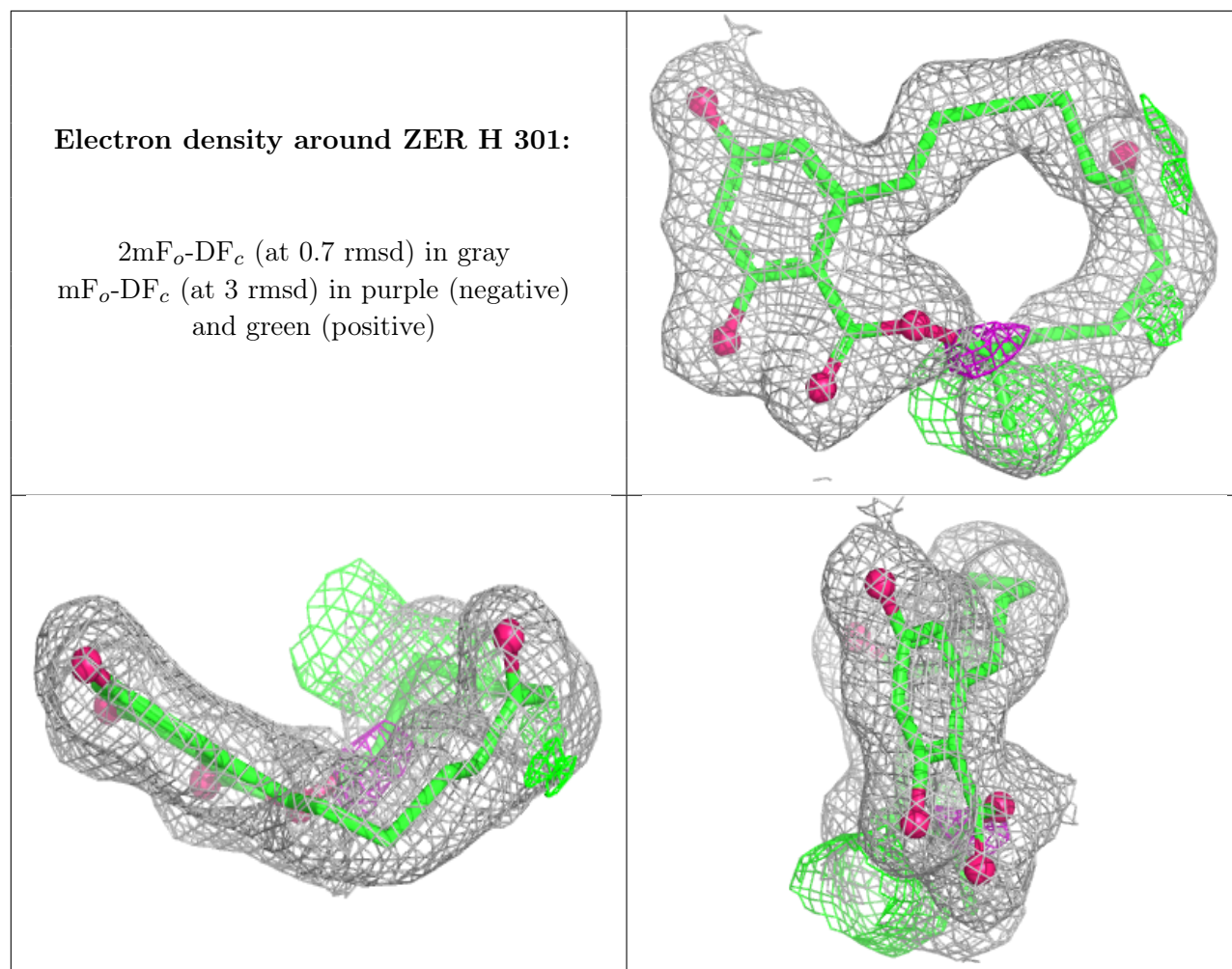
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZER B 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.