



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:01 PM UTC

PDB ID : 8Q67 / pdb_00008q67
Title : Crystal structure of a homohexameric MCM from *M. acidophilum*
Authors : Noble, O.W.; Degut, C.; Hodgkinson, M.R.; Chong, J.P.J.; Plevin, M.J.
Deposited on : 2023-08-11
Resolution : 2.59 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:

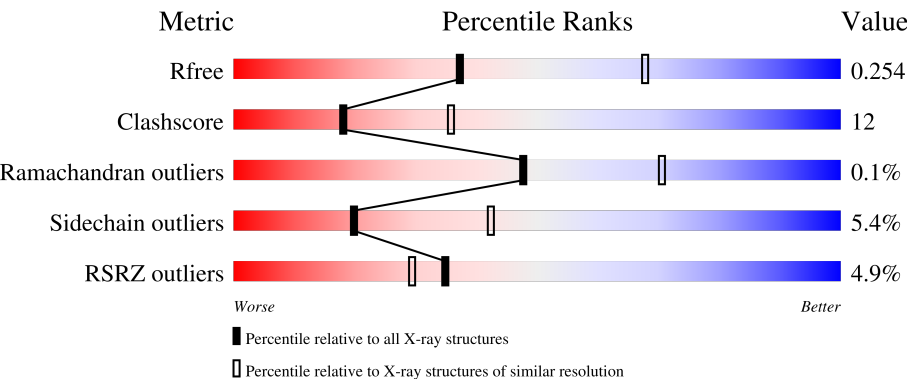
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	601	4% 72% 21% • •
1	B	601	6% 71% 23% • 5%
1	C	601	4% 72% 22% • •
1	D	601	5% 77% 18% • •
1	E	601	5% 65% 25% 5% •

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Mol	Chain	Length	Quality of chain
1	F	601	

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
3	PO4	A	702	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 54511 atoms, of which 27391 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 DNA helicase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	574	Total	C	H	N	O	S	0	2	0
			9022	2846	4546	752	864	14			
1	B	572	Total	C	H	N	O	S	0	0	0
			8988	2834	4530	750	860	14			
1	C	574	Total	C	H	N	O	S	0	0	0
			9023	2849	4545	752	863	14			
1	D	577	Total	C	H	N	O	S	0	0	0
			9065	2864	4561	757	869	14			
1	E	574	Total	C	H	N	O	S	0	0	0
			9022	2847	4547	752	862	14			
1	F	582	Total	C	H	N	O	S	0	0	0
			9146	2886	4606	762	878	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A218NN99
A	391	GLN	GLU	engineered mutation	UNP A0A218NN99
B	0	GLY	-	expression tag	UNP A0A218NN99
B	391	GLN	GLU	engineered mutation	UNP A0A218NN99
C	0	GLY	-	expression tag	UNP A0A218NN99
C	391	GLN	GLU	engineered mutation	UNP A0A218NN99
D	0	GLY	-	expression tag	UNP A0A218NN99
D	391	GLN	GLU	engineered mutation	UNP A0A218NN99
E	0	GLY	-	expression tag	UNP A0A218NN99
E	391	GLN	GLU	engineered mutation	UNP A0A218NN99
F	0	GLY	-	expression tag	UNP A0A218NN99
F	391	GLN	GLU	engineered mutation	UNP A0A218NN99

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 38	C 10	H 11	N 5	O 10	P 2	1	0
2	B	1	Total 38	C 10	H 11	N 5	O 10	P 2	1	0
2	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	7	0
2	E	1	Total 38	C 10	H 11	N 5	O 10	P 2	3	0
2	F	1	Total 38	C 10	H 11	N 5	O 10	P 2	5	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0

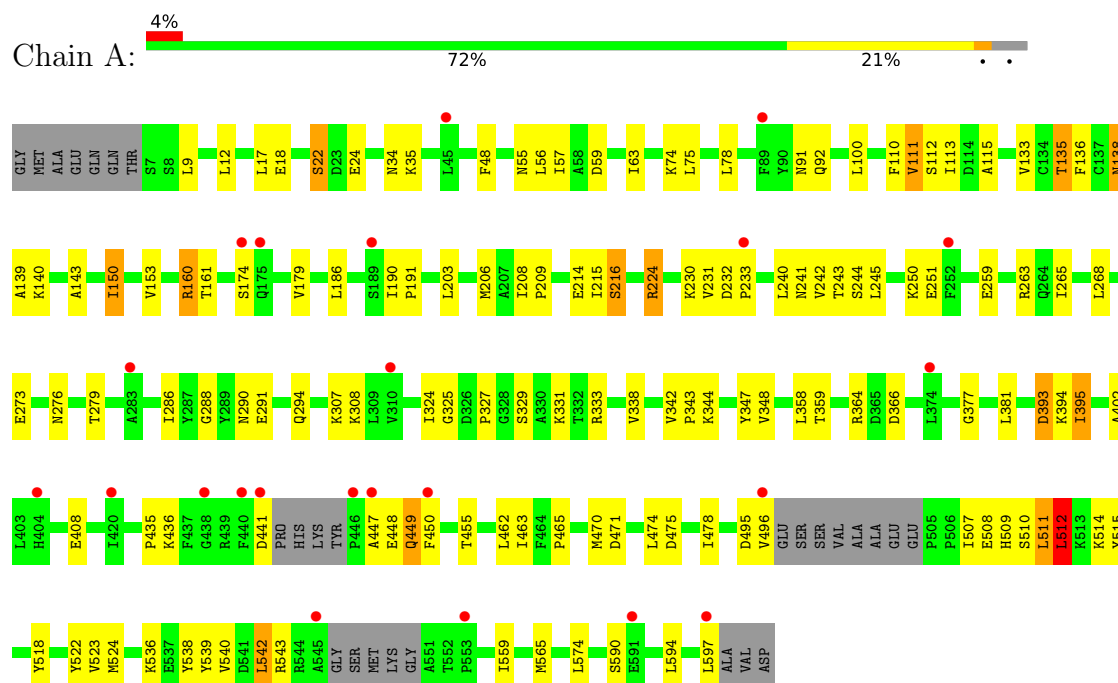
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	1	Total 1	O 1	0	0
5	C	3	Total 3	O 3	0	0
5	D	1	Total 1	O 1	0	0
5	F	2	Total 2	O 2	0	0

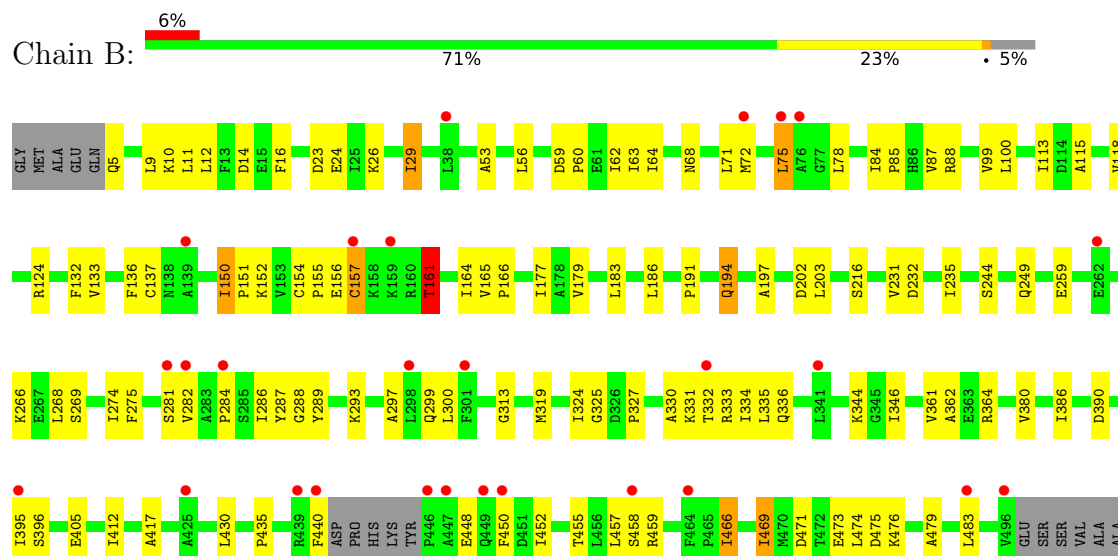
3 Residue-property plots

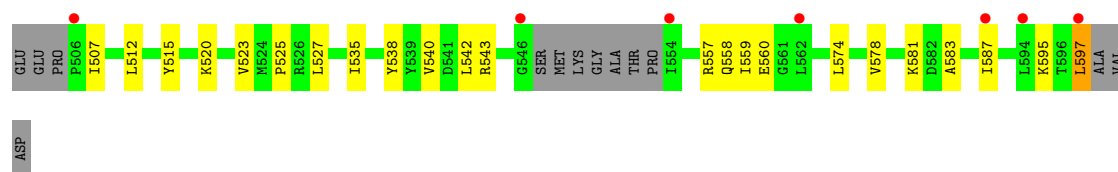
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: DNA helicase

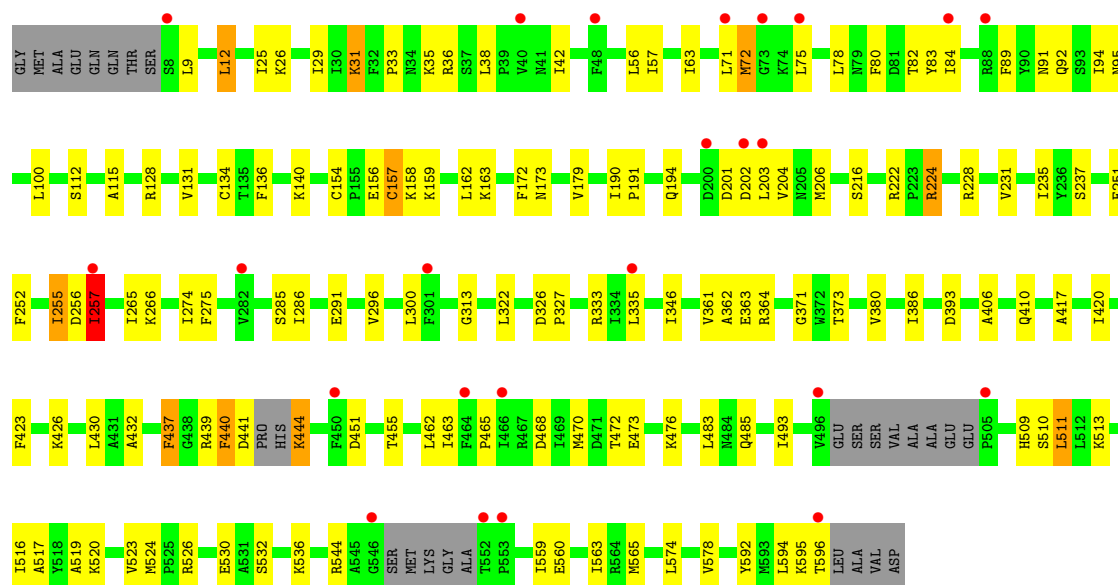


• Molecule 1: DNA helicase

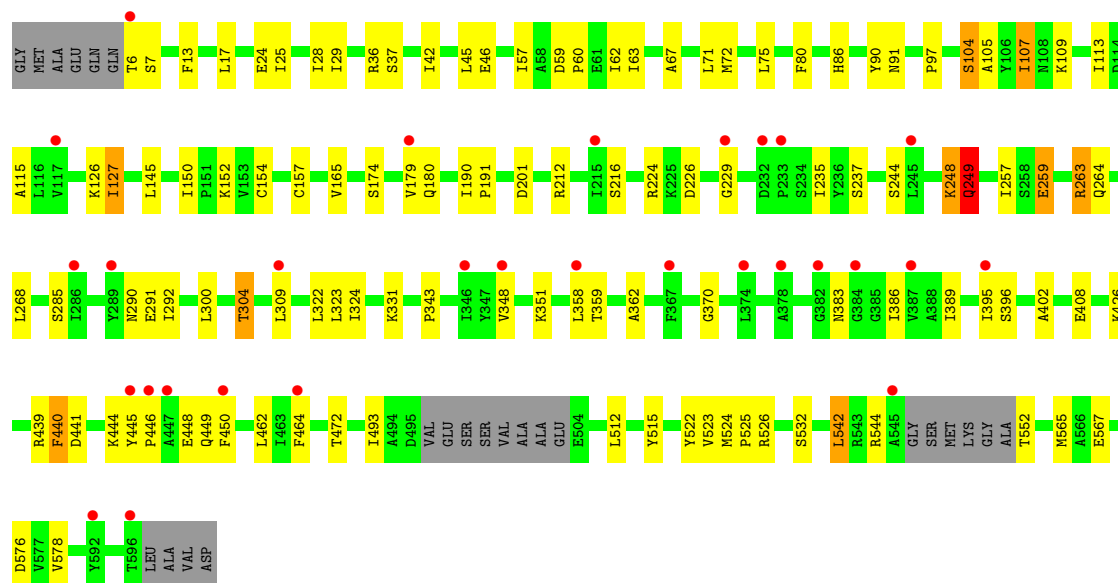
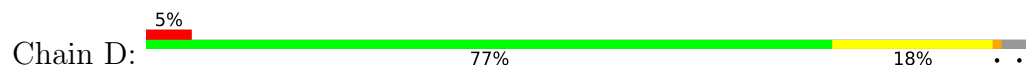




- Molecule 1: DNA helicase



- Molecule 1: DNA helicase



- Molecule 1: DNA helicase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	228.70Å 127.49Å 177.04Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	57.15 – 2.59 57.15 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.0 (57.15-2.59) 98.0 (57.15-2.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.231 , 0.253 0.232 , 0.254	Depositor DCC
R_{free} test set	2021 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	54511	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: PO4, ZN, ADP

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	1.35	43/4559 (0.9%)	0.93	11/6163 (0.2%)
1	B	1.11	10/4531 (0.2%)	0.89	6/6121 (0.1%)
1	C	1.16	24/4554 (0.5%)	0.93	15/6155 (0.2%)
1	D	1.07	12/4583 (0.3%)	0.92	11/6198 (0.2%)
1	E	1.37	34/4550 (0.7%)	1.09	19/6147 (0.3%)
1	F	1.23	19/4616 (0.4%)	0.92	10/6239 (0.2%)
All	All	1.22	142/27393 (0.5%)	0.95	72/37023 (0.2%)

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	VAL	C-O	-9.20	1.14	1.23
1	E	123	ILE	C-O	-9.01	1.14	1.24
1	A	215	ILE	C-O	-8.55	1.14	1.24
1	A	241	ASN	C-O	-8.07	1.14	1.24
1	E	154	CYS	CA-C	-7.97	1.43	1.52
1	B	560	GLU	CA-C	-7.82	1.42	1.52
1	D	107	ILE	C-O	-7.78	1.15	1.24
1	A	113	ILE	C-O	-7.75	1.16	1.24
1	A	139	ALA	C-O	-7.35	1.14	1.23
1	C	440	PHE	N-CA	-7.30	1.36	1.46
1	A	240	LEU	C-O	-7.25	1.15	1.24
1	F	154	CYS	CA-C	-7.18	1.44	1.52
1	A	112	SER	C-O	-7.04	1.15	1.24
1	A	244	SER	C-O	-6.96	1.15	1.23
1	A	510	SER	C-O	-6.70	1.16	1.24
1	E	331	LYS	CA-C	-6.70	1.44	1.52
1	D	408	GLU	C-O	-6.65	1.16	1.23
1	F	596	THR	N-CA	-6.58	1.38	1.46
1	A	242	VAL	C-O	-6.56	1.15	1.24
1	F	172	PHE	C-O	-6.54	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	154	CYS	C-O	-6.49	1.16	1.24
1	E	559	ILE	C-O	-6.47	1.16	1.24
1	A	216	SER	C-O	-6.47	1.15	1.23
1	E	523	VAL	C-O	-6.46	1.17	1.24
1	D	105	ALA	C-O	-6.45	1.15	1.24
1	D	63	ILE	C-O	-6.40	1.17	1.24
1	E	590	SER	CA-C	-6.40	1.44	1.52
1	E	125	PRO	C-O	-6.39	1.16	1.23
1	F	594	LEU	CA-C	-6.38	1.44	1.52
1	A	465	PRO	C-O	-6.38	1.17	1.23
1	A	215	ILE	CA-CB	-6.35	1.46	1.54
1	A	224	ARG	C-O	-6.33	1.16	1.23
1	F	173	ASN	C-O	-6.33	1.16	1.23
1	D	104	SER	C-O	-6.31	1.15	1.24
1	C	154	CYS	C-O	-6.28	1.15	1.23
1	F	84	ILE	C-O	-6.25	1.16	1.24
1	C	510	SER	C-O	-6.23	1.16	1.24
1	A	110	PHE	C-O	-6.22	1.16	1.24
1	A	512	LEU	C-O	-6.17	1.16	1.24
1	A	35	LYS	C-O	-6.17	1.17	1.24
1	C	509	HIS	C-O	-6.16	1.17	1.24
1	B	87	VAL	C-O	-6.14	1.17	1.24
1	A	230	LYS	C-O	-6.13	1.16	1.23
1	C	157	CYS	C-O	-6.04	1.16	1.24
1	A	463	ILE	C-O	-6.03	1.17	1.24
1	A	214	GLU	C-O	-6.00	1.16	1.24
1	E	302	GLY	C-O	-6.00	1.15	1.23
1	C	513	LYS	C-O	-5.98	1.17	1.24
1	C	519	ALA	C-O	-5.97	1.17	1.24
1	A	91	ASN	C-O	-5.96	1.16	1.24
1	E	331	LYS	C-O	-5.92	1.17	1.24
1	F	154	CYS	C-O	-5.92	1.16	1.24
1	C	72	MET	C-O	-5.91	1.17	1.24
1	F	295	ALA	CA-C	-5.91	1.45	1.52
1	A	143	ALA	C-O	-5.89	1.16	1.23
1	E	172	PHE	C-O	-5.88	1.16	1.23
1	A	245	LEU	C-O	-5.87	1.17	1.24
1	A	338	VAL	C-O	-5.82	1.17	1.24
1	E	558	GLN	C-O	-5.81	1.16	1.24
1	E	317	SER	C-O	-5.81	1.15	1.23
1	F	174	SER	C-O	-5.81	1.16	1.23
1	C	516	ILE	CA-CB	-5.80	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	305	PRO	C-O	-5.78	1.16	1.24
1	E	386	ILE	C-O	-5.75	1.17	1.24
1	A	243	THR	C-O	-5.74	1.15	1.23
1	E	56	LEU	C-O	-5.73	1.17	1.24
1	A	22	SER	C-O	-5.71	1.17	1.24
1	D	212	ARG	C-O	-5.71	1.17	1.24
1	C	134	CYS	C-O	-5.70	1.17	1.23
1	E	571	LYS	C-O	-5.69	1.17	1.24
1	C	510	SER	CA-C	-5.68	1.45	1.52
1	E	521	ARG	CA-C	-5.68	1.45	1.52
1	E	237	SER	C-O	-5.66	1.16	1.23
1	A	294	GLN	C-O	-5.62	1.17	1.24
1	F	165	VAL	N-CA	-5.62	1.39	1.46
1	F	124	ARG	C-O	-5.61	1.19	1.25
1	E	173	ASN	C-O	-5.56	1.16	1.23
1	A	509	HIS	C-O	-5.53	1.17	1.24
1	C	516	ILE	C-O	-5.53	1.17	1.24
1	D	107	ILE	CA-CB	-5.52	1.47	1.54
1	A	92	GLN	C-O	-5.50	1.16	1.23
1	C	154	CYS	CA-C	-5.49	1.46	1.53
1	A	216	SER	CA-C	-5.46	1.46	1.52
1	F	338	VAL	CA-CB	-5.45	1.47	1.54
1	F	204	VAL	C-O	-5.45	1.18	1.24
1	E	286	ILE	CA-CB	-5.43	1.47	1.54
1	D	304	THR	CA-C	-5.42	1.46	1.52
1	A	174	SER	C-O	-5.41	1.17	1.23
1	F	338	VAL	C-O	-5.40	1.17	1.24
1	C	426	LYS	C-O	-5.39	1.17	1.24
1	C	517	ALA	CA-C	-5.38	1.45	1.52
1	E	304	THR	CA-C	-5.38	1.46	1.52
1	C	520	LYS	C-O	-5.37	1.17	1.24
1	A	135	THR	CA-C	-5.36	1.45	1.52
1	D	60	PRO	C-O	-5.36	1.17	1.24
1	C	136	PHE	C-O	-5.35	1.19	1.23
1	E	595	LYS	N-CA	-5.33	1.40	1.46
1	C	523	VAL	C-O	-5.33	1.17	1.24
1	A	511	LEU	C-O	-5.32	1.17	1.24
1	B	559	ILE	C-O	-5.32	1.18	1.24
1	D	174	SER	C-O	-5.32	1.17	1.23
1	F	334	ILE	CA-C	-5.31	1.46	1.52
1	B	475	ASP	C-O	-5.30	1.17	1.24
1	C	266	LYS	C-O	-5.30	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	560	GLU	C-O	-5.27	1.17	1.24
1	A	74	LYS	C-O	-5.24	1.17	1.24
1	C	112	SER	C-O	-5.23	1.17	1.24
1	B	124	ARG	C-O	-5.23	1.19	1.24
1	F	334	ILE	C-O	-5.22	1.18	1.24
1	F	293	LYS	C-O	-5.21	1.18	1.24
1	E	524	MET	C-O	-5.21	1.18	1.24
1	E	305	PRO	CA-C	-5.21	1.45	1.52
1	A	161	THR	C-O	-5.20	1.18	1.24
1	C	509	HIS	CA-C	-5.20	1.46	1.52
1	A	112	SER	CA-C	-5.19	1.46	1.52
1	A	279	THR	C-O	-5.19	1.17	1.24
1	E	123	ILE	CA-CB	-5.19	1.48	1.54
1	A	9	LEU	C-O	-5.18	1.18	1.24
1	A	244	SER	CA-C	-5.17	1.46	1.52
1	C	519	ALA	CA-C	-5.17	1.46	1.52
1	D	59	ASP	C-O	-5.16	1.17	1.24
1	E	590	SER	C-O	-5.15	1.18	1.24
1	C	237	SER	C-O	-5.14	1.17	1.23
1	B	161	THR	N-CA	-5.14	1.41	1.46
1	B	542	LEU	CA-C	-5.14	1.46	1.52
1	E	65	ASP	N-CA	-5.13	1.40	1.46
1	E	513	LYS	N-CA	-5.13	1.40	1.46
1	E	543	ARG	N-CA	-5.12	1.40	1.46
1	D	104	SER	CA-C	-5.11	1.45	1.52
1	A	514	LYS	C-O	-5.10	1.18	1.24
1	E	525	PRO	C-O	-5.09	1.17	1.23
1	E	523	VAL	CA-CB	-5.08	1.48	1.54
1	E	340	ARG	CA-C	-5.07	1.45	1.52
1	F	590	SER	C-O	-5.06	1.18	1.24
1	B	53	ALA	C-O	-5.05	1.18	1.24
1	B	476	LYS	C-O	-5.05	1.18	1.24
1	F	335	LEU	C-O	-5.03	1.18	1.24
1	A	241	ASN	CA-C	-5.02	1.46	1.52
1	A	34	ASN	C-O	-5.02	1.18	1.24
1	C	38	LEU	C-O	-5.00	1.20	1.25
1	E	331	LYS	N-CA	-5.00	1.40	1.46
1	A	288	GLY	CA-C	-5.00	1.47	1.52

All (72) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	578	VAL	N-CA-C	11.66	122.52	110.62
1	E	450	PHE	N-CA-C	10.46	122.69	111.28
1	C	91	ASN	N-CA-C	9.88	122.47	110.91
1	E	91	ASN	N-CA-C	9.50	124.10	111.28
1	A	136	PHE	N-CA-C	8.75	120.59	111.14
1	F	91	ASN	N-CA-C	8.13	122.47	111.24
1	A	138	ASN	N-CA-C	7.11	121.34	112.24
1	E	257	ILE	CB-CA-C	-6.70	104.22	111.59
1	E	286	ILE	N-CA-C	6.65	117.70	107.99
1	A	150	ILE	CA-C-N	6.40	126.37	119.78
1	A	150	ILE	C-N-CA	6.40	126.37	119.78
1	A	449	GLN	N-CA-C	6.37	121.38	112.72
1	F	173	ASN	N-CA-C	6.21	118.79	110.35
1	F	559	ILE	CB-CA-C	-6.15	103.84	112.14
1	D	248	LYS	N-CA-C	6.10	122.04	113.56
1	A	242	VAL	N-CA-C	6.08	117.48	109.21
1	C	257	ILE	CB-CA-C	-6.06	102.24	110.42
1	E	581	LYS	N-CA-C	-6.06	104.76	111.36
1	E	38	LEU	CA-C-N	6.05	125.99	119.76
1	E	38	LEU	C-N-CA	6.05	125.99	119.76
1	C	523	VAL	CA-C-N	6.04	133.48	123.08
1	C	523	VAL	C-N-CA	6.04	133.48	123.08
1	D	523	VAL	N-CA-C	5.99	116.49	107.75
1	C	231	VAL	N-CA-C	5.95	116.44	108.11
1	B	559	ILE	CB-CA-C	-5.88	104.35	111.88
1	F	265	ILE	CB-CA-C	-5.84	104.26	112.14
1	C	362	ALA	CA-C-N	5.82	131.33	122.65
1	C	362	ALA	C-N-CA	5.82	131.33	122.65
1	F	497	GLU	N-CA-C	5.82	118.39	108.90
1	B	29	ILE	CB-CA-C	-5.81	104.54	111.97
1	F	166	PRO	CB-CA-C	-5.80	103.61	111.85
1	C	38	LEU	CA-C-N	5.78	125.69	119.85
1	C	38	LEU	C-N-CA	5.78	125.69	119.85
1	B	152	LYS	N-CA-C	5.78	117.38	111.14
1	E	29	ILE	CB-CA-C	-5.78	104.34	112.14
1	B	473	GLU	N-CA-C	-5.77	104.91	111.14
1	A	113	ILE	CB-CA-C	-5.73	101.67	110.50
1	D	104	SER	N-CA-C	5.70	120.07	113.18
1	A	232	ASP	N-CA-CB	-5.66	101.97	109.78
1	E	156	GLU	N-CA-C	5.65	117.52	111.36
1	C	313	GLY	CA-C-N	5.63	129.09	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	GLY	C-N-CA	5.63	129.09	121.05
1	E	302	GLY	N-CA-C	5.61	119.94	112.65
1	F	478	ILE	CB-CA-C	-5.60	104.58	112.14
1	B	313	GLY	O-C-N	-5.57	117.11	122.84
1	D	292	ILE	CB-CA-C	-5.46	104.98	111.97
1	D	249	GLN	N-CA-C	-5.44	99.22	110.80
1	E	201	ASP	CB-CA-C	-5.39	110.38	116.63
1	F	273	GLU	N-CA-C	5.38	118.68	112.97
1	C	35	LYS	N-CA-C	-5.37	99.53	108.34
1	E	294	GLN	CB-CA-C	-5.30	101.83	110.85
1	F	535	ILE	CB-CA-C	-5.30	104.91	112.22
1	E	329	SER	N-CA-C	5.27	118.72	112.72
1	E	561	GLY	CA-C-O	-5.27	115.31	121.00
1	D	544	ARG	N-CA-C	-5.26	102.07	109.96
1	E	279	THR	CB-CA-C	-5.25	102.07	110.79
1	E	20	TYR	N-CA-C	5.24	120.54	114.04
1	A	478	ILE	CB-CA-C	-5.23	105.28	111.97
1	D	440	PHE	CB-CA-C	5.22	119.98	112.05
1	C	72	MET	N-CA-C	-5.22	105.49	111.07
1	D	257	ILE	CB-CA-C	-5.20	102.94	110.63
1	D	127	ILE	N-CA-C	5.20	116.28	109.21
1	A	214	GLU	N-CA-C	-5.19	100.62	108.67
1	B	535	ILE	CB-CA-C	-5.18	105.06	112.22
1	E	31	LYS	N-CA-C	5.15	119.55	113.16
1	F	161	THR	CB-CA-C	-5.14	101.81	110.44
1	D	46	GLU	N-CA-C	-5.12	105.61	111.14
1	D	522	TYR	N-CA-C	5.08	119.58	113.17
1	C	173	ASN	N-CA-C	5.07	117.24	110.35
1	C	31	LYS	N-CA-C	5.05	117.52	111.71
1	E	286	ILE	CB-CA-C	-5.04	104.08	110.98
1	A	471	ASP	N-CA-C	-5.03	101.11	109.46

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	4476	4546	4541	102	0
1	B	4458	4530	4530	124	0
1	C	4478	4545	4545	101	0
1	D	4504	4561	4560	93	0
1	E	4475	4547	4547	161	0
1	F	4540	4606	4606	112	0
2	A	27	11	12	2	0
2	B	27	11	12	5	0
2	C	27	12	12	1	0
2	E	27	11	12	3	0
2	F	27	11	12	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	6	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
All	All	27120	27391	27389	667	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 12.

All (667) 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:F:324:ILE:HD13	1:F:450:PHE:CD2	1.50	1.47
1:F:324:ILE:HD13	1:F:450:PHE:CE2	1.59	1.38
1:F:324:ILE:CD1	1:F:450:PHE:CE2	2.21	1.23
1:E:324:ILE:HG12	1:E:450:PHE:CD1	1.78	1.17
1:E:324:ILE:HG21	1:E:450:PHE:CE1	1.80	1.16
1:E:324:ILE:HG12	1:E:450:PHE:CE1	1.80	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:558:GLN:O	1:F:562:LEU:HD23	1.44	1.14
1:E:324:ILE:HG21	1:E:450:PHE:HE1	1.10	1.13
1:E:324:ILE:CG2	1:E:450:PHE:HE1	1.71	1.04
1:B:75:LEU:HD12	1:B:78:LEU:HD23	1.39	1.02
1:E:324:ILE:CG1	1:E:450:PHE:CE1	2.43	1.01
1:E:322:LEU:HD22	1:E:324:ILE:HD12	1.40	1.01
1:F:330:ALA:HA	2:F:701:ADP:H5'2	1.40	1.00
1:B:29:ILE:HG12	1:B:75:LEU:HB2	1.42	1.00
1:A:436:LYS:HE2	1:A:449:GLN:HA	1.45	0.98
1:E:228:ARG:HD2	1:E:230:LYS:HD2	1.45	0.98
1:E:228:ARG:CD	1:E:230:LYS:HD2	1.94	0.97
1:B:75:LEU:HD12	1:B:78:LEU:CD2	1.94	0.97
1:B:115:ALA:HB1	1:B:179:VAL:HG13	1.47	0.96
1:D:322:LEU:HD22	1:D:324:ILE:HG13	1.44	0.96
1:B:132:PHE:CE2	1:B:164:ILE:HG12	2.01	0.96
1:E:9:LEU:CD2	1:E:66:ALA:HB1	1.95	0.95
1:E:9:LEU:HD22	1:E:66:ALA:CB	1.98	0.94
1:F:324:ILE:CD1	1:F:450:PHE:CD2	2.45	0.93
1:E:361:VAL:HG11	1:E:423:PHE:CD1	2.05	0.92
1:E:527:LEU:HD22	1:E:578:VAL:HG21	1.51	0.90
1:E:9:LEU:CD2	1:E:66:ALA:CB	2.49	0.90
1:A:436:LYS:HE2	1:A:449:GLN:CA	2.01	0.90
1:E:9:LEU:HD22	1:E:66:ALA:HB1	1.52	0.90
1:B:88:ARG:CZ	1:B:203:LEU:HD11	2.02	0.90
1:B:479:ALA:O	1:B:483:LEU:HD13	1.72	0.89
1:A:55:ASN:OD1	1:A:63:ILE:HD11	1.72	0.89
1:F:324:ILE:HG21	1:F:450:PHE:CD2	2.09	0.87
1:E:9:LEU:HD11	1:E:63:ILE:HG12	1.56	0.86
1:E:71:LEU:HD12	1:E:71:LEU:O	1.76	0.85
1:C:84:ILE:HD12	1:C:128:ARG:CZ	2.06	0.85
1:E:346:ILE:CD1	1:F:420:ILE:HD13	2.07	0.85
1:E:115:ALA:HB1	1:E:179:VAL:HG13	1.59	0.84
1:C:224:ARG:HG2	1:C:224:ARG:HH11	1.41	0.84
1:F:324:ILE:HD12	1:F:450:PHE:CE2	2.12	0.84
1:B:88:ARG:CZ	1:B:203:LEU:CD1	2.56	0.83
1:E:324:ILE:CB	1:E:450:PHE:HE1	1.91	0.83
1:A:160:ARG:HG3	1:A:160:ARG:HH11	1.44	0.83
1:B:469:ILE:HD11	1:B:474:LEU:HD22	1.59	0.83
1:F:324:ILE:CD1	1:F:450:PHE:CZ	2.61	0.83
1:F:527:LEU:HD12	1:F:578:VAL:HG21	1.60	0.82
1:D:45:LEU:O	1:D:45:LEU:HD23	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:THR:CG2	1:E:422:THR:HG22	2.10	0.81
1:D:115:ALA:HB1	1:D:179:VAL:HG13	1.63	0.81
1:E:322:LEU:HD23	1:E:323:LEU:N	1.95	0.80
1:E:585:LEU:HD12	1:E:585:LEU:O	1.81	0.80
1:D:324:ILE:HG21	1:D:450:PHE:CZ	2.17	0.80
1:D:24:GLU:OE1	1:D:24:GLU:N	2.14	0.80
1:C:56:LEU:HB2	1:C:63:ILE:HD11	1.63	0.79
1:E:324:ILE:CG2	1:E:450:PHE:CE1	2.56	0.79
1:E:361:VAL:CG1	1:E:423:PHE:CE1	2.66	0.78
1:D:512:LEU:HD12	1:D:512:LEU:O	1.83	0.78
1:F:324:ILE:HG21	1:F:450:PHE:HD2	1.49	0.77
1:D:322:LEU:HD23	1:D:323:LEU:N	2.00	0.77
1:C:56:LEU:CB	1:C:63:ILE:HD11	2.15	0.77
1:B:56:LEU:HA	1:B:63:ILE:HD13	1.67	0.76
1:B:88:ARG:NH2	1:B:203:LEU:HD13	1.99	0.76
1:F:259:GLU:CD	1:F:259:GLU:H	1.94	0.76
1:E:277:LYS:HB3	1:E:507:ILE:HD11	1.67	0.76
1:F:224:ARG:HG2	1:F:224:ARG:HH11	1.51	0.76
1:E:325:GLY:O	1:E:435:PRO:HD3	1.86	0.76
1:E:12:LEU:O	1:E:12:LEU:HD12	1.86	0.76
1:F:523:VAL:HG21	1:F:574:LEU:HA	1.68	0.76
1:C:25:ILE:O	1:C:29:ILE:HD12	1.86	0.76
1:D:322:LEU:CD2	1:D:324:ILE:HG13	2.15	0.76
1:E:75:LEU:HD12	1:E:80:PHE:HZ	1.50	0.76
1:E:322:LEU:HD22	1:E:324:ILE:CD1	2.17	0.75
1:E:512:LEU:O	1:E:512:LEU:HD12	1.86	0.75
1:C:511:LEU:HD12	1:C:511:LEU:O	1.86	0.75
1:A:333:ARG:HH11	1:A:333:ARG:HG3	1.51	0.75
1:A:511:LEU:HD23	1:A:511:LEU:O	1.87	0.75
1:E:324:ILE:CB	1:E:450:PHE:CE1	2.69	0.75
1:F:167:GLU:OE1	1:F:167:GLU:N	2.21	0.74
1:A:56:LEU:HD12	1:A:56:LEU:O	1.87	0.74
1:D:304:THR:HG22	1:D:525:PRO:HD2	1.69	0.74
1:E:68:ASN:OD1	1:E:87:VAL:HG23	1.88	0.74
1:F:151:PRO:HB2	1:F:162:LEU:HD13	1.70	0.74
1:A:75:LEU:HD12	1:A:78:LEU:HD12	1.67	0.74
1:D:462:LEU:HD11	1:D:565:MET:HE3	1.69	0.74
1:E:411:THR:CG2	1:E:422:THR:CG2	2.66	0.74
1:A:333:ARG:HG3	1:A:333:ARG:NH1	2.02	0.74
1:B:88:ARG:NH2	1:B:203:LEU:CD1	2.51	0.74
1:D:291:GLU:N	1:D:291:GLU:OE1	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:GLN:O	1:E:268:LEU:HD22	1.87	0.73
1:B:324:ILE:HD12	1:B:450:PHE:CE1	2.23	0.73
1:E:21:TYR:O	1:E:25:ILE:HG13	1.89	0.73
1:E:346:ILE:HD13	1:F:420:ILE:HD13	1.68	0.73
1:B:448:GLU:O	1:B:448:GLU:HG2	1.87	0.73
1:B:29:ILE:CG1	1:B:75:LEU:HB2	2.18	0.73
1:E:361:VAL:CG1	1:E:423:PHE:CD1	2.71	0.72
1:F:324:ILE:HD13	1:F:450:PHE:CG	2.22	0.72
1:B:115:ALA:HB1	1:B:179:VAL:CG1	2.18	0.72
1:C:224:ARG:HG2	1:C:224:ARG:NH1	2.01	0.72
1:E:78:LEU:HD12	1:E:78:LEU:N	2.04	0.72
1:E:469:ILE:HG22	1:E:469:ILE:O	1.89	0.72
1:C:72:MET:HE3	1:C:80:PHE:CD2	2.23	0.72
1:A:436:LYS:HE2	1:A:449:GLN:CB	2.20	0.72
1:E:247:THR:HG22	1:E:250:LYS:HE3	1.72	0.72
1:E:71:LEU:HD12	1:E:71:LEU:C	2.15	0.72
1:E:75:LEU:HD12	1:E:75:LEU:O	1.90	0.71
1:F:115:ALA:HB1	1:F:179:VAL:HG13	1.72	0.71
1:F:330:ALA:CA	2:F:701:ADP:H5'2	2.20	0.71
1:E:228:ARG:HD3	1:E:230:LYS:HD2	1.71	0.70
1:E:539:TYR:CE2	1:E:559:ILE:HD11	2.27	0.70
1:F:158:LYS:O	1:F:158:LYS:HG2	1.91	0.70
1:A:436:LYS:CE	1:A:449:GLN:HA	2.21	0.70
1:B:132:PHE:CE2	1:B:164:ILE:CG1	2.74	0.70
1:B:11:LEU:O	1:B:14:ASP:HB2	1.91	0.70
1:F:291:GLU:N	1:F:291:GLU:OE1	2.25	0.69
1:C:115:ALA:HB1	1:C:179:VAL:CG1	2.23	0.69
1:F:186:LEU:HD21	1:F:191:PRO:HD3	1.75	0.69
1:C:56:LEU:CA	1:C:63:ILE:HD11	2.23	0.69
1:D:542:LEU:HD12	1:D:542:LEU:O	1.91	0.69
1:A:115:ALA:HB1	1:A:179:VAL:HG13	1.74	0.68
1:A:324:ILE:HD13	1:A:450:PHE:CE1	2.29	0.68
1:F:330:ALA:HA	2:F:701:ADP:C5'	2.21	0.68
1:F:537:GLU:O	1:F:540:VAL:HG23	1.93	0.68
1:A:523:VAL:HG21	1:A:574:LEU:HD23	1.75	0.68
1:C:462:LEU:HD11	1:C:565:MET:SD	2.33	0.68
1:B:75:LEU:O	1:B:78:LEU:HD23	1.93	0.68
1:C:115:ALA:HB1	1:C:179:VAL:HG13	1.75	0.68
1:E:75:LEU:CD1	1:E:80:PHE:HZ	2.05	0.68
1:E:268:LEU:HB3	1:E:274:ILE:CD1	2.24	0.67
1:B:558:GLN:OE1	1:B:558:GLN:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:585:LEU:HD12	1:E:585:LEU:C	2.19	0.67
1:F:560:GLU:HA	1:F:563:ILE:HD12	1.76	0.67
1:B:523:VAL:HG12	1:B:525:PRO:HD3	1.77	0.67
1:F:558:GLN:N	1:F:558:GLN:OE1	2.28	0.67
1:C:485:GLN:CD	1:D:309:LEU:HD11	2.19	0.66
1:F:186:LEU:HD21	1:F:191:PRO:CD	2.26	0.66
1:A:523:VAL:C	1:A:524:MET:HE2	2.21	0.66
1:B:330:ALA:HA	2:B:701:ADP:H5'2	1.77	0.66
1:A:308:LYS:HD3	1:A:308:LYS:N	2.11	0.66
1:B:232:ASP:HB3	1:B:235:ILE:HB	1.77	0.66
1:A:436:LYS:HE2	1:A:449:GLN:HB3	1.78	0.65
1:B:583:ALA:O	1:B:587:ILE:HG12	1.96	0.65
1:E:122:ASP:N	1:E:122:ASP:OD1	2.24	0.65
1:E:335:LEU:HD11	1:E:432:ALA:HB3	1.79	0.65
1:E:335:LEU:HD11	1:E:432:ALA:CB	2.26	0.65
1:C:257:ILE:HD12	1:C:257:ILE:O	1.96	0.65
1:C:36:ARG:HG2	1:C:36:ARG:HH11	1.62	0.65
1:D:6:THR:HG23	1:D:7:SER:H	1.62	0.65
1:B:249:GLN:N	1:B:249:GLN:OE1	2.28	0.64
1:C:235:ILE:HG13	1:D:126:LYS:HG3	1.77	0.64
1:D:71:LEU:HD12	1:D:71:LEU:O	1.97	0.64
1:C:285:SER:OG	1:D:309:LEU:HD21	1.98	0.64
1:F:56:LEU:CB	1:F:63:ILE:HD11	2.28	0.64
1:F:56:LEU:CA	1:F:63:ILE:HD11	2.28	0.64
1:B:137:CYS:HB3	1:B:157:CYS:SG	2.37	0.64
1:B:186:LEU:HD13	1:B:191:PRO:HD3	1.79	0.64
1:C:559:ILE:O	1:C:563:ILE:HD12	1.97	0.64
1:E:361:VAL:HG21	1:E:412:ILE:HG21	1.80	0.64
1:D:324:ILE:HG21	1:D:450:PHE:CE1	2.32	0.64
1:D:115:ALA:HB1	1:D:179:VAL:CG1	2.28	0.63
1:E:361:VAL:HG11	1:E:423:PHE:CE1	2.31	0.63
1:F:311:ASP:C	1:F:311:ASP:OD1	2.41	0.63
1:F:56:LEU:HB2	1:F:63:ILE:HD11	1.80	0.62
1:D:28:ILE:HG22	1:D:75:LEU:HD11	1.80	0.62
1:E:411:THR:HG21	1:E:422:THR:CG2	2.29	0.62
1:D:440:PHE:HZ	1:D:446:PRO:HB3	1.64	0.62
1:A:160:ARG:HH11	1:A:160:ARG:CG	2.11	0.62
1:E:268:LEU:HB3	1:E:274:ILE:HD11	1.80	0.62
1:E:129:ASP:H	1:E:170:SER:HB3	1.63	0.62
1:E:359:THR:O	1:E:361:VAL:HG23	1.99	0.62
1:A:115:ALA:HB1	1:A:179:VAL:CG1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:GLU:N	1:A:291:GLU:OE1	2.32	0.62
1:E:322:LEU:HD23	1:E:323:LEU:H	1.64	0.62
1:E:115:ALA:HB1	1:E:179:VAL:CG1	2.27	0.61
1:F:541:ASP:OD1	1:F:541:ASP:N	2.29	0.61
1:C:296:VAL:O	1:C:300:LEU:HD13	2.00	0.61
1:D:71:LEU:HD11	1:D:75:LEU:HD23	1.80	0.61
1:C:574:LEU:N	1:C:574:LEU:HD12	2.13	0.61
1:A:539:TYR:CD2	1:A:559:ILE:HD11	2.35	0.61
1:B:538:TYR:CG	1:B:587:ILE:HD12	2.35	0.61
1:F:489:ALA:O	1:F:493:ILE:HG12	2.00	0.61
1:A:12:LEU:C	1:A:12:LEU:HD23	2.26	0.61
1:F:115:ALA:HB1	1:F:179:VAL:CG1	2.31	0.61
1:B:289:TYR:CE1	1:B:466:ILE:HD13	2.35	0.61
1:C:42:ILE:HD13	1:C:92:GLN:HB3	1.83	0.61
1:E:127:ILE:HD13	1:E:164:ILE:HD11	1.81	0.61
1:C:286:ILE:HD11	1:C:333:ARG:HG2	1.83	0.61
1:E:346:ILE:CD1	1:F:420:ILE:CD1	2.79	0.61
1:E:361:VAL:HG12	1:E:423:PHE:CE1	2.35	0.60
1:F:75:LEU:HB3	1:F:78:LEU:HD12	1.82	0.60
1:A:333:ARG:HH11	1:A:333:ARG:CG	2.14	0.60
1:C:201:ASP:O	1:C:204:VAL:HG23	2.01	0.60
1:F:5:GLN:OE1	1:F:5:GLN:N	2.34	0.60
1:B:100:LEU:HD12	1:B:191:PRO:HG3	1.83	0.60
1:A:543:ARG:HE	1:F:475:ASP:CG	2.10	0.60
1:D:235:ILE:HD12	1:D:235:ILE:N	2.16	0.60
1:D:150:ILE:O	1:D:152:LYS:HD3	2.00	0.60
1:E:247:THR:HG23	1:E:247:THR:O	2.01	0.60
1:C:559:ILE:C	1:C:563:ILE:HD12	2.27	0.60
1:E:411:THR:HG23	1:E:422:THR:HG22	1.83	0.60
2:E:701:ADP:O1A	2:E:701:ADP:H4'	2.02	0.60
1:B:469:ILE:HD12	1:B:471:ASP:CB	2.32	0.59
1:C:25:ILE:HG22	1:C:29:ILE:HD11	1.83	0.59
1:C:71:LEU:O	1:C:75:LEU:HD13	2.03	0.59
1:E:21:TYR:O	1:E:25:ILE:CG1	2.49	0.59
1:E:508:GLU:HG2	1:E:509:HIS:N	2.17	0.59
1:B:231:VAL:O	1:B:231:VAL:HG13	2.01	0.59
1:E:13:PHE:HE2	1:E:63:ILE:HG23	1.67	0.59
1:D:440:PHE:CZ	1:D:446:PRO:HB3	2.38	0.59
1:B:132:PHE:HE2	1:B:164:ILE:CG1	2.15	0.59
1:B:469:ILE:HD12	1:B:471:ASP:HB2	1.83	0.59
1:B:10:LYS:HD3	1:B:14:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:HD12	1:B:75:LEU:O	2.03	0.58
1:E:338:VAL:HG11	1:E:430:LEU:CD2	2.33	0.58
1:C:559:ILE:HG22	1:C:563:ILE:HD11	1.85	0.58
1:D:493:ILE:O	1:D:493:ILE:HG22	2.02	0.58
1:A:324:ILE:HD13	1:A:450:PHE:CZ	2.38	0.58
1:E:271:ASP:HB3	1:E:274:ILE:HB	1.86	0.58
1:B:595:LYS:C	1:B:597:LEU:H	2.09	0.58
1:C:92:GLN:NE2	1:C:95:ASN:O	2.36	0.58
1:D:322:LEU:HD22	1:D:324:ILE:CG1	2.26	0.58
1:E:9:LEU:HD21	1:E:66:ALA:CB	2.32	0.57
1:C:12:LEU:O	1:C:12:LEU:HD12	2.04	0.57
1:B:346:ILE:HG12	1:C:420:ILE:HD13	1.86	0.57
1:C:256:ASP:OD1	1:C:256:ASP:N	2.21	0.57
1:C:26:LYS:HA	1:C:29:ILE:CD1	2.35	0.57
1:E:469:ILE:O	1:E:469:ILE:CG2	2.53	0.57
1:E:224:ARG:HG2	1:E:224:ARG:HH11	1.70	0.57
1:A:186:LEU:HD13	1:A:191:PRO:HD3	1.86	0.57
1:B:71:LEU:O	1:B:71:LEU:HD12	2.04	0.57
1:B:289:TYR:HE1	1:B:466:ILE:HG23	1.70	0.57
1:C:251:GLU:O	1:C:255:ILE:HG12	2.04	0.57
1:A:394:LYS:HA	1:A:394:LYS:HE2	1.86	0.56
1:D:359:THR:HG21	1:D:402:ALA:HB3	1.86	0.56
1:A:543:ARG:NE	1:F:475:ASP:OD2	2.36	0.56
1:C:291:GLU:HG2	1:C:592:TYR:CD1	2.40	0.56
1:D:97:PRO:O	1:D:113:ILE:HG22	2.05	0.56
1:D:552:THR:HG22	1:D:552:THR:O	2.04	0.56
1:E:346:ILE:HD11	1:F:420:ILE:CD1	2.35	0.56
1:E:542:LEU:HD13	1:E:542:LEU:O	2.04	0.56
1:B:364:ARG:HB3	1:B:417:ALA:HB1	1.88	0.56
1:E:9:LEU:C	1:E:9:LEU:HD23	2.29	0.56
1:E:574:LEU:HD12	1:E:574:LEU:N	2.19	0.56
1:F:144:ASN:OD1	1:F:146:GLU:N	2.38	0.56
1:B:324:ILE:CD1	1:B:450:PHE:CD1	2.89	0.56
1:D:71:LEU:CD1	1:D:75:LEU:HD23	2.35	0.56
1:E:539:TYR:CD2	1:E:559:ILE:HD11	2.40	0.56
1:C:56:LEU:HA	1:C:63:ILE:HD11	1.88	0.56
1:C:560:GLU:HA	1:C:563:ILE:CD1	2.35	0.56
1:F:56:LEU:HA	1:F:63:ILE:HD11	1.88	0.56
1:B:88:ARG:CZ	1:B:203:LEU:HD13	2.30	0.56
1:E:268:LEU:O	1:E:274:ILE:HD13	2.06	0.56
1:C:194:GLN:NE2	1:D:370:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:289:TYR:CD2	1:F:292:ILE:HD12	2.41	0.56
1:F:224:ARG:HG2	1:F:224:ARG:NH1	2.20	0.56
1:B:483:LEU:HD23	1:C:532:SER:OG	2.06	0.55
1:D:37:SER:OG	1:D:86:HIS:HB2	2.07	0.55
1:D:216:SER:HB2	1:D:244:SER:OG	2.07	0.55
1:D:512:LEU:HD12	1:D:512:LEU:C	2.27	0.55
1:C:82:THR:HG1	1:C:83:TYR:HD1	1.52	0.55
1:D:224:ARG:HG2	1:D:224:ARG:HH11	1.71	0.55
1:C:252:PHE:HA	1:C:255:ILE:HG13	1.87	0.55
1:A:536:LYS:O	1:A:540:VAL:HG23	2.06	0.55
1:F:298:LEU:HD22	1:F:568:ALA:HB3	1.88	0.55
1:B:56:LEU:CA	1:B:63:ILE:HD13	2.36	0.55
1:F:29:ILE:CG1	1:F:75:LEU:HD22	2.37	0.55
1:A:251:GLU:HG3	1:A:344:LYS:HG3	1.89	0.54
1:C:12:LEU:HD12	1:C:12:LEU:C	2.32	0.54
1:F:324:ILE:HD12	1:F:450:PHE:CZ	2.36	0.54
1:E:512:LEU:HD12	1:E:512:LEU:C	2.29	0.54
1:E:462:LEU:HB3	1:E:464:PHE:CE1	2.41	0.54
1:B:12:LEU:HD23	1:B:12:LEU:C	2.33	0.54
1:C:526:ARG:O	1:C:578:VAL:HG23	2.08	0.54
1:B:268:LEU:HD12	1:B:274:ILE:HD11	1.90	0.54
1:B:512:LEU:HD12	1:B:512:LEU:O	2.08	0.54
1:E:346:ILE:HD11	1:F:420:ILE:HD13	1.85	0.54
1:B:299:GLN:HA	1:B:319:MET:HE3	1.90	0.54
1:B:327:PRO:HG3	1:C:455:THR:HG22	1.90	0.54
1:E:361:VAL:HG12	1:E:423:PHE:CZ	2.43	0.54
1:A:12:LEU:HD23	1:A:12:LEU:O	2.07	0.54
1:D:45:LEU:HD23	1:D:45:LEU:C	2.31	0.54
1:A:347:TYR:HE2	1:B:405:GLU:OE2	1.91	0.53
1:C:203:LEU:O	1:C:206:MET:HB2	2.07	0.53
1:E:575:ARG:HH12	1:E:579:SER:HB3	1.74	0.53
1:E:75:LEU:CD1	1:E:80:PHE:CZ	2.90	0.53
1:A:447:ALA:HA	1:A:450:PHE:CE2	2.42	0.53
1:E:63:ILE:O	1:E:63:ILE:CG2	2.57	0.53
1:E:257:ILE:O	1:E:257:ILE:HG13	2.08	0.53
1:A:111:VAL:O	1:A:111:VAL:HG23	2.09	0.53
1:A:208:ILE:HG23	1:A:209:PRO:HD2	1.90	0.53
1:C:100:LEU:HD13	1:C:191:PRO:HG3	1.90	0.53
1:B:216:SER:HB2	1:B:244:SER:OG	2.09	0.53
1:B:288:GLY:O	1:B:293:LYS:HE3	2.09	0.53
1:B:330:ALA:O	1:B:334:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:C	1:C:84:ILE:HG13	2.34	0.53
1:A:408:GLU:OE1	1:A:408:GLU:HA	2.09	0.53
1:F:523:VAL:HG11	1:F:571:LYS:HA	1.91	0.53
1:B:29:ILE:HA	1:B:75:LEU:HD13	1.89	0.53
1:F:491:ALA:HB1	1:F:496:VAL:O	2.08	0.52
1:F:562:LEU:N	1:F:562:LEU:CD2	2.72	0.52
1:A:329:SER:HB2	1:A:331:LYS:HG3	1.90	0.52
1:A:518:TYR:CE1	1:A:522:TYR:CD2	2.98	0.52
1:B:458:SER:O	1:B:557:ARG:HD3	2.10	0.52
1:E:338:VAL:HG11	1:E:430:LEU:HD23	1.90	0.52
1:A:359:THR:HG21	1:A:402:ALA:HB3	1.91	0.52
1:D:324:ILE:HD13	1:D:450:PHE:CD2	2.43	0.52
1:A:56:LEU:HD12	1:A:56:LEU:C	2.28	0.52
1:A:342:VAL:HG13	1:A:343:PRO:HD2	1.92	0.52
1:B:515:TYR:OH	1:B:574:LEU:HD13	2.09	0.52
1:B:75:LEU:CD1	1:B:78:LEU:CD2	2.81	0.52
1:B:483:LEU:HD22	1:C:536:LYS:HE2	1.92	0.52
1:C:335:LEU:HD11	1:C:432:ALA:HB2	1.91	0.52
1:E:63:ILE:O	1:E:63:ILE:HG22	2.10	0.52
1:A:462:LEU:HD11	1:A:565:MET:SD	2.49	0.52
1:E:324:ILE:HG21	1:E:450:PHE:CD1	2.40	0.52
1:A:324:ILE:HG21	1:A:450:PHE:CE1	2.45	0.52
1:C:31:LYS:HE2	1:C:31:LYS:CA	2.40	0.51
1:D:180:GLN:NE2	1:D:190:ILE:HG23	2.25	0.51
1:C:574:LEU:N	1:C:574:LEU:CD1	2.73	0.51
1:D:285:SER:OG	1:E:311:ASP:OD2	2.29	0.51
1:F:363:GLU:O	1:F:373:THR:HG23	2.10	0.51
1:A:366:ASP:CG	1:F:374:LEU:HD11	2.36	0.51
1:F:268:LEU:N	1:F:268:LEU:CD2	2.73	0.51
1:C:530:GLU:OE1	1:C:530:GLU:N	2.35	0.51
1:D:165:VAL:O	1:D:165:VAL:HG13	2.11	0.51
1:E:24:GLU:HA	1:E:24:GLU:OE1	2.10	0.51
1:F:523:VAL:HG12	1:F:525:PRO:HD3	1.93	0.51
1:B:75:LEU:HD12	1:B:78:LEU:HD21	1.87	0.51
1:C:406:ALA:O	1:C:410:GLN:HA	2.11	0.51
1:E:268:LEU:C	1:E:274:ILE:HD13	2.35	0.51
1:E:324:ILE:CD1	1:E:450:PHE:CE1	2.94	0.51
1:F:136:PHE:CD1	1:F:136:PHE:C	2.89	0.51
1:F:158:LYS:O	1:F:159:LYS:HD3	2.11	0.51
1:A:273:GLU:OE1	1:A:276:ASN:ND2	2.44	0.51
1:A:393:ASP:OD1	1:A:393:ASP:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:PHE:CE2	1:D:67:ALA:HB2	2.45	0.50
1:E:9:LEU:HD21	1:E:66:ALA:HB3	1.92	0.50
1:E:286:ILE:HD11	1:E:333:ARG:HD2	1.93	0.50
1:F:308:LYS:HG3	1:F:313:GLY:O	2.11	0.50
1:A:48:PHE:CD1	1:A:48:PHE:C	2.89	0.50
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.76	0.50
1:A:590:SER:O	1:A:594:LEU:HD23	2.11	0.50
1:E:318:ASP:HB3	1:E:428:SER:OG	2.10	0.50
1:E:361:VAL:CG1	1:E:423:PHE:CZ	2.94	0.50
1:B:324:ILE:CD1	1:B:450:PHE:CE1	2.93	0.50
1:B:595:LYS:C	1:B:597:LEU:N	2.70	0.50
1:C:560:GLU:HA	1:C:563:ILE:HD13	1.93	0.50
1:D:462:LEU:HD11	1:D:565:MET:CE	2.40	0.50
1:E:381:LEU:HD13	1:F:420:ILE:HG13	1.93	0.50
1:F:265:ILE:HG23	1:F:515:TYR:HD1	1.76	0.50
1:F:289:TYR:HD2	1:F:292:ILE:HD12	1.75	0.50
1:D:36:ARG:NH1	1:D:201:ASP:OD2	2.42	0.50
1:E:183:LEU:HD12	1:E:190:ILE:HD12	1.94	0.50
1:E:440:PHE:CD1	1:E:440:PHE:C	2.90	0.50
1:E:523:VAL:HG12	1:E:525:PRO:HD3	1.93	0.50
1:A:325[A]:GLY:O	1:A:435:PRO:HD3	2.11	0.50
1:A:325[B]:GLY:O	1:A:435:PRO:HD3	2.11	0.50
1:B:405:GLU:OE1	1:B:412:ILE:HA	2.12	0.50
1:D:145:LEU:N	1:D:145:LEU:HD23	2.27	0.50
1:C:333:ARG:NH2	2:C:701:ADP:O2'	2.45	0.50
1:C:12:LEU:C	1:C:12:LEU:CD1	2.85	0.50
1:D:180:GLN:HE22	1:D:190:ILE:HG23	1.74	0.50
1:A:475:ASP:OD2	1:B:543:ARG:HG3	2.12	0.49
1:A:538:TYR:CZ	1:A:542:LEU:HD13	2.47	0.49
1:B:56:LEU:HA	1:B:63:ILE:CD1	2.39	0.49
1:F:29:ILE:HG12	1:F:75:LEU:HD22	1.93	0.49
1:C:84:ILE:HD12	1:C:128:ARG:NE	2.27	0.49
1:D:36:ARG:NH1	1:D:201:ASP:CG	2.71	0.49
1:E:78:LEU:N	1:E:78:LEU:CD1	2.73	0.49
1:E:145:LEU:HD23	1:E:145:LEU:N	2.27	0.49
1:D:395:ILE:HG22	1:D:396:SER:O	2.12	0.49
1:E:394:LYS:HE2	1:E:394:LYS:HA	1.93	0.49
1:B:364:ARG:HB3	1:B:417:ALA:CB	2.41	0.49
1:A:190:ILE:HD12	1:B:362:ALA:HB3	1.95	0.49
1:A:327:PRO:HG3	1:B:455:THR:HG22	1.95	0.49
1:D:304:THR:HG23	1:D:567:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:TYR:CD1	1:E:592:TYR:C	2.91	0.49
1:E:291:GLU:HG2	1:E:592:TYR:CE2	2.47	0.49
1:F:439:ARG:O	1:F:440:PHE:C	2.56	0.49
1:F:447:ALA:HA	1:F:450:PHE:CE1	2.48	0.49
1:C:26:LYS:HA	1:C:29:ILE:HD13	1.95	0.49
1:D:493:ILE:N	1:D:493:ILE:HD13	2.28	0.49
1:A:347:TYR:CE2	1:B:405:GLU:OE2	2.66	0.48
1:A:523:VAL:N	1:A:524:MET:HE2	2.28	0.48
1:C:451:ASP:OD1	1:C:451:ASP:O	2.31	0.48
1:B:88:ARG:NE	1:B:203:LEU:HD11	2.28	0.48
1:E:258:SER:N	1:E:261:GLU:OE2	2.46	0.48
1:E:581:LYS:O	1:E:584:ASN:HB2	2.13	0.48
1:A:538:TYR:CE1	1:A:542:LEU:CD1	2.96	0.48
1:F:538:TYR:CE2	1:F:587:ILE:HG12	2.47	0.48
1:B:161:THR:O	1:B:161:THR:OG1	2.32	0.48
1:C:172:PHE:CD1	1:C:172:PHE:C	2.91	0.48
1:F:75:LEU:HB3	1:F:78:LEU:CD1	2.43	0.48
1:D:57:ILE:O	1:D:57:ILE:HG22	2.13	0.48
1:E:12:LEU:HD12	1:E:12:LEU:C	2.34	0.48
1:A:512:LEU:HD12	1:A:512:LEU:O	2.14	0.48
1:A:538:TYR:CZ	1:A:542:LEU:CD1	2.97	0.48
1:C:190:ILE:HD12	1:D:362:ALA:CB	2.44	0.48
1:C:473:GLU:HA	1:C:476:LYS:HD3	1.95	0.48
1:E:364:ARG:NH2	1:E:366:ASP:OD1	2.46	0.48
1:E:398:GLU:CD	1:E:398:GLU:H	2.22	0.48
1:E:542:LEU:CD1	1:E:542:LEU:C	2.87	0.48
1:A:436:LYS:HG2	1:A:449:GLN:HB2	1.95	0.48
1:D:331:LYS:HZ3	1:D:331:LYS:HB2	1.79	0.48
1:E:137:CYS:SG	1:E:157:CYS:HB3	2.54	0.48
1:A:307:LYS:C	1:A:308:LYS:HD3	2.38	0.48
1:A:515:TYR:CD1	1:A:515:TYR:C	2.91	0.48
1:C:33:PRO:O	1:C:36:ARG:NH1	2.47	0.48
1:E:228:ARG:HH11	1:E:230:LYS:HE3	1.79	0.48
1:E:225:LYS:HG2	1:E:231:VAL:HG22	1.96	0.48
1:E:322:LEU:O	1:E:323:LEU:HD12	2.14	0.47
1:B:325:GLY:O	1:B:435:PRO:HD3	2.14	0.47
1:C:57:ILE:HG13	1:C:94:ILE:HD12	1.96	0.47
1:E:287:TYR:H	2:E:701:ADP:HN62	1.62	0.47
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.59	0.47
1:B:249:GLN:N	1:B:249:GLN:CD	2.72	0.47
1:A:18:GLU:O	1:A:22:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:CG2	1:B:275:PHE:N	2.77	0.47
1:D:300:LEU:HD23	1:D:386:ILE:HD11	1.97	0.47
1:D:472:THR:O	1:D:472:THR:HG22	2.15	0.47
1:F:186:LEU:CD2	1:F:191:PRO:HD3	2.43	0.47
1:A:474:LEU:C	1:A:474:LEU:HD23	2.39	0.47
1:B:286:ILE:HD11	1:B:333:ARG:HG2	1.97	0.47
1:E:462:LEU:HD13	1:E:464:PHE:CZ	2.50	0.47
1:D:6:THR:HG23	1:D:7:SER:N	2.28	0.47
1:F:202:ASP:OD1	1:F:202:ASP:N	2.47	0.47
1:F:203:LEU:HD22	1:F:245:LEU:HD12	1.97	0.47
1:B:202:ASP:N	1:B:202:ASP:OD1	2.47	0.47
1:C:326:ASP:HB3	1:C:327:PRO:HD2	1.96	0.47
1:B:16:PHE:CD1	1:B:16:PHE:C	2.89	0.47
1:D:13:PHE:O	1:D:17:LEU:HG	2.15	0.47
1:D:29:ILE:O	1:D:29:ILE:HG22	2.13	0.47
1:D:248:LYS:O	1:D:248:LYS:HG2	2.15	0.47
1:F:325:GLY:O	1:F:435:PRO:HD3	2.15	0.46
1:A:597:LEU:HD23	1:A:597:LEU:H	1.79	0.46
1:C:36:ARG:HG2	1:C:36:ARG:NH1	2.29	0.46
1:C:78:LEU:N	1:C:78:LEU:HD22	2.30	0.46
1:A:224:ARG:HG2	1:A:224:ARG:NH1	2.30	0.46
1:F:539:TYR:CD2	1:F:559:ILE:HD11	2.51	0.46
1:A:12:LEU:C	1:A:12:LEU:CD2	2.88	0.46
1:E:172:PHE:N	1:E:172:PHE:CD1	2.83	0.46
1:F:279:THR:O	1:F:279:THR:HG22	2.16	0.46
1:A:455:THR:HG22	1:F:327:PRO:HG3	1.97	0.46
1:D:439:ARG:O	1:D:449:GLN:OE1	2.34	0.46
1:E:447:ALA:HA	1:E:450:PHE:CD2	2.51	0.46
1:B:331:LYS:N	2:B:701:ADP:O1A	2.47	0.46
1:E:30:ILE:HG22	1:E:31:LYS:HG2	1.96	0.46
1:D:322:LEU:CD2	1:D:324:ILE:CG1	2.90	0.46
1:F:286:ILE:HD12	1:F:286:ILE:HG23	1.70	0.46
1:A:12:LEU:HD21	1:A:48:PHE:HE1	1.81	0.46
1:B:23:ASP:OD1	1:B:24:GLU:OE1	2.34	0.46
1:E:228:ARG:HD3	1:E:230:LYS:CD	2.43	0.46
1:B:12:LEU:HD23	1:B:12:LEU:O	2.16	0.45
1:B:574:LEU:HD12	1:B:574:LEU:N	2.30	0.45
1:F:186:LEU:HD21	1:F:191:PRO:HD2	1.97	0.45
1:D:71:LEU:HD11	1:D:75:LEU:CD2	2.46	0.45
1:B:469:ILE:HD11	1:B:474:LEU:CD2	2.41	0.45
1:C:84:ILE:CD1	1:C:128:ARG:NE	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:ILE:HD13	1:F:420:ILE:CD1	2.40	0.45
1:C:75:LEU:HB3	1:C:78:LEU:HD23	1.97	0.45
1:C:511:LEU:HD12	1:C:511:LEU:C	2.31	0.45
1:D:29:ILE:O	1:D:29:ILE:CG2	2.64	0.45
1:D:29:ILE:HG12	1:D:75:LEU:HD13	1.99	0.45
1:F:268:LEU:N	1:F:268:LEU:HD22	2.31	0.45
1:C:462:LEU:HD21	1:C:565:MET:HE1	1.98	0.45
1:D:42:ILE:HD12	1:D:91:ASN:N	2.32	0.45
1:B:297:ALA:HA	1:B:300:LEU:HD12	1.99	0.45
1:D:180:GLN:HE22	1:D:190:ILE:CG2	2.30	0.45
1:E:462:LEU:HB3	1:E:464:PHE:HE1	1.82	0.45
1:F:224:ARG:NH1	1:F:224:ARG:CG	2.78	0.45
1:A:394:LYS:HE2	1:A:394:LYS:CA	2.46	0.45
1:B:16:PHE:CD1	1:B:16:PHE:O	2.70	0.45
1:B:154:CYS:SG	1:B:155:PRO:HD2	2.56	0.45
1:C:560:GLU:HA	1:C:563:ILE:HD12	1.99	0.45
1:D:351:LYS:HD2	1:D:351:LYS:HA	1.79	0.45
1:F:400:THR:O	1:F:404:HIS:ND1	2.49	0.45
1:A:250:LYS:O	1:A:343:PRO:HB3	2.17	0.45
1:C:172:PHE:CD1	1:C:172:PHE:O	2.70	0.45
1:D:71:LEU:HD12	1:D:71:LEU:C	2.39	0.45
1:D:358:LEU:HD13	1:D:389:ILE:HD13	1.99	0.45
1:A:377:GLY:O	1:A:381:LEU:HG	2.17	0.44
1:B:274:ILE:HG23	1:B:275:PHE:N	2.31	0.44
1:B:282:VAL:C	1:B:284:PRO:HD3	2.43	0.44
1:E:538:TYR:CZ	1:E:587:ILE:HG23	2.52	0.44
1:F:163:LYS:HB3	1:F:163:LYS:HE3	1.56	0.44
1:B:452:ILE:HB	1:B:457:LEU:HD11	1.98	0.44
1:C:31:LYS:HE2	1:C:31:LYS:HA	1.99	0.44
1:E:203:LEU:HD22	1:E:245:LEU:HD12	1.98	0.44
1:F:137:CYS:SG	1:F:157:CYS:HB3	2.56	0.44
1:B:59:ASP:O	1:B:63:ILE:HD12	2.16	0.44
1:A:348:VAL:HG11	1:A:358:LEU:CD2	2.48	0.44
1:B:150:ILE:HA	1:B:151:PRO:HD3	1.78	0.44
1:B:268:LEU:O	1:B:269:SER:C	2.60	0.44
1:B:60:PRO:O	1:B:64:ILE:HG13	2.17	0.44
1:B:154:CYS:SG	1:B:156:GLU:N	2.88	0.44
1:B:232:ASP:CB	1:B:235:ILE:HB	2.47	0.44
1:B:581:LYS:HD2	1:B:581:LYS:HA	1.74	0.44
1:E:305:PRO:O	1:E:305:PRO:HG2	2.17	0.44
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ILE:HD12	1:B:471:ASP:HB3	1.99	0.44
1:C:363:GLU:H	1:C:373:THR:HG22	1.82	0.44
1:A:538:TYR:CE1	1:A:542:LEU:HD13	2.53	0.44
1:E:9:LEU:HD22	1:E:66:ALA:HB2	1.92	0.44
1:B:335:LEU:CD2	1:B:430:LEU:HG	2.48	0.44
1:D:179:VAL:CG1	1:D:180:GLN:N	2.80	0.44
1:D:190:ILE:HG22	1:D:191:PRO:O	2.17	0.44
1:F:136:PHE:CD1	1:F:136:PHE:O	2.70	0.44
1:B:330:ALA:HA	2:B:701:ADP:C5'	2.46	0.43
1:C:274:ILE:HG23	1:C:275:PHE:N	2.33	0.43
1:C:82:THR:OG1	1:C:83:TYR:CD1	2.70	0.43
1:D:42:ILE:HD12	1:D:42:ILE:H	1.83	0.43
1:E:335:LEU:HD11	1:E:432:ALA:HB2	1.97	0.43
1:F:382:GLY:O	1:F:383:ASN:OD1	2.35	0.43
1:A:436:LYS:NZ	1:A:448:GLU:OE1	2.39	0.43
1:A:511:LEU:HD23	1:A:511:LEU:C	2.36	0.43
1:B:68:ASN:O	1:B:72:MET:HG3	2.19	0.43
1:E:40:VAL:O	1:E:40:VAL:HG12	2.19	0.43
1:E:216:SER:HB2	1:E:244:SER:HB3	2.00	0.43
1:E:559:ILE:HD13	1:E:559:ILE:HG21	1.82	0.43
1:C:203:LEU:HA	1:C:203:LEU:HD23	1.74	0.43
1:D:383:ASN:HA	1:D:426:LYS:O	2.18	0.43
1:E:562:LEU:HA	1:E:565:MET:HE3	2.00	0.43
1:A:331:LYS:NZ	2:A:701:ADP:O2B	2.52	0.43
1:B:332:THR:O	1:B:336:GLN:HG3	2.19	0.43
1:D:226:ASP:HB3	1:D:229:GLY:H	1.83	0.43
1:D:263:ARG:HH11	1:D:263:ARG:CG	2.29	0.43
1:C:83:TYR:CD1	1:C:83:TYR:N	2.86	0.43
1:D:542:LEU:HD12	1:D:542:LEU:C	2.41	0.43
1:F:98:MET:O	1:F:102:VAL:HG23	2.19	0.43
1:A:190:ILE:HG22	1:A:191:PRO:O	2.18	0.43
1:B:118:VAL:HG11	1:B:194:GLN:OE1	2.18	0.43
1:C:82:THR:OG1	1:C:83:TYR:HD1	2.01	0.43
1:E:364:ARG:NH1	1:E:366:ASP:OD1	2.52	0.43
1:A:518:TYR:CD1	1:A:522:TYR:CD2	3.06	0.43
1:E:344:LYS:HA	1:E:344:LYS:HD3	1.88	0.43
1:F:400:THR:O	1:F:404:HIS:CE1	2.72	0.43
1:C:364:ARG:HD2	1:C:371:GLY:O	2.18	0.43
1:C:524:MET:SD	1:C:524:MET:N	2.92	0.43
1:F:158:LYS:O	1:F:158:LYS:CG	2.59	0.43
1:D:462:LEU:HD13	1:D:464:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ASN:OD1	1:F:144:ASN:C	2.62	0.43
1:B:287:TYR:CD1	1:B:287:TYR:C	2.97	0.42
1:B:346:ILE:HG12	1:C:420:ILE:CD1	2.49	0.42
1:C:56:LEU:CD2	1:C:89:PHE:CD2	3.02	0.42
1:D:263:ARG:CG	1:D:263:ARG:NH1	2.81	0.42
1:E:33:PRO:C	1:E:35:LYS:N	2.76	0.42
1:E:118:VAL:HG12	1:E:119:LYS:HG3	2.01	0.42
1:E:142:LYS:HB2	1:E:142:LYS:HE3	1.82	0.42
1:F:382:GLY:C	1:F:383:ASN:OD1	2.62	0.42
1:E:98:MET:O	1:E:102:VAL:HG23	2.19	0.42
1:F:145:LEU:HD22	1:F:150:ILE:HG12	1.99	0.42
1:A:331:LYS:HE2	1:A:331:LYS:HB2	1.80	0.42
2:A:701:ADP:O3B	1:B:459:ARG:NH2	2.52	0.42
1:B:99:VAL:HG22	1:B:113:ILE:HD12	2.01	0.42
1:F:75:LEU:O	1:F:78:LEU:HD12	2.19	0.42
1:F:265:ILE:HG23	1:F:515:TYR:CD1	2.53	0.42
1:A:441:ASP:N	1:A:449:GLN:OE1	2.47	0.42
1:B:183:LEU:HD13	1:C:423:PHE:CZ	2.55	0.42
1:D:268:LEU:HD23	1:D:515:TYR:CD2	2.54	0.42
1:F:228:ARG:HG3	1:F:228:ARG:HH11	1.84	0.42
1:F:316:ARG:NH2	1:F:564:ARG:NH2	2.68	0.42
1:D:62:ILE:HD12	1:D:62:ILE:HA	1.90	0.42
1:F:298:LEU:HD22	1:F:568:ALA:CB	2.48	0.42
1:B:344:LYS:HA	1:B:344:LYS:HD2	1.80	0.42
1:B:395:ILE:HG22	1:B:396:SER:O	2.19	0.42
1:D:107:ILE:O	1:D:109:LYS:HG2	2.19	0.42
1:E:224:ARG:HG2	1:E:224:ARG:NH1	2.32	0.42
2:E:701:ADP:H8	2:E:701:ADP:H3'	1.84	0.42
1:F:160:ARG:HE	1:F:160:ARG:HB3	1.60	0.42
1:F:231:VAL:O	1:F:231:VAL:HG23	2.20	0.42
1:C:361:VAL:HG12	1:C:380:VAL:HG21	2.01	0.42
1:C:560:GLU:CA	1:C:563:ILE:HD12	2.50	0.42
1:D:72:MET:HG2	1:D:80:PHE:CE2	2.54	0.42
1:E:557:ARG:HG3	1:E:557:ARG:NH1	2.34	0.42
1:B:165:VAL:HA	1:B:166:PRO:HD3	1.86	0.42
1:C:468:ASP:OD2	1:C:470:MET:HG3	2.20	0.42
1:D:259:GLU:H	1:D:259:GLU:HG2	1.58	0.42
1:D:324:ILE:CG2	1:D:450:PHE:CE1	3.01	0.42
1:E:193:TRP:CD1	1:E:193:TRP:C	2.98	0.42
1:E:268:LEU:O	1:E:274:ILE:CD1	2.68	0.42
1:E:361:VAL:CG1	1:E:423:PHE:CG	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HD13	1:A:395:ILE:HA	1.71	0.42
1:A:590:SER:O	1:A:594:LEU:CD2	2.68	0.42
1:B:177:ILE:CG1	1:B:197:ALA:HB3	2.49	0.42
1:E:589:LEU:HD23	1:E:589:LEU:HA	1.81	0.42
1:F:29:ILE:HG13	1:F:75:LEU:HD22	2.01	0.42
1:B:100:LEU:CD1	1:B:191:PRO:HG3	2.49	0.42
1:C:544:ARG:HE	1:C:544:ARG:HB3	1.66	0.42
1:E:307:LYS:HB3	1:E:315:ILE:HD12	2.02	0.42
1:E:542:LEU:O	1:E:542:LEU:CD1	2.68	0.42
1:F:290:ASN:OD1	1:F:290:ASN:O	2.38	0.42
1:A:150:ILE:HD11	1:F:233:PRO:HB2	2.02	0.41
1:B:203:LEU:N	1:B:203:LEU:HD12	2.35	0.41
1:C:72:MET:HE3	1:C:80:PHE:CE2	2.55	0.41
1:E:331:LYS:HZ3	1:E:331:LYS:HB2	1.85	0.41
1:F:56:LEU:HA	1:F:63:ILE:CD1	2.49	0.41
1:F:157:CYS:O	1:F:157:CYS:SG	2.77	0.41
1:F:167:GLU:N	1:F:167:GLU:CD	2.76	0.41
1:A:160:ARG:CG	1:A:160:ARG:NH1	2.73	0.41
1:B:474:LEU:HD12	1:B:474:LEU:HA	1.86	0.41
1:C:322:LEU:HD23	1:C:463:ILE:HG23	2.03	0.41
1:F:519:ALA:HB1	1:F:571:LYS:HG2	2.02	0.41
1:A:364:ARG:NH1	1:A:366:ASP:OD1	2.53	0.41
1:A:436:LYS:HG2	1:A:449:GLN:O	2.20	0.41
1:C:465:PRO:HD2	1:C:596:THR:HG23	2.02	0.41
1:F:230:LYS:HZ3	1:F:230:LYS:HG2	1.76	0.41
1:B:26:LYS:HA	1:B:29:ILE:HD12	2.02	0.41
1:B:361:VAL:HG12	1:B:380:VAL:HG11	2.03	0.41
1:D:154:CYS:HB3	1:D:157:CYS:SG	2.60	0.41
1:D:441:ASP:OD2	1:D:444:LYS:N	2.43	0.41
1:D:526:ARG:O	1:D:578:VAL:HG23	2.20	0.41
1:D:576:ASP:N	1:D:576:ASP:OD1	2.51	0.41
1:F:562:LEU:HD23	1:F:562:LEU:H	1.85	0.41
1:F:589:LEU:HA	1:F:589:LEU:HD23	1.78	0.41
1:A:100:LEU:HD12	1:A:100:LEU:C	2.45	0.41
1:A:324:ILE:CD1	1:A:450:PHE:CZ	3.03	0.41
2:B:701:ADP:N3	2:B:701:ADP:C2'	2.83	0.41
1:C:31:LYS:HA	1:C:31:LYS:CE	2.50	0.41
1:E:33:PRO:C	1:E:35:LYS:H	2.27	0.41
1:E:559:ILE:HG22	1:E:563:ILE:CD1	2.50	0.41
1:F:538:TYR:CZ	1:F:587:ILE:HG23	2.56	0.41
1:A:24:GLU:OE1	1:A:24:GLU:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HG13	1:B:85:PRO:HD2	2.02	0.41
1:E:97:PRO:O	1:E:113:ILE:HG22	2.20	0.41
1:A:286:ILE:O	1:A:286:ILE:HG13	2.20	0.41
1:B:5:GLN:O	1:B:9:LEU:HG	2.20	0.41
1:E:251:GLU:H	1:E:251:GLU:HG3	1.47	0.41
1:A:203:LEU:O	1:A:206:MET:HB2	2.21	0.41
1:A:523:VAL:CG2	1:A:574:LEU:HD23	2.46	0.41
1:B:332:THR:HG22	1:B:390:ASP:OD2	2.21	0.41
1:B:527:LEU:HD12	1:B:578:VAL:HB	2.02	0.41
1:C:140:LYS:HE2	1:C:140:LYS:HB2	1.64	0.41
1:C:190:ILE:HG22	1:C:191:PRO:O	2.21	0.41
1:D:42:ILE:HD12	1:D:91:ASN:H	1.86	0.41
1:D:445:TYR:HB3	1:D:446:PRO:HD2	2.03	0.41
1:D:446:PRO:C	1:D:448:GLU:H	2.28	0.41
1:E:404:HIS:NE2	1:E:455:THR:OG1	2.39	0.41
1:E:575:ARG:NH1	1:E:579:SER:HB3	2.34	0.41
1:B:59:ASP:HB3	1:B:62:ILE:HD12	2.03	0.41
1:E:92:GLN:C	1:E:92:GLN:CD	2.89	0.41
1:E:154:CYS:SG	1:E:156:GLU:N	2.94	0.41
1:E:396:SER:HB2	1:E:398:GLU:OE1	2.21	0.41
1:F:483:LEU:N	1:F:483:LEU:HD22	2.35	0.41
1:B:100:LEU:HD12	1:B:191:PRO:CG	2.50	0.40
1:C:393:ASP:OD1	1:C:393:ASP:N	2.54	0.40
1:E:526:ARG:O	1:E:578:VAL:HG23	2.22	0.40
1:C:437:PHE:HD1	1:C:437:PHE:HA	1.75	0.40
1:D:42:ILE:CD1	1:D:91:ASN:N	2.84	0.40
1:E:258:SER:H	1:E:261:GLU:CG	2.34	0.40
1:A:57:ILE:O	1:A:57:ILE:HG22	2.20	0.40
1:A:590:SER:C	1:A:594:LEU:HD23	2.46	0.40
1:C:364:ARG:HB3	1:C:417:ALA:CB	2.50	0.40
1:C:441:ASP:CG	1:C:444:LYS:HG3	2.46	0.40
1:C:444:LYS:CD	1:C:444:LYS:O	2.69	0.40
1:F:316:ARG:HB3	1:F:564:ARG:NH1	2.36	0.40
1:B:281:SER:HB2	1:B:507:ILE:HG22	2.04	0.40
1:B:286:ILE:HG23	2:B:701:ADP:C6	2.57	0.40
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.84	0.40
1:E:331:LYS:HB2	1:E:331:LYS:NZ	2.36	0.40
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.80	0.40
1:A:597:LEU:HD23	1:A:597:LEU:N	2.36	0.40
1:B:75:LEU:O	1:B:75:LEU:CG	2.70	0.40
1:C:72:MET:HE3	1:C:80:PHE:HD2	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ILE:HD11	1:D:90:TYR:N	2.37	0.40
1:E:13:PHE:CE2	1:E:63:ILE:HG23	2.53	0.40
1:F:289:TYR:HD2	1:F:292:ILE:CD1	2.34	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	568/601 (94%)	547 (96%)	20 (4%)	1 (0%)	43	66
1	B	564/601 (94%)	543 (96%)	21 (4%)	0	100	100
1	C	566/601 (94%)	546 (96%)	19 (3%)	1 (0%)	43	66
1	D	571/601 (95%)	547 (96%)	23 (4%)	1 (0%)	43	66
1	E	566/601 (94%)	542 (96%)	23 (4%)	1 (0%)	43	66
1	F	574/601 (96%)	557 (97%)	16 (3%)	1 (0%)	43	66
All	All	3409/3606 (94%)	3282 (96%)	122 (4%)	5 (0%)	48	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	202	ASP
1	D	249	GLN
1	E	189	SER
1	F	343	PRO
1	A	233	PRO

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	494/513 (96%)	472 (96%)	22 (4%)	24	50
1	B	491/513 (96%)	475 (97%)	16 (3%)	33	61
1	C	493/513 (96%)	465 (94%)	28 (6%)	18	40
1	D	496/513 (97%)	482 (97%)	14 (3%)	38	66
1	E	492/513 (96%)	453 (92%)	39 (8%)	11	26
1	F	501/513 (98%)	459 (92%)	42 (8%)	10	23
All	All	2967/3078 (96%)	2806 (95%)	161 (5%)	20	42

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	133	VAL
1	A	135	THR
1	A	138	ASN
1	A	140	LYS
1	A	153	VAL
1	A	160	ARG
1	A	216	SER
1	A	231	VAL
1	A	259	GLU
1	A	263	ARG
1	A	265	ILE
1	A	290	ASN
1	A	393	ASP
1	A	395	ILE
1	A	470	MET
1	A	495	ASP
1	A	496	VAL
1	A	507	ILE
1	A	508	GLU
1	A	512	LEU
1	A	542	LEU

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Mol	Chain	Res	Type
1	B	75	LEU
1	B	133	VAL
1	B	136	PHE
1	B	150	ILE
1	B	157	CYS
1	B	161	THR
1	B	194	GLN
1	B	259	GLU
1	B	266	LYS
1	B	386	ILE
1	B	440	PHE
1	B	466	ILE
1	B	469	ILE
1	B	520	LYS
1	B	540	VAL
1	B	597	LEU
1	C	9	LEU
1	C	12	LEU
1	C	131	VAL
1	C	156	GLU
1	C	157	CYS
1	C	158	LYS
1	C	159	LYS
1	C	163	LYS
1	C	216	SER
1	C	222	ARG
1	C	224	ARG
1	C	228	ARG
1	C	255	ILE
1	C	257	ILE
1	C	265	ILE
1	C	346	ILE
1	C	386	ILE
1	C	430	LEU
1	C	437	PHE
1	C	439	ARG
1	C	440	PHE
1	C	444	LYS
1	C	472	THR
1	C	483	LEU
1	C	493	ILE
1	C	511	LEU

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Mol	Chain	Res	Type
1	C	594	LEU
1	C	595	LYS
1	D	25	ILE
1	D	104	SER
1	D	127	ILE
1	D	237	SER
1	D	249	GLN
1	D	259	GLU
1	D	263	ARG
1	D	264	GLN
1	D	290	ASN
1	D	343	PRO
1	D	348	VAL
1	D	524	MET
1	D	532	SER
1	D	542	LEU
1	E	25	ILE
1	E	26	LYS
1	E	28	ILE
1	E	29	ILE
1	E	30	ILE
1	E	31	LYS
1	E	35	LYS
1	E	42	ILE
1	E	43	SER
1	E	71	LEU
1	E	74	LYS
1	E	75	LEU
1	E	123	ILE
1	E	161	THR
1	E	189	SER
1	E	246	GLU
1	E	247	THR
1	E	248	LYS
1	E	250	LYS
1	E	251	GLU
1	E	255	ILE
1	E	409	SER
1	E	436	LYS
1	E	439	ARG
1	E	444	LYS
1	E	467	ARG

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Mol	Chain	Res	Type
1	E	524	MET
1	E	525	PRO
1	E	527	LEU
1	E	532	SER
1	E	536	LYS
1	E	541	ASP
1	E	542	LEU
1	E	543	ARG
1	E	577	VAL
1	E	579	SER
1	E	580	VAL
1	E	591	GLU
1	E	597	LEU
1	F	9	LEU
1	F	10	LYS
1	F	93	SER
1	F	133	VAL
1	F	135	THR
1	F	157	CYS
1	F	160	ARG
1	F	163	LYS
1	F	216	SER
1	F	224	ARG
1	F	228	ARG
1	F	230	LYS
1	F	231	VAL
1	F	243	THR
1	F	247	THR
1	F	248	LYS
1	F	249	GLN
1	F	259	GLU
1	F	261	GLU
1	F	263	ARG
1	F	266	LYS
1	F	274	ILE
1	F	439	ARG
1	F	440	PHE
1	F	444	LYS
1	F	466	ILE
1	F	469	ILE
1	F	470	MET
1	F	493	ILE

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Mol	Chain	Res	Type
1	F	496	VAL
1	F	497	GLU
1	F	526	ARG
1	F	540	VAL
1	F	541	ASP
1	F	542	LEU
1	F	543	ARG
1	F	554	ILE
1	F	558	GLN
1	F	562	LEU
1	F	577	VAL
1	F	580	VAL
1	F	599	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	280	GLN
1	A	290	ASN
1	A	299	GLN
1	A	383	ASN
1	A	410	GLN
1	B	91	ASN
1	B	175	GLN
1	B	410	GLN
1	B	449	GLN
1	C	55	ASN
1	C	91	ASN
1	D	138	ASN
1	D	175	GLN
1	D	205	ASN
1	D	280	GLN
1	D	290	ASN
1	D	404	HIS
1	D	485	GLN
1	D	509	HIS
1	E	280	GLN
1	F	299	GLN

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 ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	B	702	-	4,4,4	1.86	2 (50%)	6,6,6	0.68	0
3	PO4	C	702	-	4,4,4	1.73	1 (25%)	6,6,6	1.12	0
2	ADP	F	701	-	28,29,29	2.22	5 (17%)	43,45,45	2.53	14 (32%)
2	ADP	C	701	-	28,29,29	1.38	4 (14%)	43,45,45	1.85	10 (23%)
2	ADP	E	701	-	28,29,29	1.78	9 (32%)	43,45,45	2.26	14 (32%)
3	PO4	E	702	-	4,4,4	1.89	2 (50%)	6,6,6	0.69	0
3	PO4	F	702	-	4,4,4	1.99	3 (75%)	6,6,6	0.78	0
3	PO4	D	702	-	4,4,4	0.98	0	6,6,6	0.50	0
2	ADP	B	701	-	28,29,29	1.48	5 (17%)	43,45,45	1.78	7 (16%)
3	PO4	A	702	-	4,4,4	3.31	4 (100%)	6,6,6	1.00	0
3	PO4	D	701	-	4,4,4	1.73	0	6,6,6	0.63	0
2	ADP	A	701	-	28,29,29	1.77	6 (21%)	43,45,45	2.20	17 (39%)

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	ADP	F	701	-	-	6/16/32/32	0/3/3/3
2	ADP	C	701	-	-	7/16/32/32	0/3/3/3
2	ADP	E	701	-	-	4/16/32/32	0/3/3/3
2	ADP	B	701	-	-	7/16/32/32	0/3/3/3
2	ADP	A	701	-	-	9/16/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	ADP	PA-O3A	-8.19	1.50	1.59
2	F	701	ADP	C5-N7	-4.90	1.30	1.39
2	C	701	ADP	C5-C4	4.43	1.47	1.39
2	A	701	ADP	C4-N9	-4.02	1.29	1.37
2	B	701	ADP	C5-C4	3.74	1.45	1.39
2	F	701	ADP	C5-C4	3.72	1.45	1.39
2	E	701	ADP	PA-O3A	-3.67	1.55	1.59
3	A	702	PO4	P-O3	-3.48	1.44	1.54
2	B	701	ADP	C5-N7	-3.47	1.32	1.39
2	E	701	ADP	C5-N7	-3.43	1.32	1.39
3	A	702	PO4	P-O2	-3.35	1.44	1.54
3	A	702	PO4	P-O4	-3.33	1.44	1.54
2	F	701	ADP	C8-N9	-3.06	1.32	1.37
3	A	702	PO4	P-O1	-3.05	1.43	1.50
2	A	701	ADP	C5-N7	-3.03	1.33	1.39
2	A	701	ADP	PB-O2B	-3.00	1.43	1.54
2	E	701	ADP	PB-O2B	-2.86	1.44	1.54
2	E	701	ADP	C4-N9	-2.83	1.31	1.37
2	A	701	ADP	C5-C4	2.78	1.44	1.39
2	B	701	ADP	C4-N9	-2.64	1.32	1.37
2	E	701	ADP	C8-N9	-2.61	1.33	1.37
2	A	701	ADP	PB-O3B	-2.59	1.45	1.54
2	E	701	ADP	PB-O3B	-2.58	1.45	1.54
2	C	701	ADP	C5-C6	2.50	1.47	1.41
2	C	701	ADP	C8-N7	2.38	1.36	1.31
3	E	702	PO4	P-O3	-2.35	1.47	1.54
2	B	701	ADP	PB-O2B	-2.33	1.46	1.54
2	F	701	ADP	PA-O2A	-2.31	1.44	1.55
2	E	701	ADP	C5-C4	2.26	1.43	1.39
3	F	702	PO4	P-O3	-2.26	1.48	1.54
2	A	701	ADP	C3'-C4'	-2.23	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	702	PO4	P-O2	-2.22	1.48	1.54
2	E	701	ADP	PA-O2A	-2.19	1.45	1.55
3	F	702	PO4	P-O4	-2.19	1.48	1.54
2	C	701	ADP	C5-N7	-2.19	1.35	1.39
2	B	701	ADP	C8-N9	-2.18	1.33	1.37
3	B	702	PO4	P-O4	-2.18	1.48	1.54
3	B	702	PO4	P-O2	-2.14	1.48	1.54
3	C	702	PO4	P-O2	-2.14	1.48	1.54
2	E	701	ADP	PB-O1B	-2.11	1.43	1.50
3	E	702	PO4	P-O2	-2.08	1.48	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	ADP	C5-C4-N3	-8.97	114.37	126.72
2	F	701	ADP	N3-C4-N9	7.53	139.97	127.17
2	B	701	ADP	C5-C4-N3	-5.97	118.49	126.72
2	E	701	ADP	C5-C4-N3	-5.82	118.70	126.72
2	C	701	ADP	C5-C4-N3	-5.39	119.30	126.72
2	E	701	ADP	N3-C4-N9	5.08	135.81	127.17
2	A	701	ADP	N3-C2-N1	-4.81	121.30	128.58
2	E	701	ADP	O2A-PA-O3A	-4.73	94.49	107.27
2	F	701	ADP	C2-N3-C4	4.65	123.18	111.83
2	C	701	ADP	N3-C4-N9	4.57	134.94	127.17
2	E	701	ADP	N3-C2-N1	-4.55	121.69	128.58
2	B	701	ADP	N3-C4-N9	4.51	134.83	127.17
2	A	701	ADP	C5-C4-N3	-4.41	120.64	126.72
2	A	701	ADP	C2-N3-C4	4.20	122.08	111.83
2	E	701	ADP	C2-N3-C4	4.19	122.05	111.83
2	E	701	ADP	C4-N9-C8	4.09	110.03	105.74
2	A	701	ADP	O2B-PB-O1B	-4.07	94.97	110.83
2	A	701	ADP	C6-C5-N7	4.07	139.93	132.09
2	C	701	ADP	N3-C2-N1	-3.94	122.61	128.58
2	C	701	ADP	C2-N3-C4	3.78	121.07	111.83
2	B	701	ADP	C2-N3-C4	3.69	120.83	111.83
2	A	701	ADP	C4-C5-N7	-3.44	106.65	110.58
2	C	701	ADP	C4-N9-C8	3.44	109.34	105.74
2	E	701	ADP	N9-C8-N7	-3.34	109.19	113.94
2	F	701	ADP	N3-C2-N1	-3.33	123.54	128.58
2	A	701	ADP	O4'-C1'-N9	3.20	114.24	108.09
2	A	701	ADP	C5'-C4'-C3'	-3.19	103.73	115.21
2	E	701	ADP	O2B-PB-O3A	-3.15	94.06	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ADP	C4-C5-N7	-3.10	107.04	110.58
2	C	701	ADP	C4-C5-N7	-3.02	107.13	110.58
2	F	701	ADP	C4-C5-N7	-2.97	107.19	110.58
2	A	701	ADP	O3'-C3'-C4'	-2.94	102.64	111.08
2	B	701	ADP	N3-C2-N1	-2.94	124.13	128.58
2	F	701	ADP	C5-N7-C8	2.92	108.04	103.45
2	E	701	ADP	C5-N7-C8	2.86	107.95	103.45
2	E	701	ADP	C4-C5-N7	-2.83	107.34	110.58
2	F	701	ADP	C1'-N9-C8	-2.83	120.81	127.09
2	A	701	ADP	C4-N9-C1'	-2.80	120.08	126.63
2	F	701	ADP	O3B-PB-O2B	2.77	118.20	107.80
2	A	701	ADP	C6-C5-C4	-2.76	113.42	117.18
2	C	701	ADP	N9-C8-N7	-2.57	110.29	113.94
2	C	701	ADP	C5-N7-C8	2.56	107.47	103.45
2	F	701	ADP	C3'-C2'-C1'	2.50	106.19	101.46
2	F	701	ADP	C6-C5-C4	2.45	120.52	117.18
2	A	701	ADP	N3-C4-N9	2.43	131.30	127.17
2	E	701	ADP	C6-C5-N7	2.41	136.74	132.09
2	F	701	ADP	N6-C6-N1	2.38	123.67	118.38
2	F	701	ADP	C4-N9-C1'	2.37	132.18	126.63
2	F	701	ADP	O3B-PB-O3A	-2.37	96.69	104.64
2	E	701	ADP	O2B-PB-O1B	2.28	119.70	110.83
2	A	701	ADP	C1'-N9-C8	2.25	132.09	127.09
2	E	701	ADP	C2-N1-C6	2.23	122.40	118.73
2	B	701	ADP	C5-N7-C8	2.17	106.86	103.45
2	A	701	ADP	N9-C8-N7	-2.16	110.86	113.94
2	B	701	ADP	O4'-C1'-N9	2.16	112.24	108.09
2	A	701	ADP	C2-N1-C6	2.16	122.27	118.73
2	F	701	ADP	C2'-C3'-C4'	2.14	106.75	102.61
2	C	701	ADP	C6-C5-N7	2.12	136.18	132.09
2	C	701	ADP	C2-N1-C6	2.08	122.15	118.73
2	E	701	ADP	O2'-C2'-C1'	-2.07	102.97	110.10
2	A	701	ADP	C5-C4-N9	2.06	108.06	105.81
2	A	701	ADP	C5-N7-C8	2.04	106.66	103.45

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ADP	C5'-O5'-PA-O1A
2	A	701	ADP	C5'-O5'-PA-O3A
2	B	701	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	701	ADP	C5'-O5'-PA-O2A
2	B	701	ADP	C5'-O5'-PA-O3A
2	C	701	ADP	C5'-O5'-PA-O1A
2	E	701	ADP	C4'-C5'-O5'-PA
2	E	701	ADP	O4'-C4'-C5'-O5'
2	E	701	ADP	C3'-C4'-C5'-O5'
2	A	701	ADP	C3'-C4'-C5'-O5'
2	C	701	ADP	O4'-C4'-C5'-O5'
2	F	701	ADP	O4'-C4'-C5'-O5'
2	F	701	ADP	C3'-C4'-C5'-O5'
2	C	701	ADP	C3'-C4'-C5'-O5'
2	A	701	ADP	O4'-C4'-C5'-O5'
2	F	701	ADP	C2'-C1'-N9-C8
2	C	701	ADP	PA-O3A-PB-O1B
2	A	701	ADP	O4'-C1'-N9-C8
2	B	701	ADP	PB-O3A-PA-O1A
2	B	701	ADP	C2'-C1'-N9-C4
2	C	701	ADP	C5'-O5'-PA-O3A
2	B	701	ADP	C2'-C1'-N9-C8
2	A	701	ADP	O4'-C1'-N9-C4
2	A	701	ADP	PB-O3A-PA-O1A
2	C	701	ADP	PA-O3A-PB-O2B
2	C	701	ADP	PA-O3A-PB-O3B
2	A	701	ADP	C2'-C1'-N9-C8
2	F	701	ADP	C2'-C1'-N9-C4
2	A	701	ADP	PB-O3A-PA-O2A
2	F	701	ADP	O4'-C1'-N9-C8
2	F	701	ADP	O4'-C1'-N9-C4
2	E	701	ADP	C2'-C1'-N9-C8
2	B	701	ADP	PB-O3A-PA-O2A

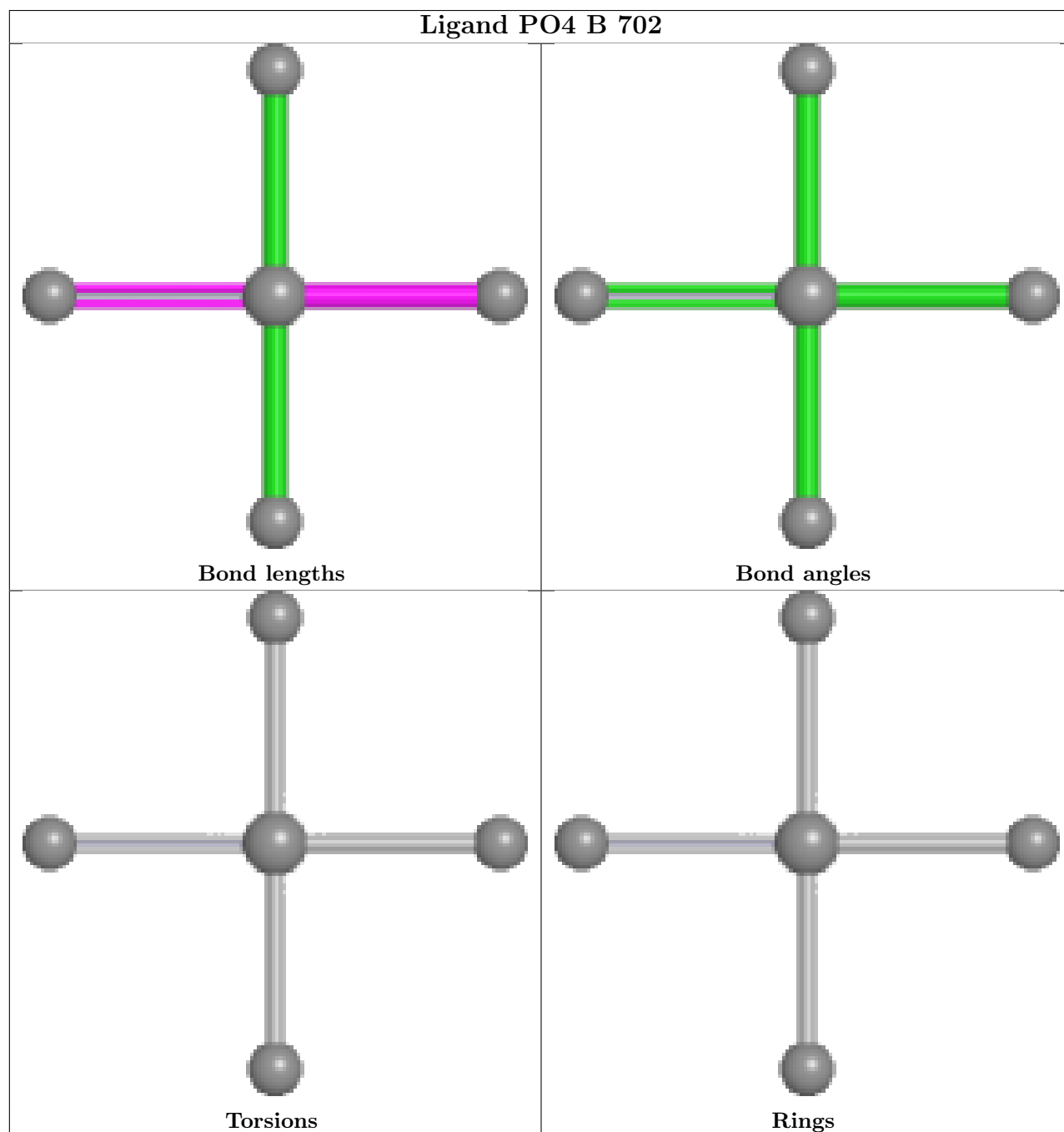
There are no ring outliers.

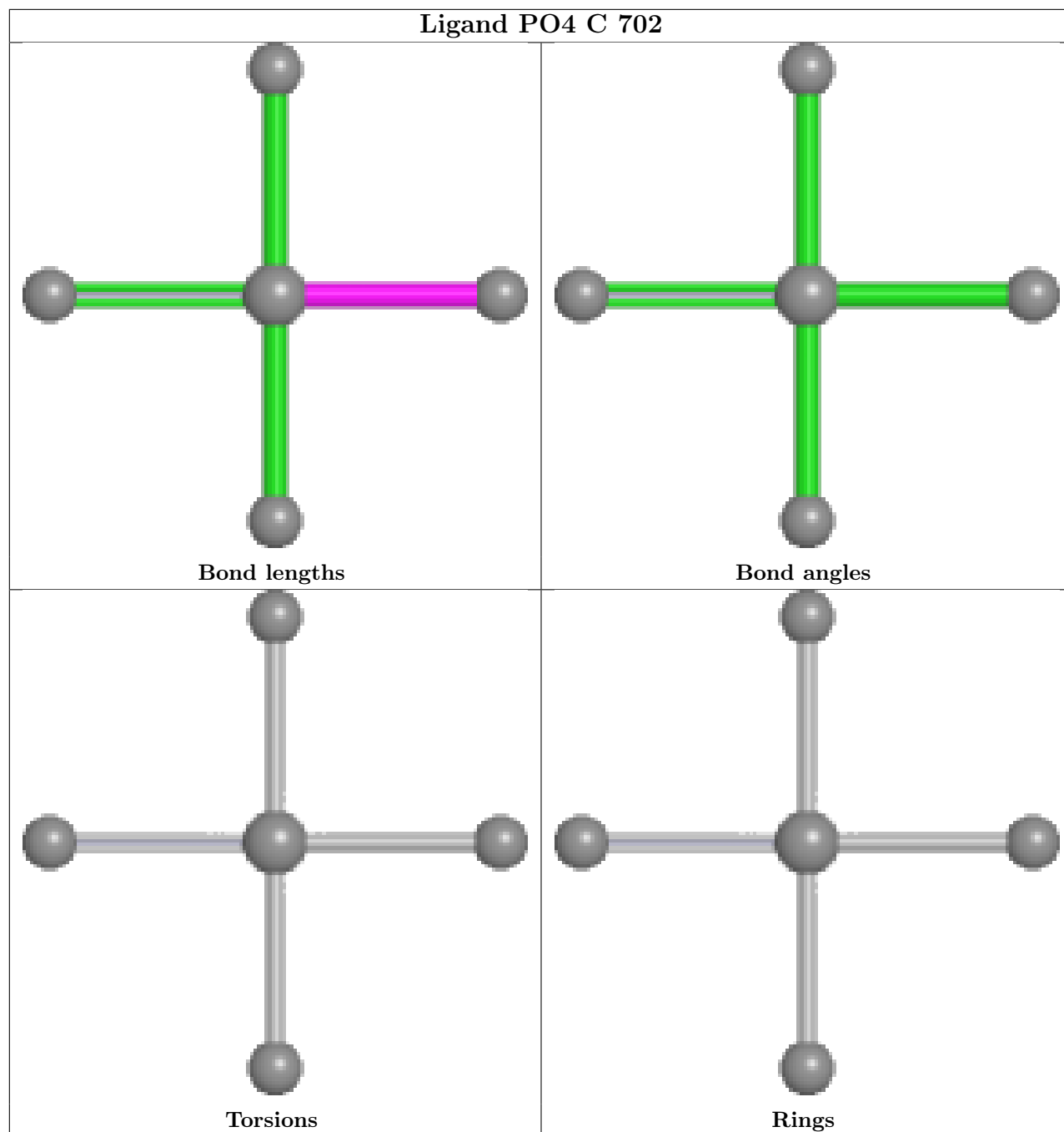
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	ADP	3	0
2	C	701	ADP	1	0
2	E	701	ADP	3	0
2	B	701	ADP	5	0
2	A	701	ADP	2	0

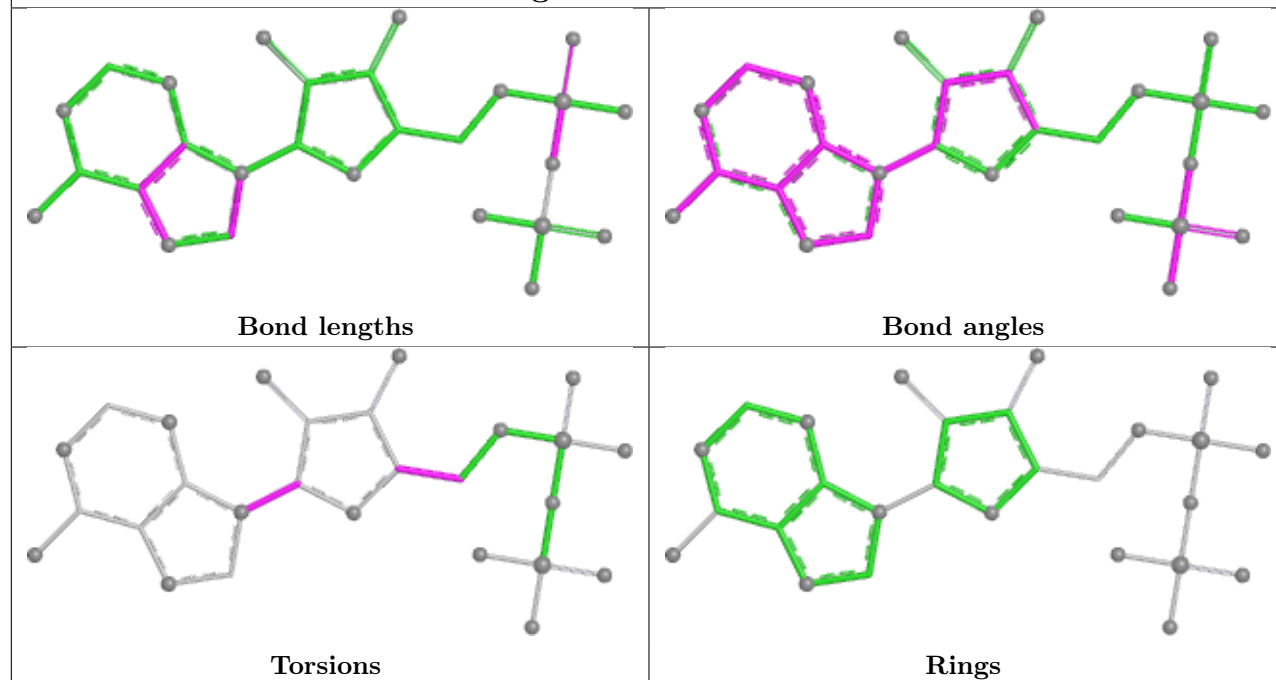
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

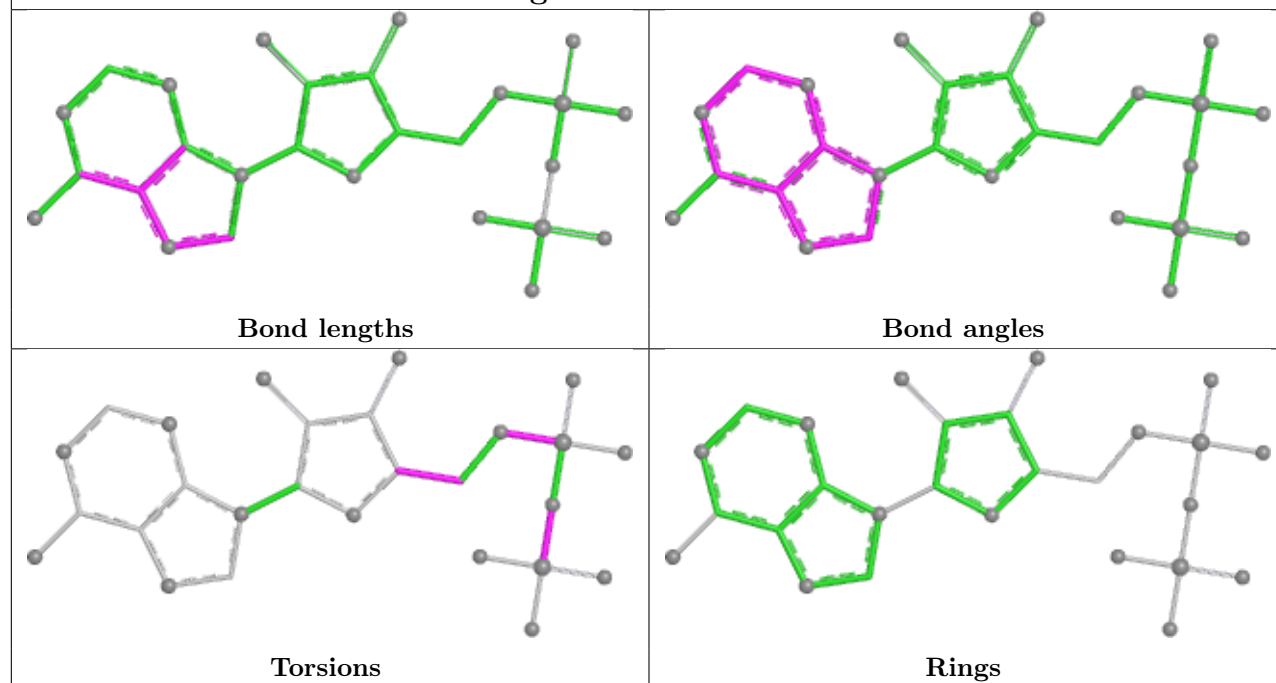


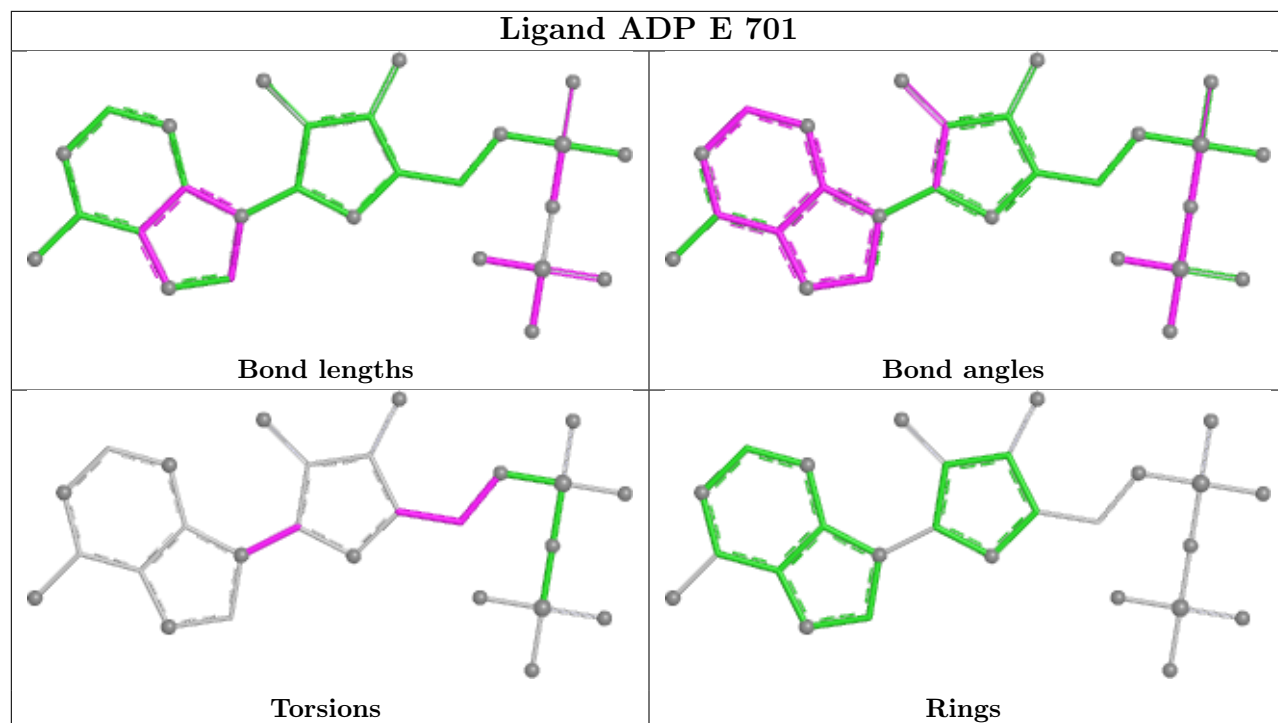


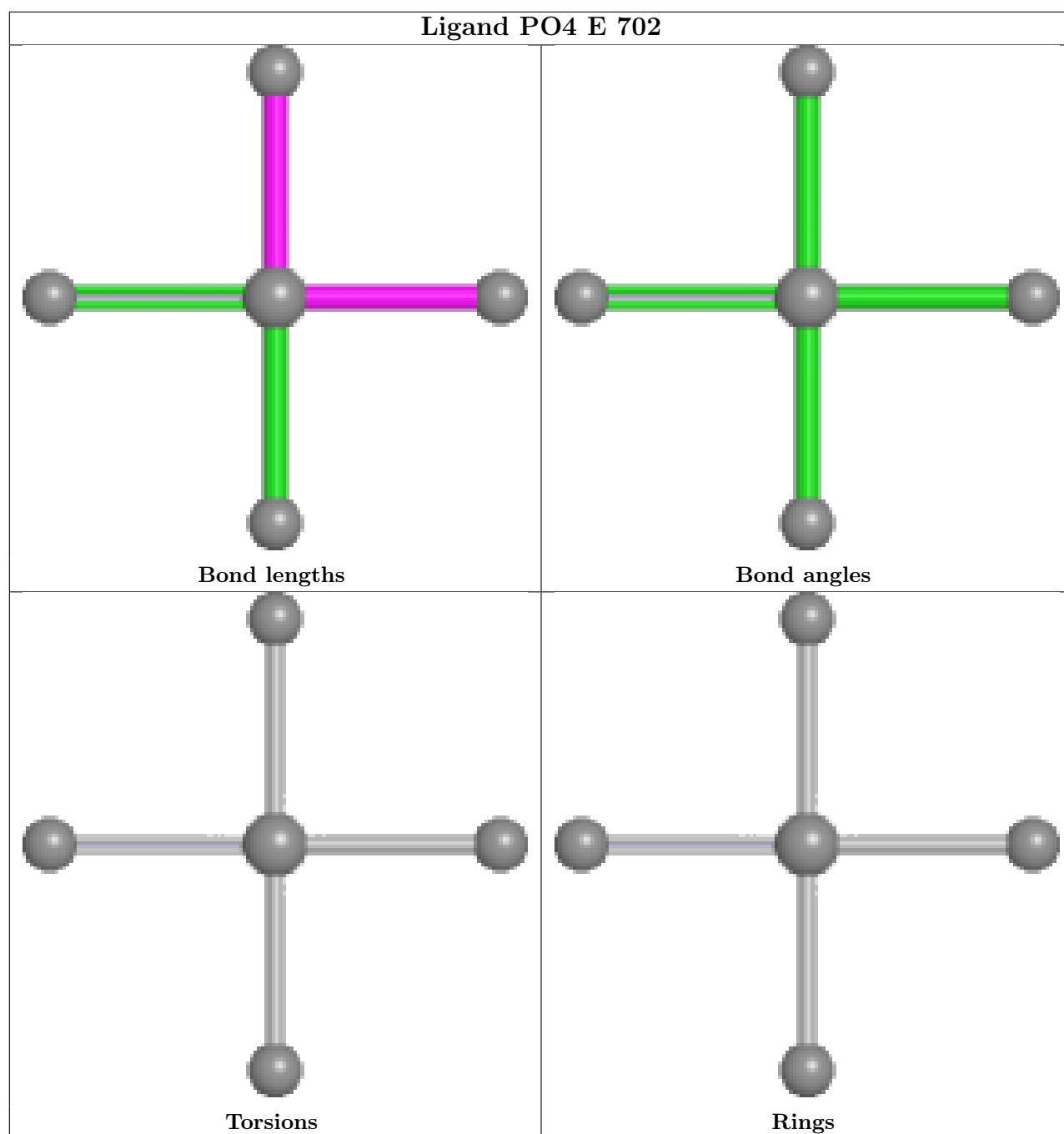
Ligand ADP F 701

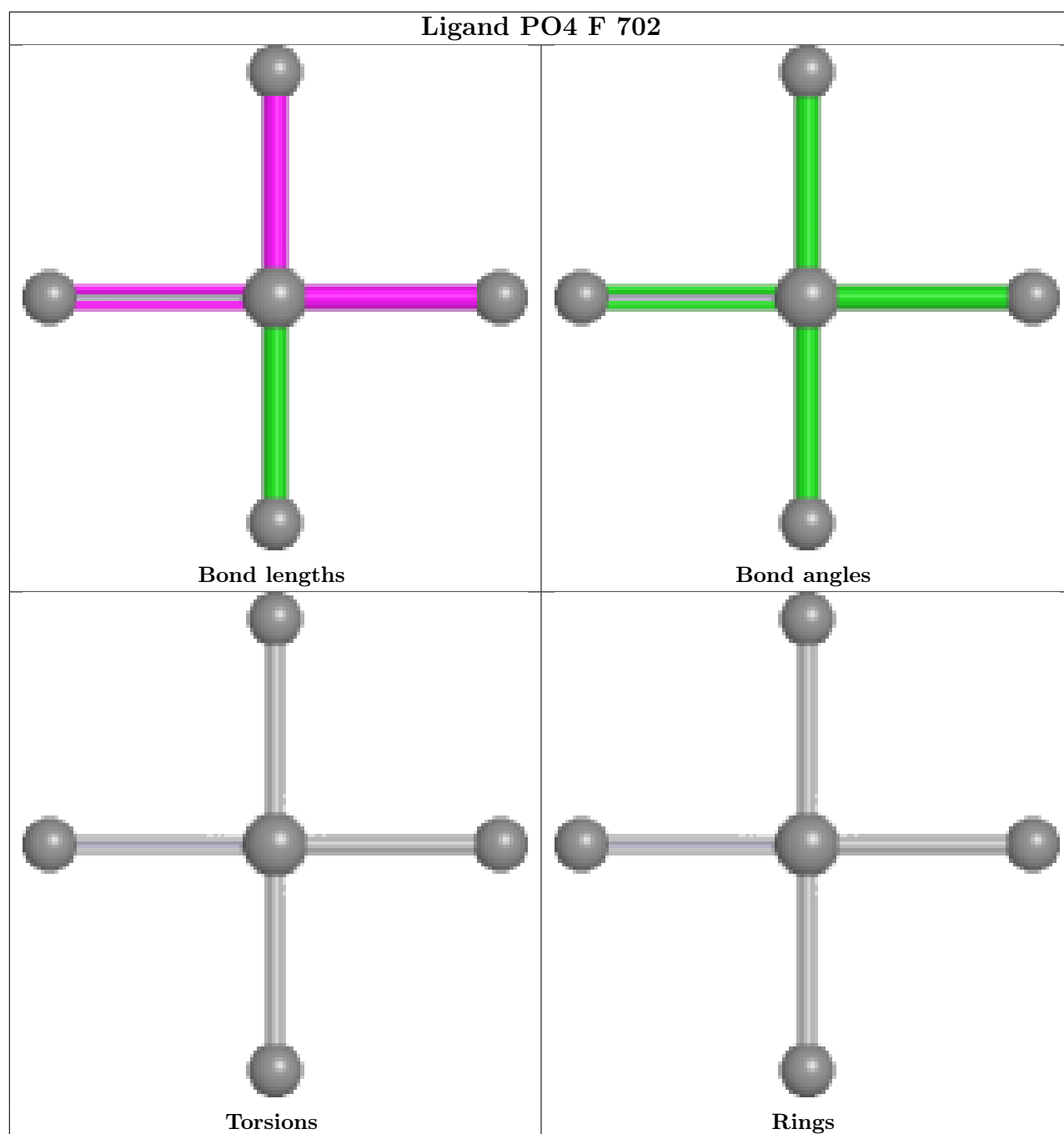


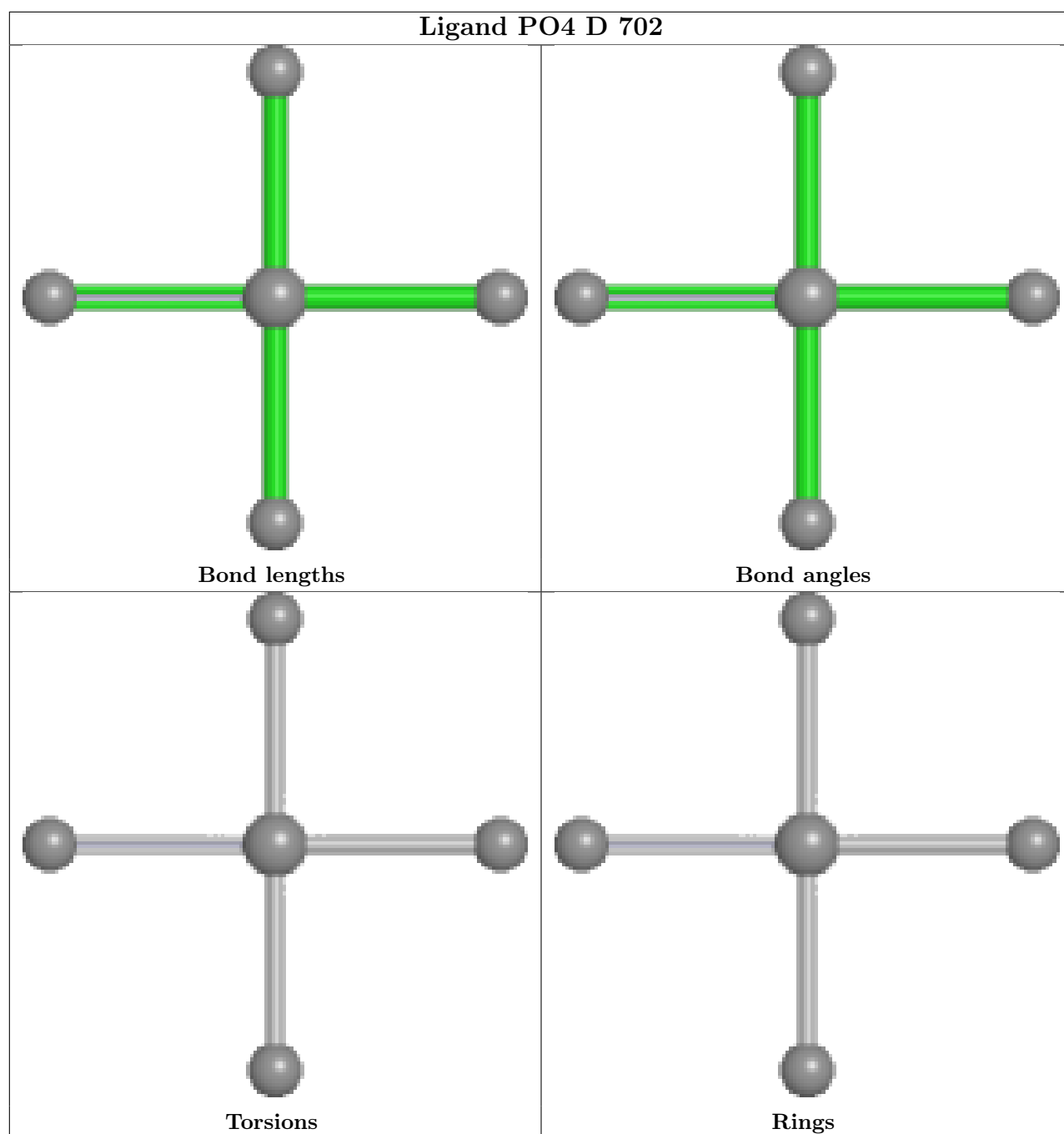
Ligand ADP C 701

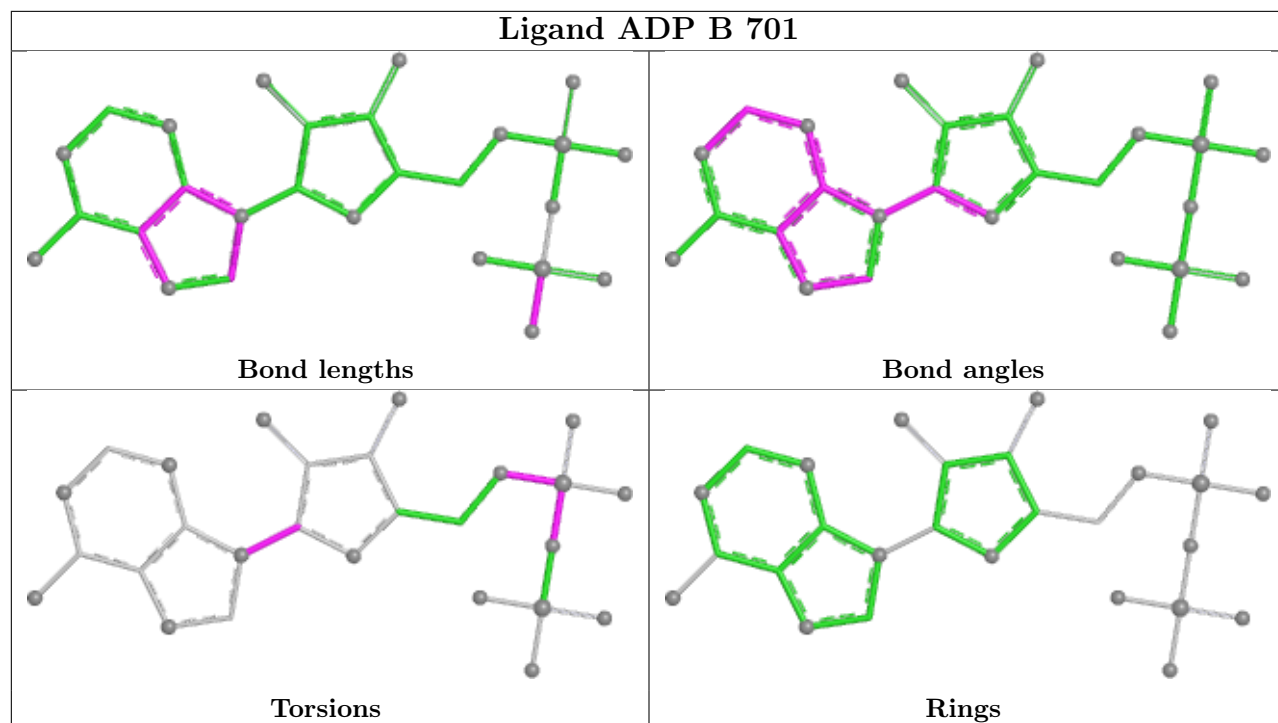


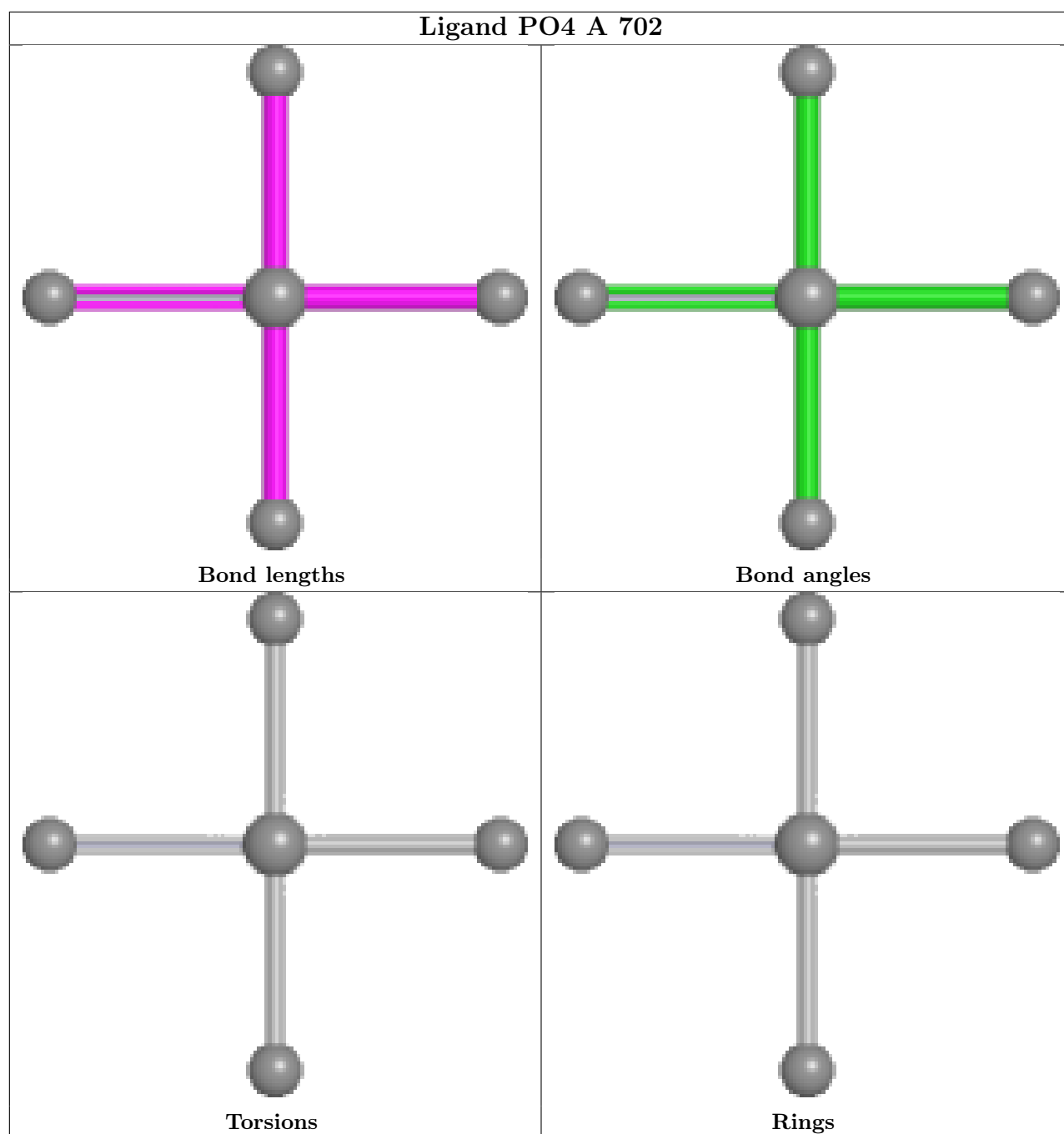


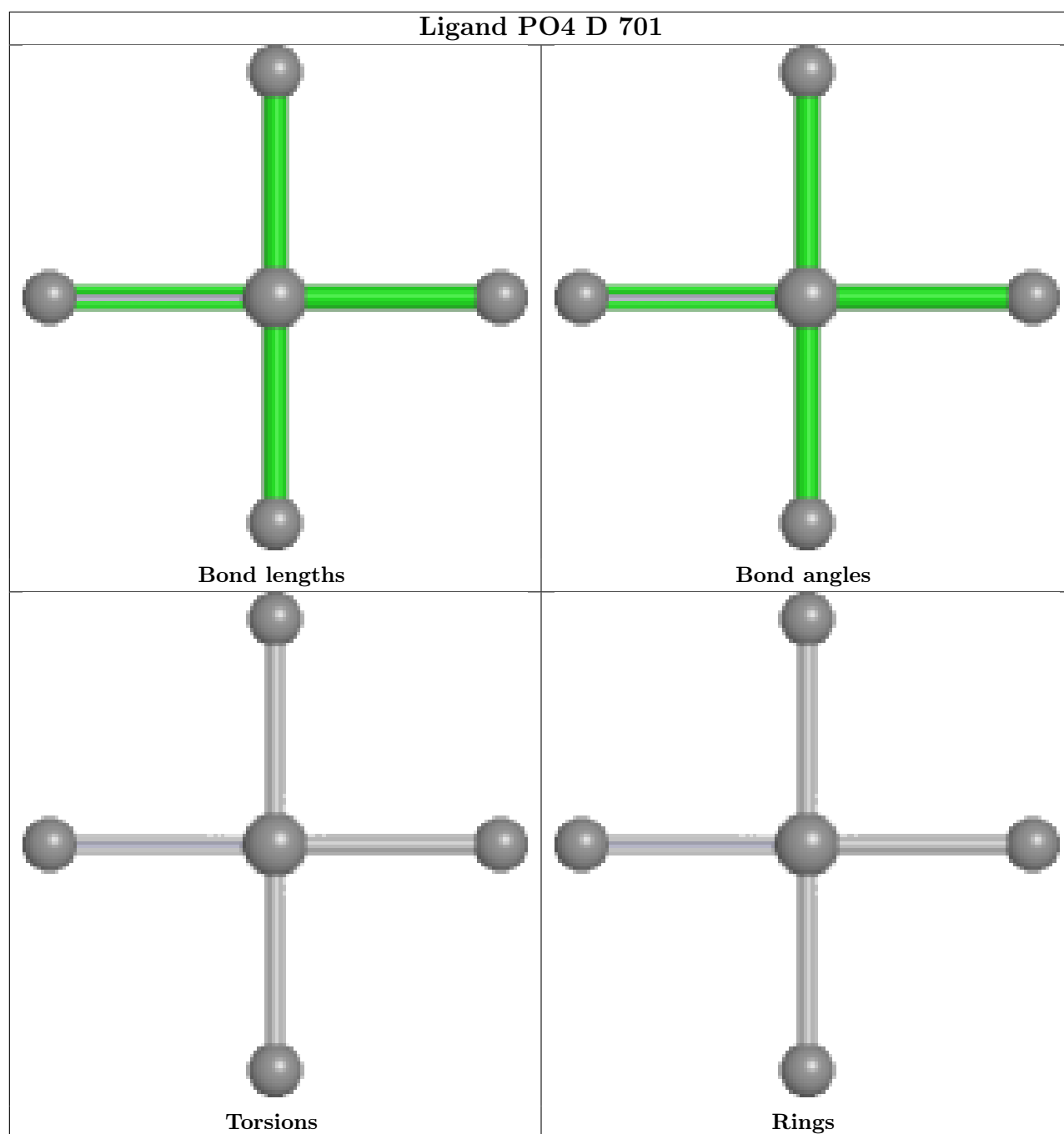


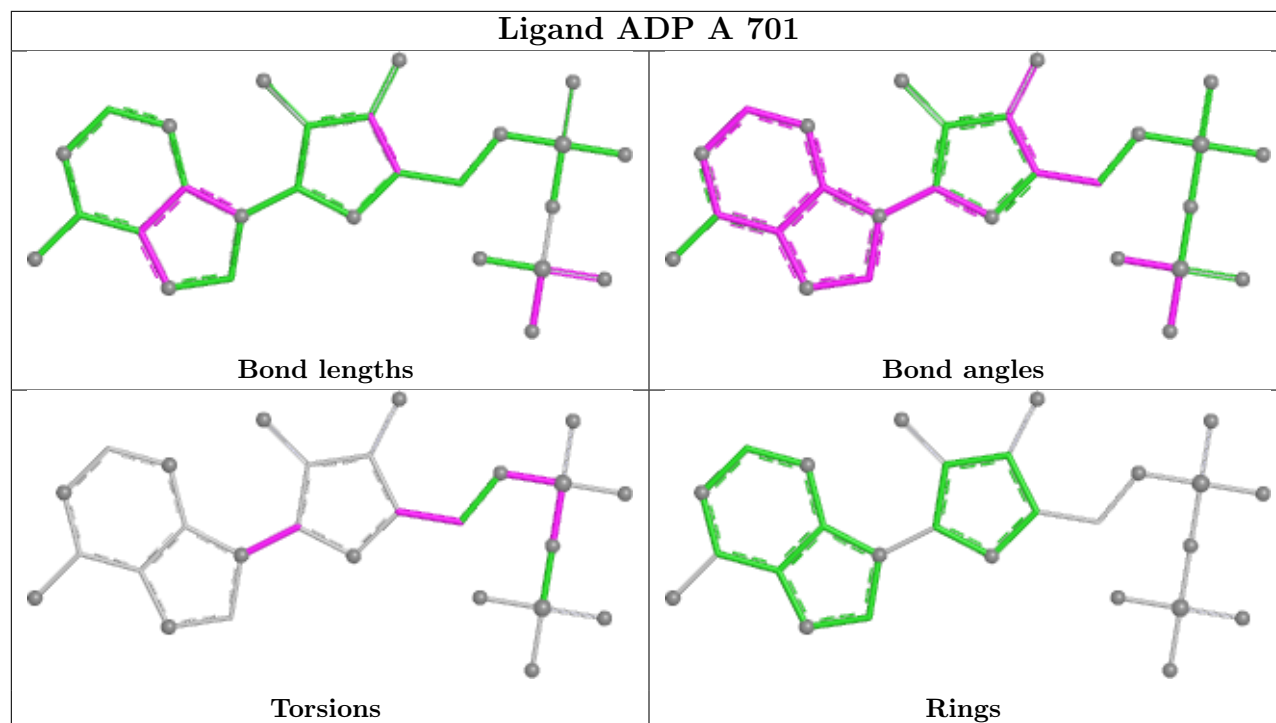












5.7 Other polymers [i](#)

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	574/601 (95%)	0.42	23 (4%)	42	37	49, 95, 127, 159	1 (0%)
1	B	572/601 (95%)	0.68	34 (5%)	28	23	76, 108, 143, 160	0
1	C	574/601 (95%)	0.44	24 (4%)	40	35	71, 102, 130, 167	0
1	D	577/601 (96%)	0.49	29 (5%)	34	28	76, 100, 138, 177	0
1	E	574/601 (95%)	0.58	29 (5%)	33	28	71, 115, 145, 181	0
1	F	582/601 (96%)	0.51	29 (4%)	34	28	65, 104, 139, 169	0
All	All	3453/3606 (95%)	0.52	168 (4%)	35	29	49, 103, 139, 181	1 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	596	THR	6.5
1	B	446	PRO	6.1
1	F	545	ALA	5.7
1	B	282	VAL	5.6
1	E	282	VAL	5.0
1	A	496	VAL	4.6
1	E	450	PHE	4.6
1	B	447	ALA	4.5
1	A	597	LEU	4.4
1	B	139	ALA	4.4
1	B	440	PHE	4.2
1	B	75	LEU	4.2
1	B	554	ILE	4.2
1	A	446	PRO	4.0
1	B	281	SER	4.0
1	E	506	PRO	3.9
1	A	441	ASP	3.8
1	D	215	ILE	3.8
1	A	450	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	308	LYS	3.7
1	F	553	PRO	3.7
1	C	71	LEU	3.7
1	B	506	PRO	3.6
1	F	450	PHE	3.6
1	B	341	LEU	3.5
1	B	450	PHE	3.5
1	E	189	SER	3.4
1	F	599	VAL	3.4
1	A	438	GLY	3.4
1	D	447	ALA	3.4
1	E	324	ILE	3.3
1	B	439	ARG	3.3
1	C	496	VAL	3.2
1	D	245	LEU	3.2
1	A	89	PHE	3.2
1	D	450	PHE	3.2
1	F	313	GLY	3.2
1	D	6	THR	3.2
1	D	395	ILE	3.1
1	F	282	VAL	3.0
1	B	594	LEU	3.0
1	E	464	PHE	3.0
1	C	282	VAL	2.9
1	D	545	ALA	2.9
1	E	558	GLN	2.9
1	B	546	GLY	2.9
1	D	286	ILE	2.9
1	A	447	ALA	2.9
1	B	449	GLN	2.8
1	F	190	ILE	2.8
1	C	450	PHE	2.8
1	C	552	THR	2.8
1	A	252	PHE	2.8
1	D	384	GLY	2.8
1	A	404	HIS	2.8
1	B	464	PHE	2.8
1	C	546	GLY	2.7
1	E	598	ALA	2.7
1	E	446	PRO	2.7
1	D	179	VAL	2.7
1	B	262	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	63	ILE	2.6
1	A	374	LEU	2.6
1	E	539	TYR	2.6
1	F	233	PRO	2.6
1	E	466	ILE	2.6
1	B	38	LEU	2.6
1	B	496	VAL	2.6
1	E	281	SER	2.6
1	B	587	ILE	2.6
1	E	554	ILE	2.6
1	A	553	PRO	2.5
1	C	466	ILE	2.5
1	F	420	ILE	2.5
1	C	335	LEU	2.5
1	D	346	ILE	2.5
1	F	309	LEU	2.5
1	D	233	PRO	2.5
1	C	257	ILE	2.5
1	E	553	PRO	2.4
1	F	159	LYS	2.4
1	F	386	ILE	2.4
1	B	562	LEU	2.4
1	A	310	VAL	2.4
1	C	40	VAL	2.4
1	D	348	VAL	2.4
1	A	283	ALA	2.4
1	B	72	MET	2.4
1	E	440	PHE	2.4
1	C	73	GLY	2.4
1	E	527	LEU	2.4
1	C	203	LEU	2.4
1	F	310	VAL	2.4
1	A	545	ALA	2.4
1	A	174	SER	2.3
1	A	189	SER	2.3
1	F	438	GLY	2.3
1	B	483	LEU	2.3
1	F	158	LYS	2.3
1	F	440	PHE	2.3
1	E	411	THR	2.3
1	F	312	GLY	2.3
1	A	45	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	420	ILE	2.3
1	C	48	PHE	2.3
1	D	464	PHE	2.3
1	E	353	VAL	2.3
1	D	446	PRO	2.3
1	A	175	GLN	2.3
1	D	229	GLY	2.3
1	D	309	LEU	2.3
1	F	248	LYS	2.3
1	A	591	GLU	2.3
1	D	117	VAL	2.3
1	C	505	PRO	2.3
1	F	459	ARG	2.3
1	B	301	PHE	2.2
1	B	157	CYS	2.2
1	B	597	LEU	2.2
1	F	193	TRP	2.2
1	D	289	TYR	2.2
1	D	445	TYR	2.2
1	E	190	ILE	2.2
1	E	563	ILE	2.2
1	C	8	SER	2.2
1	A	233	PRO	2.2
1	B	284	PRO	2.2
1	C	301	PHE	2.2
1	C	464	PHE	2.2
1	E	301	PHE	2.2
1	B	159	LYS	2.2
1	B	425	ALA	2.2
1	C	596	THR	2.2
1	B	395	ILE	2.2
1	D	382	GLY	2.1
1	E	188	GLY	2.1
1	D	592	TYR	2.1
1	C	202	ASP	2.1
1	F	252	PHE	2.1
1	D	378	ALA	2.1
1	D	374	LEU	2.1
1	F	456	LEU	2.1
1	B	458	SER	2.1
1	F	271	ASP	2.1
1	F	464	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	75	LEU	2.1
1	E	445	TYR	2.1
1	D	387	VAL	2.1
1	E	546	GLY	2.1
1	E	369	GLU	2.1
1	C	84	ILE	2.1
1	C	553	PRO	2.1
1	F	153	VAL	2.0
1	B	76	ALA	2.0
1	E	421	ALA	2.0
1	D	358	LEU	2.0
1	E	344	LYS	2.0
1	D	232	ASP	2.0
1	A	440	PHE	2.0
1	C	88	ARG	2.0
1	D	367	PHE	2.0
1	F	136	PHE	2.0
1	B	298	LEU	2.0
1	F	403	LEU	2.0
1	B	332	THR	2.0
1	E	292	ILE	2.0
1	C	200	ASP	2.0
1	F	576	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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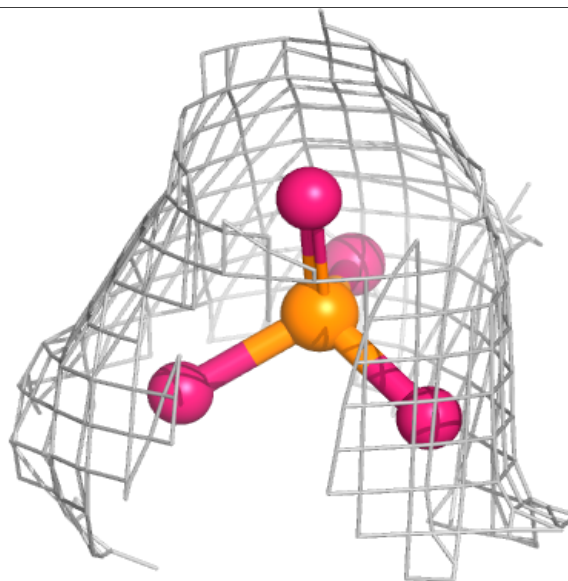
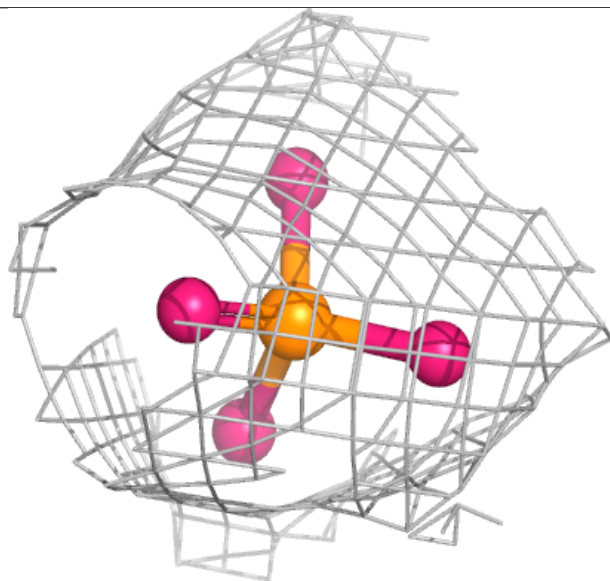
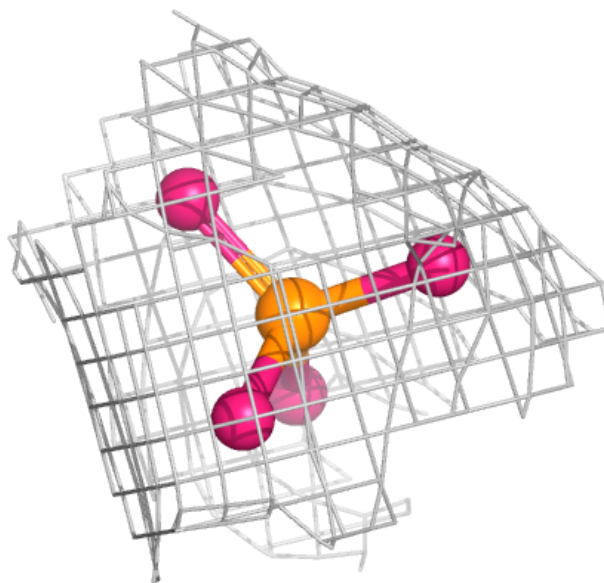
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	C	702	5/5	0.66	0.11	109,112,122,134	0
3	PO4	B	702	5/5	0.78	0.09	102,107,119,125	0
3	PO4	D	701	5/5	0.83	0.09	101,101,123,125	0
3	PO4	A	702	5/5	0.85	0.07	97,106,115,119	0
3	PO4	F	702	5/5	0.87	0.07	95,95,102,107	0
3	PO4	E	702	5/5	0.88	0.08	100,101,103,117	0
2	ADP	A	701	27/27	0.88	0.18	85,102,126,129	19
2	ADP	C	701	27/27	0.89	0.15	82,96,117,124	17
3	PO4	D	702	5/5	0.90	0.08	97,98,102,104	0
2	ADP	B	701	27/27	0.92	0.12	88,100,126,127	13
4	ZN	B	703	1/1	0.92	0.06	152,152,152,152	0
2	ADP	E	701	27/27	0.93	0.14	98,113,138,143	15
2	ADP	F	701	27/27	0.94	0.15	88,97,121,128	18
4	ZN	D	703	1/1	0.97	0.07	68,68,68,68	1
4	ZN	C	703	1/1	0.98	0.05	107,107,107,107	0
4	ZN	F	703	1/1	0.98	0.05	118,118,118,118	1
4	ZN	E	703	1/1	0.99	0.03	127,127,127,127	0
4	ZN	A	703	1/1	0.99	0.05	95,95,95,95	1

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.

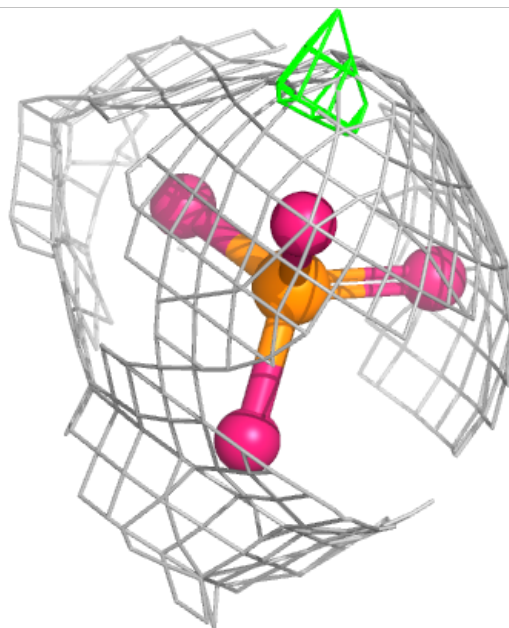
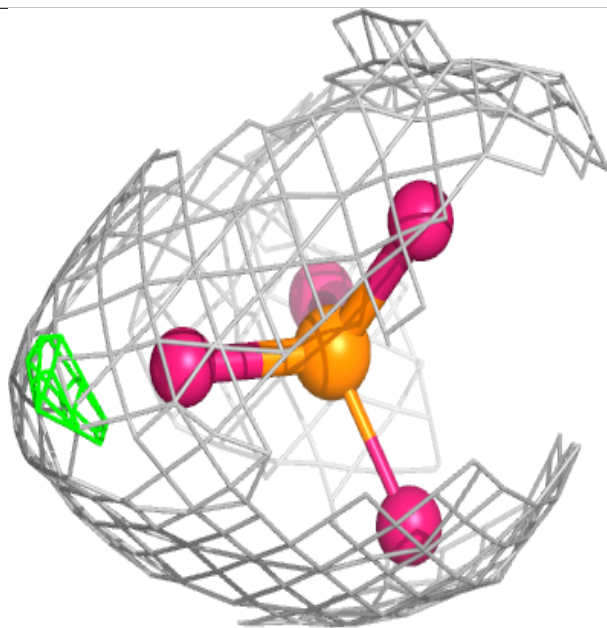
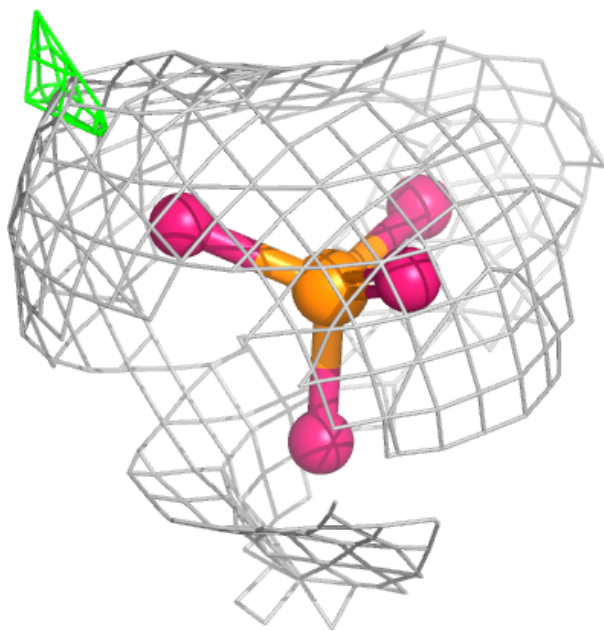
Electron density around PO4 C 702:

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



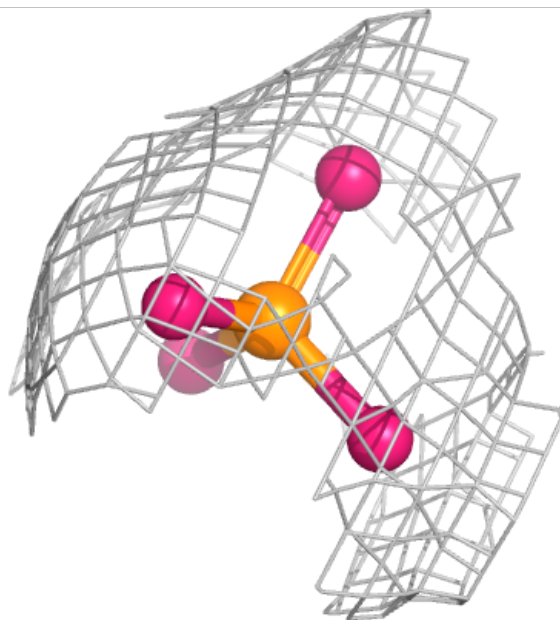
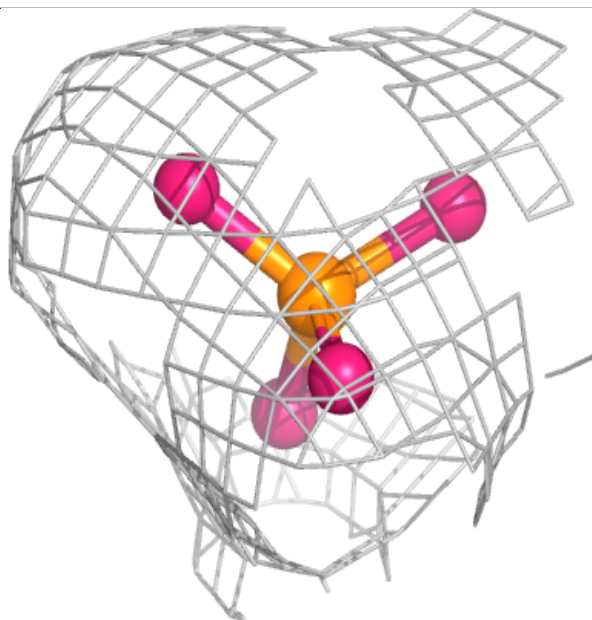
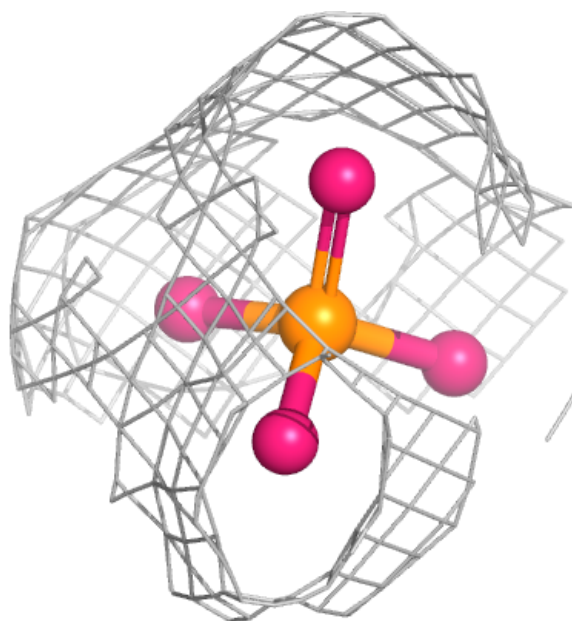
Electron density around PO4 B 702:

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



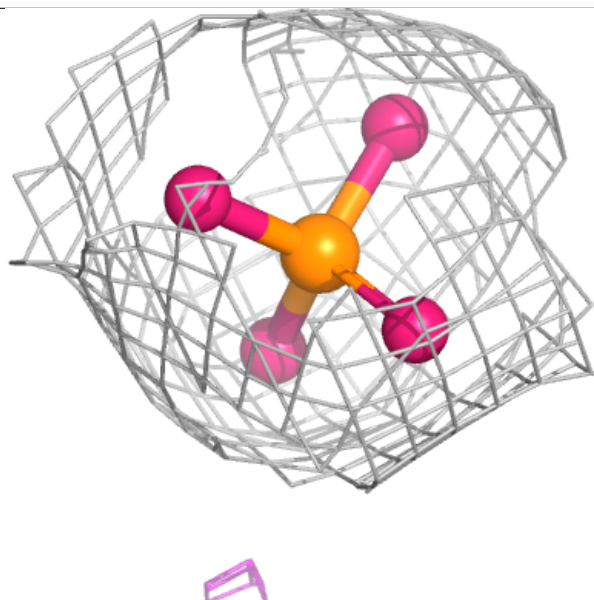
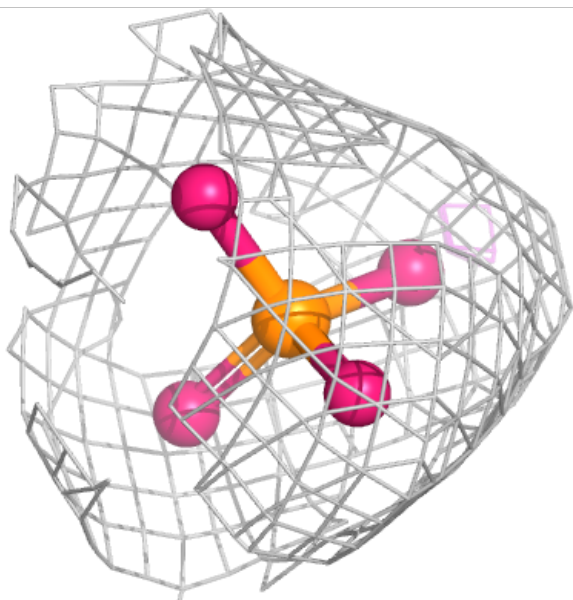
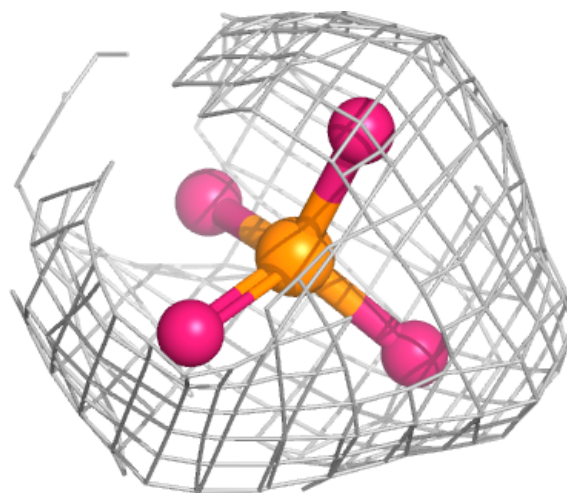
Electron density around PO4 D 701:

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



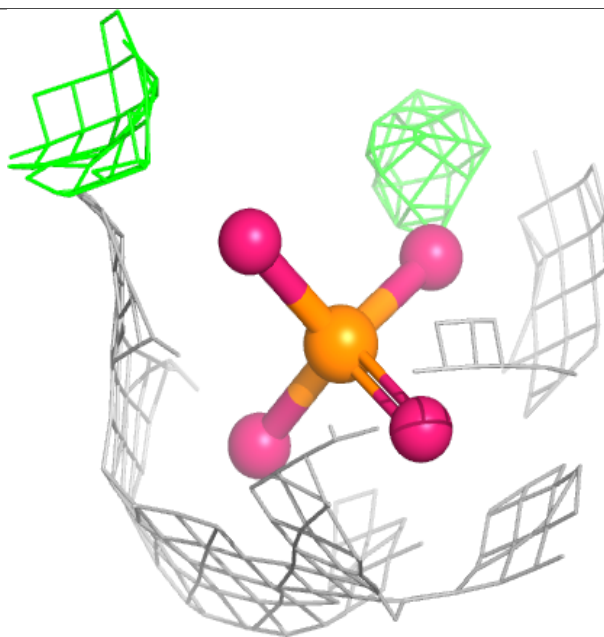
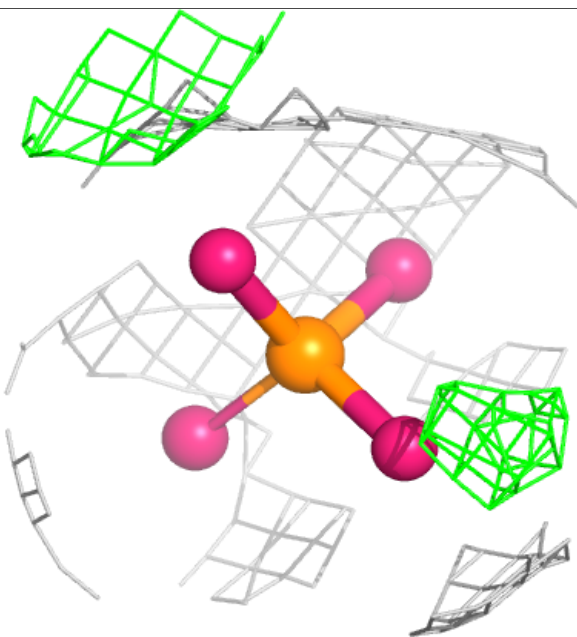
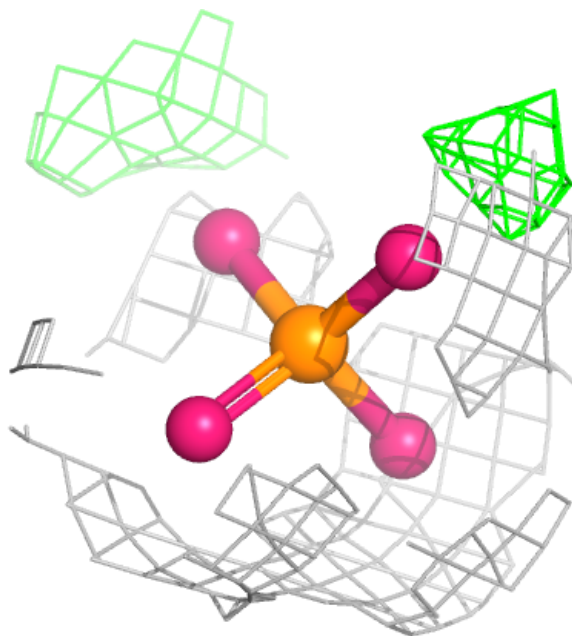
Electron density around PO4 A 702:

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



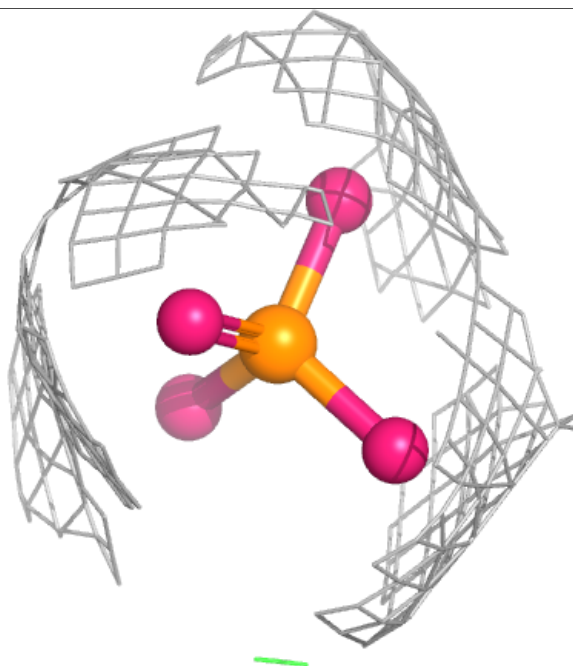
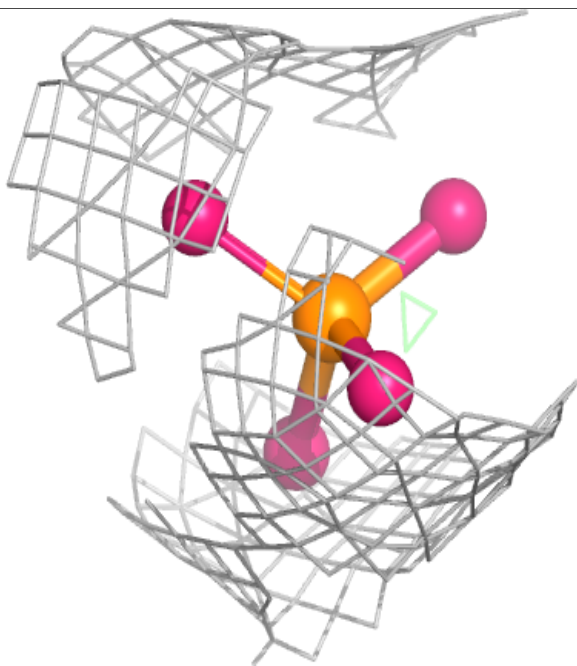
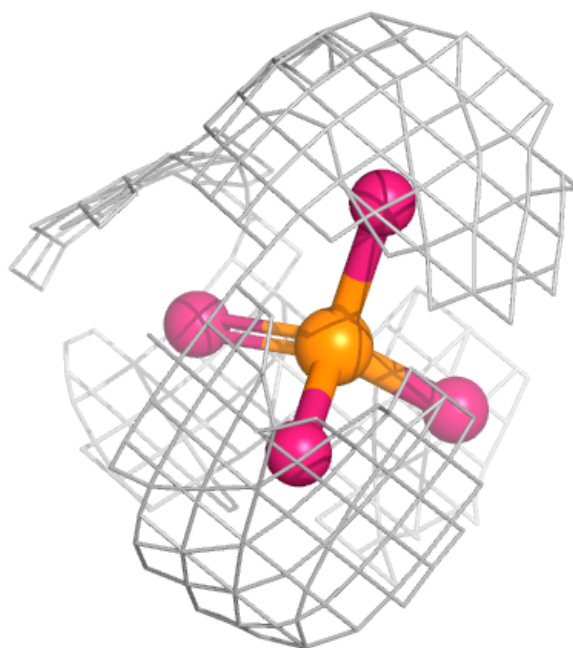
Electron density around PO4 F 702:

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



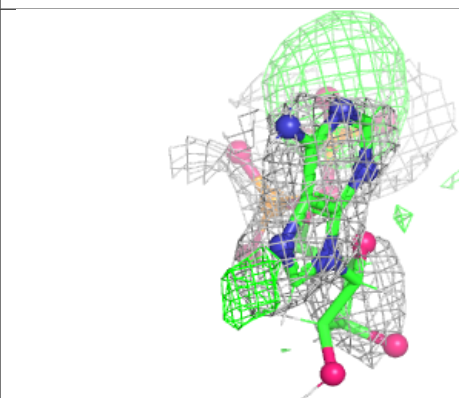
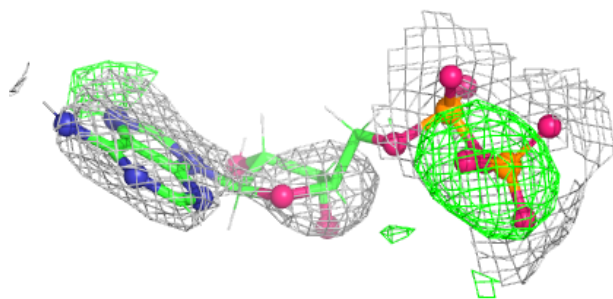
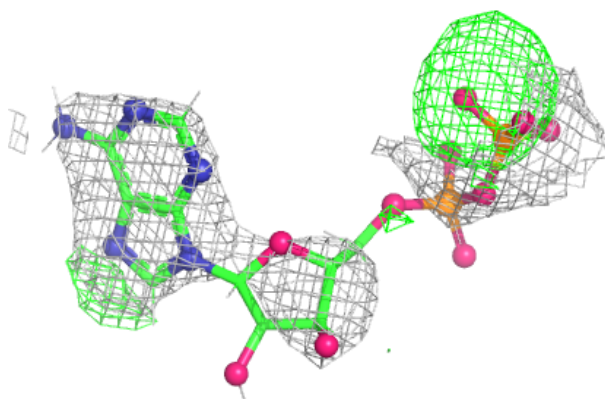
Electron density around PO4 E 702:

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and green (positive)

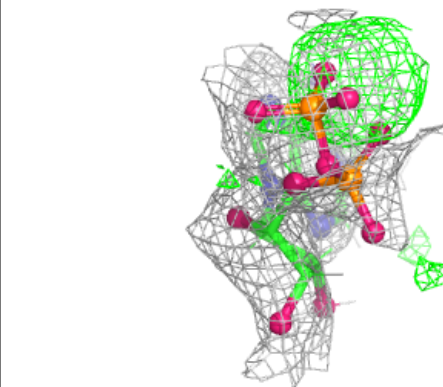
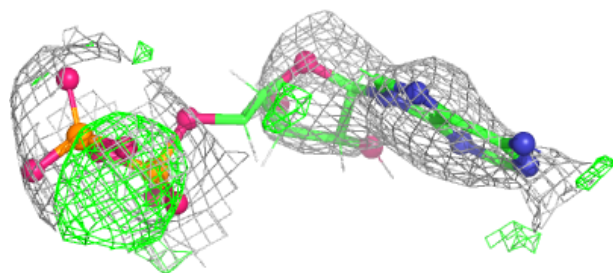
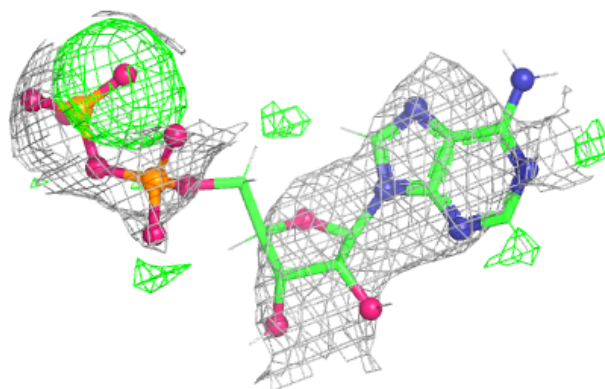


Electron density around ADP A 701:

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

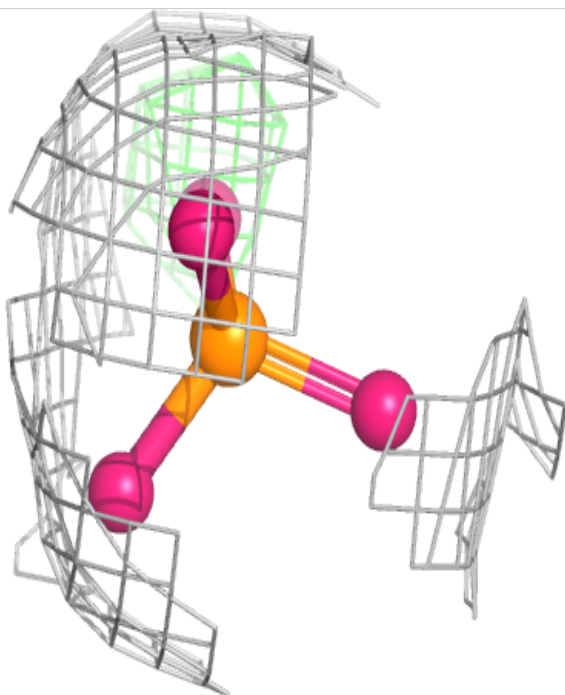
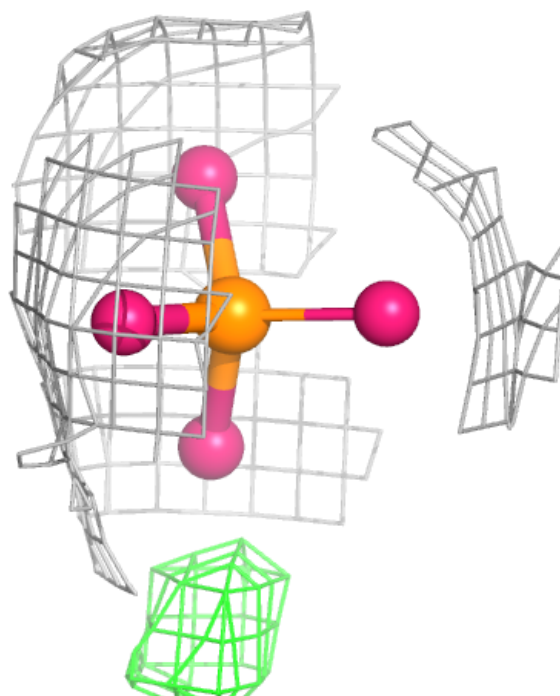
**Electron density around ADP C 701:**

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



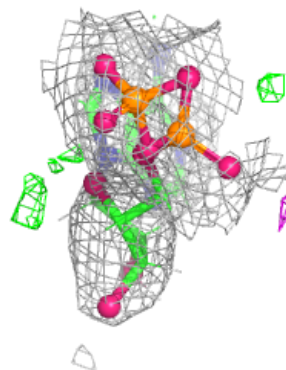
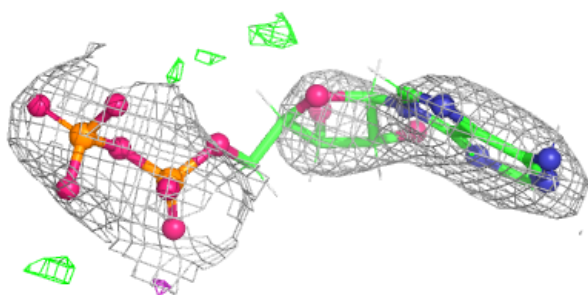
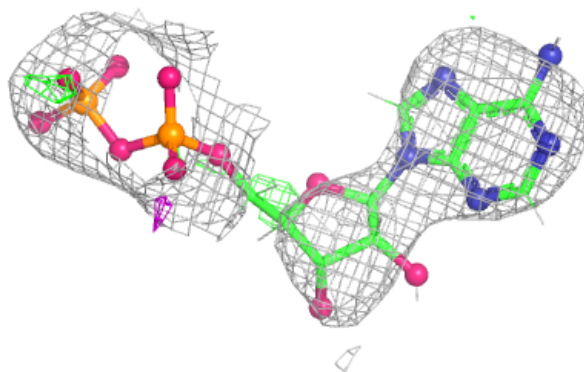
Electron density around PO4 D 702:

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



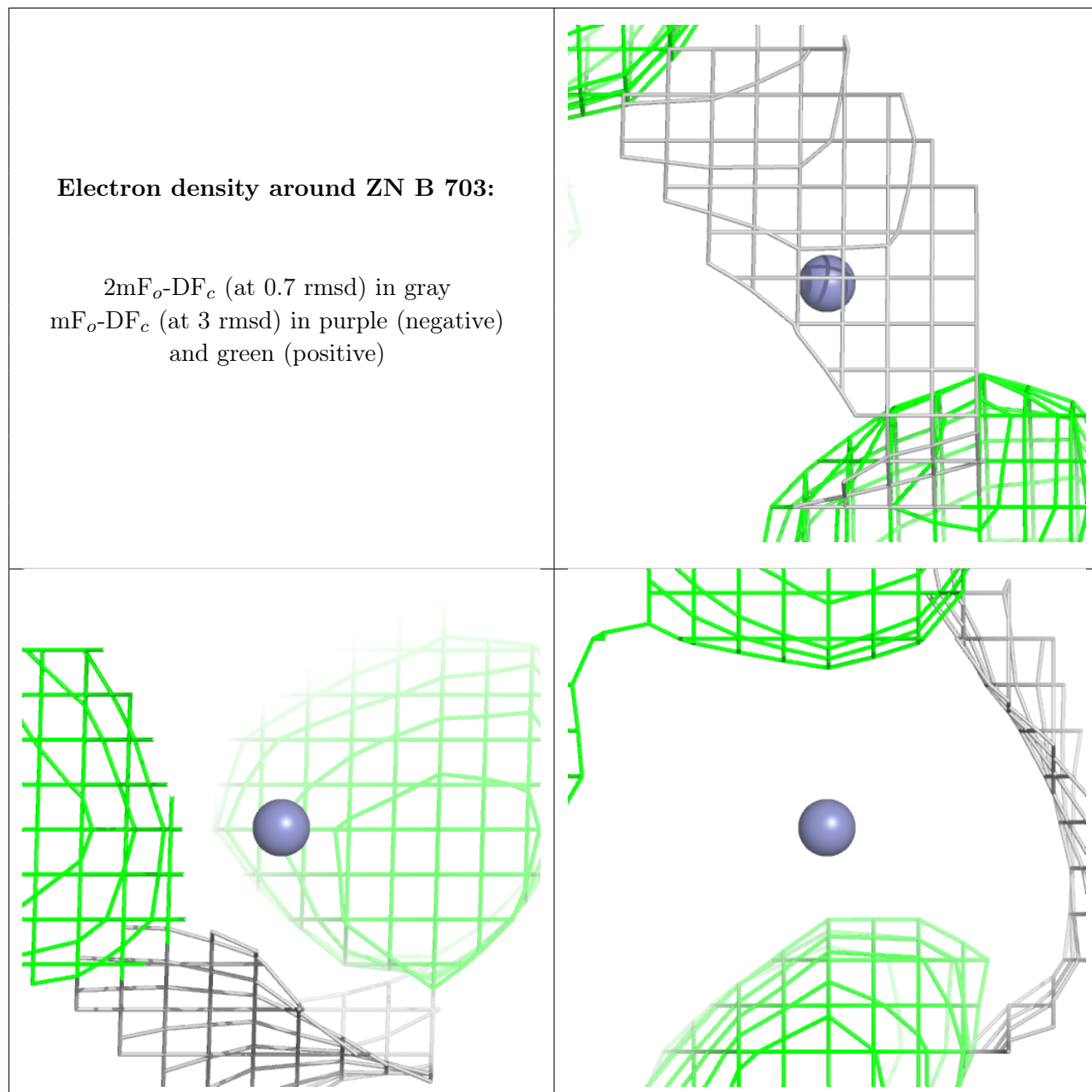
Electron density around ADP B 701:

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



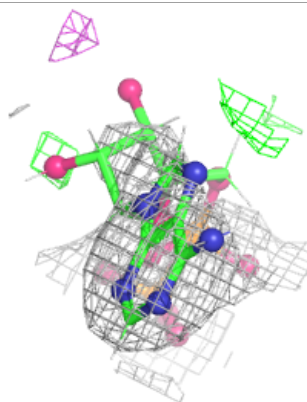
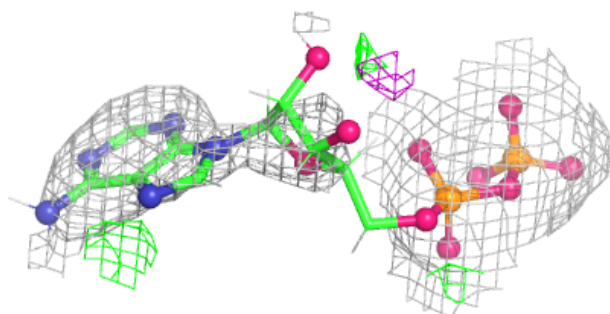
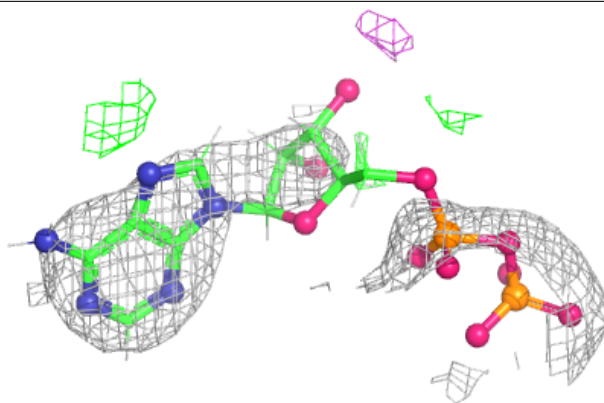
Electron density around ZN B 703:

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

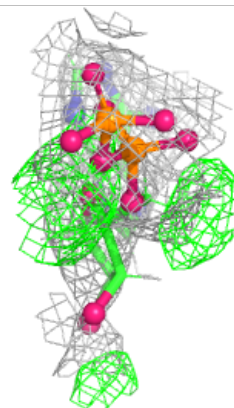
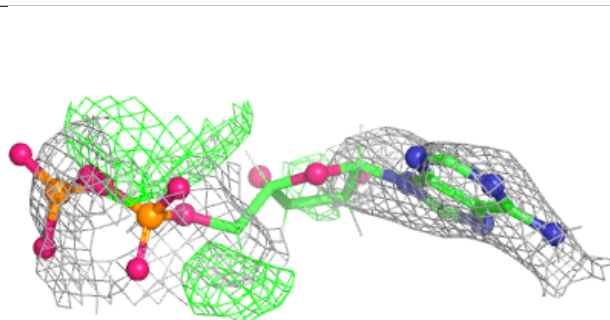
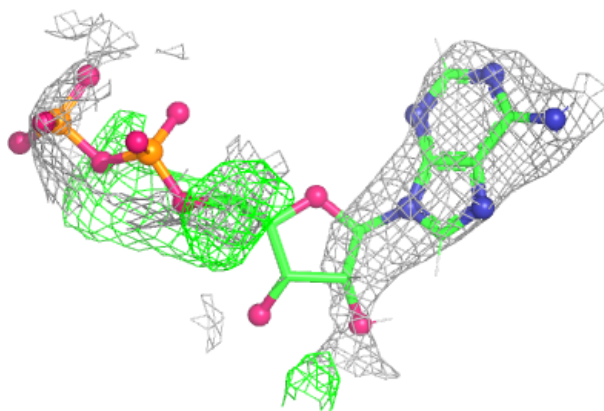


Electron density around ADP E 701:

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

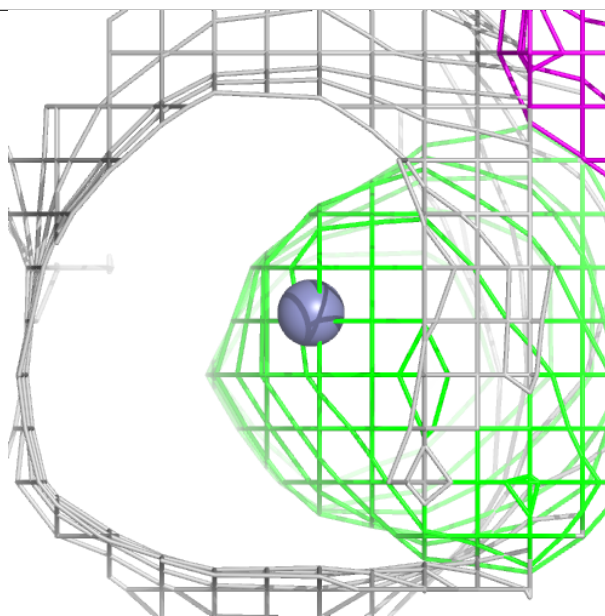
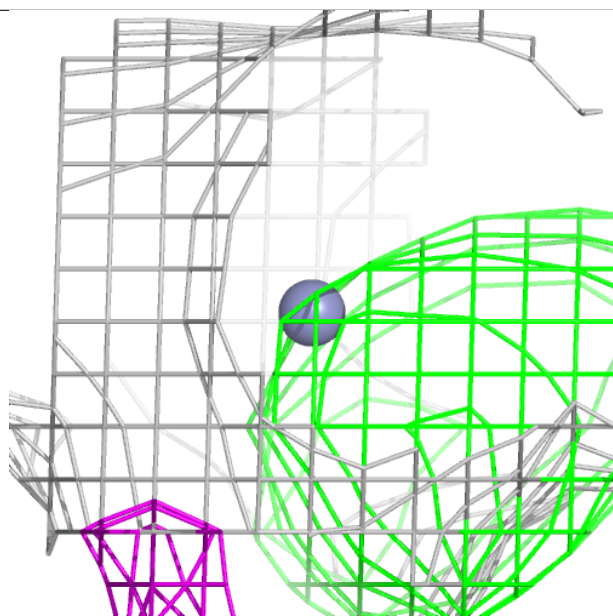
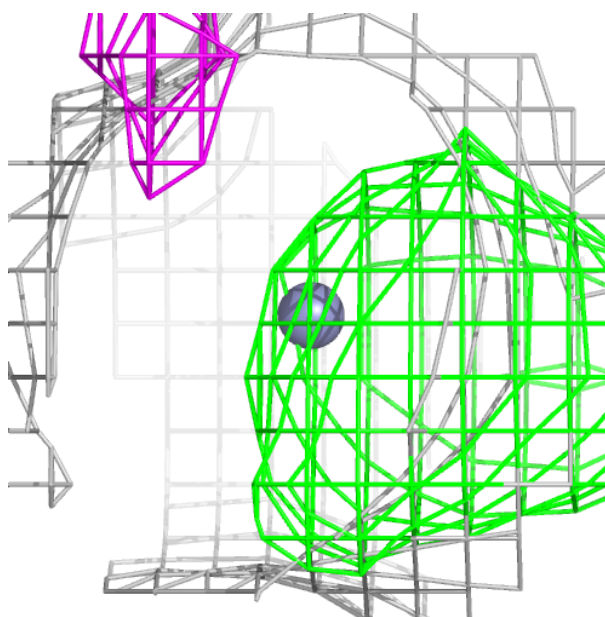
**Electron density around ADP F 701:**

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



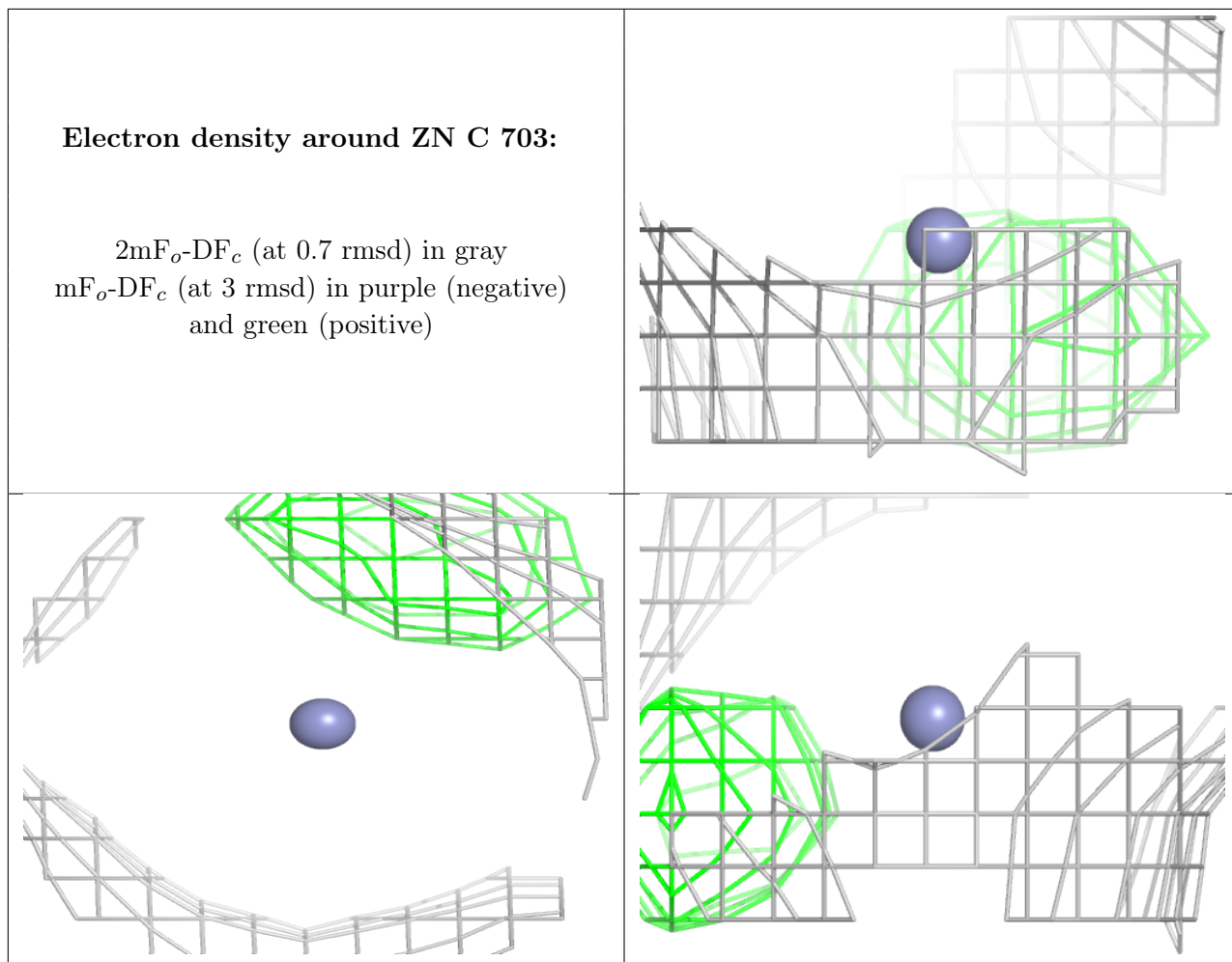
Electron density around ZN D 703:

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



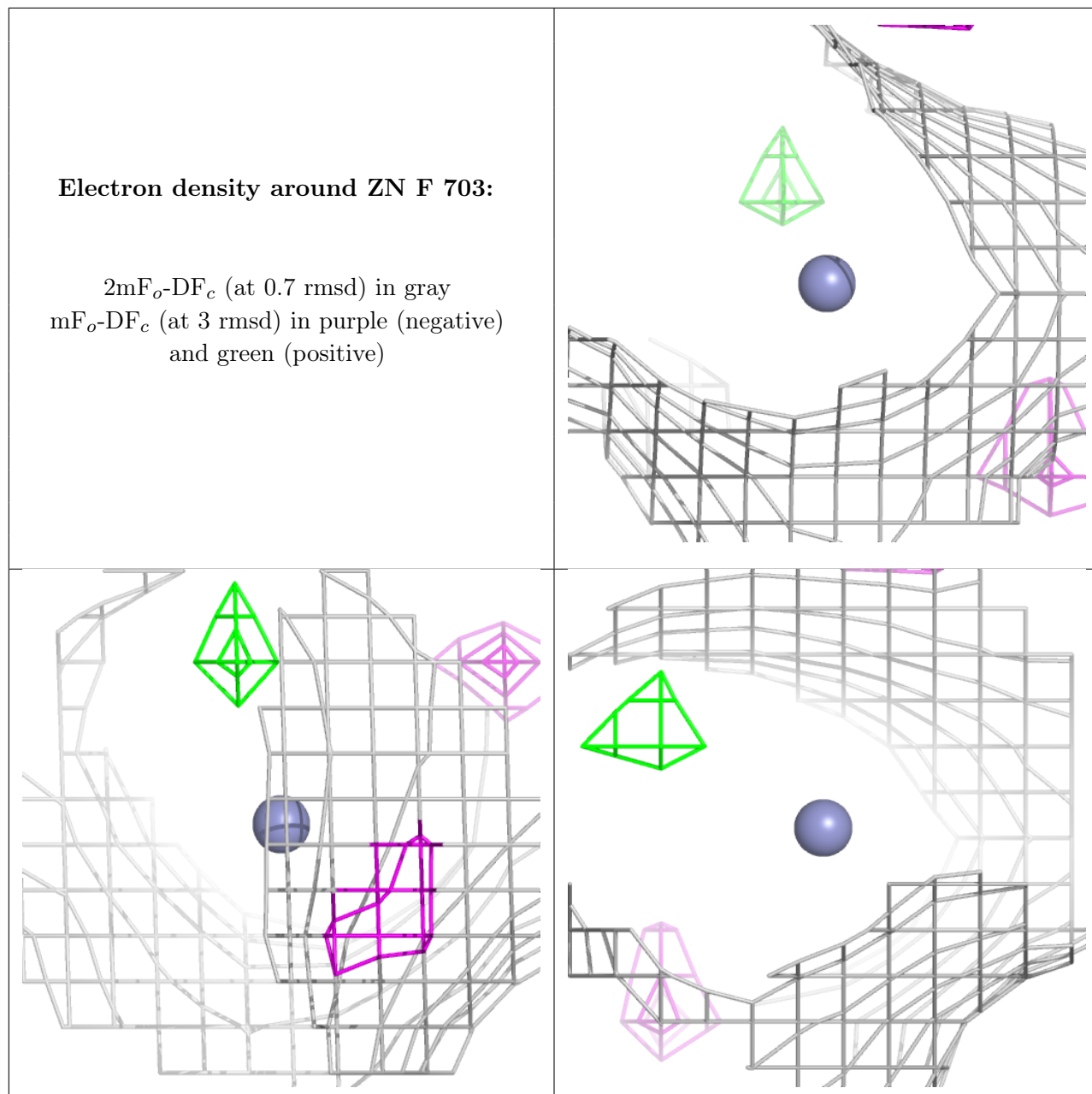
Electron density around ZN C 703:

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



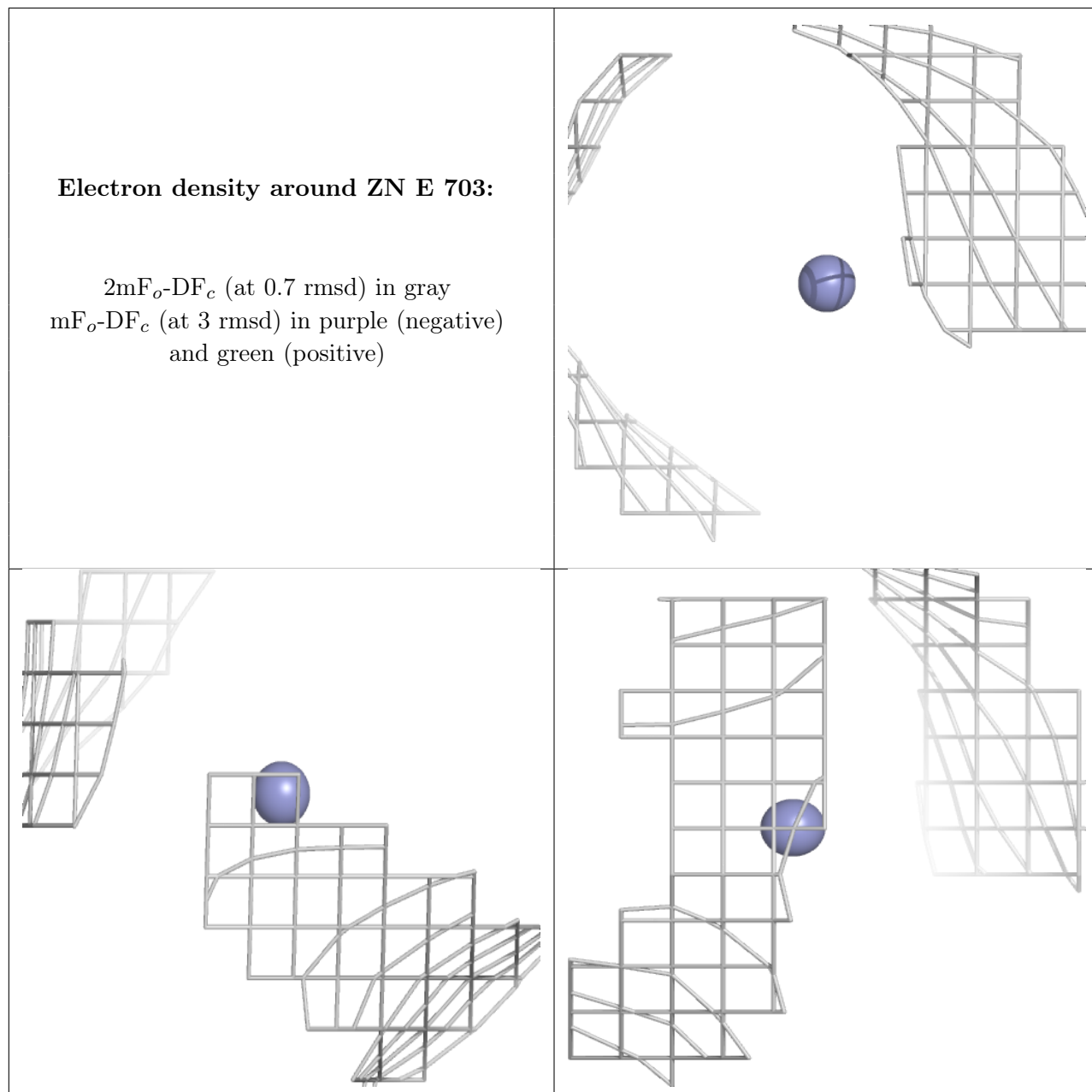
Electron density around ZN F 703:

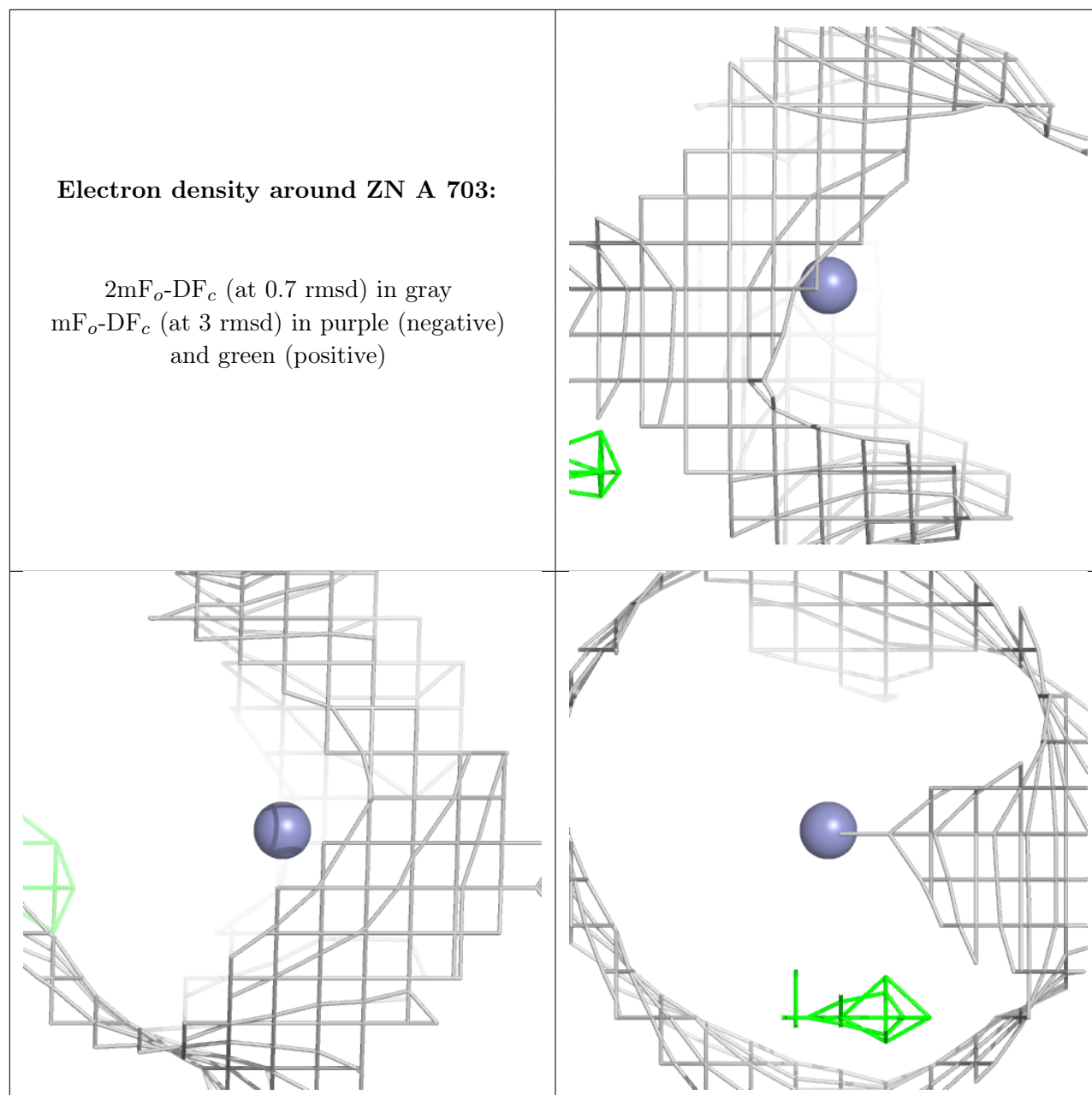
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN E 703:

$2mF_o-DF_c$ (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.