



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:20 AM UTC

PDB ID : 9E6M / pdb_00009e6m
Title : Crystal structure of the G200R mutant from the maize chloroplastic photo-synthetic NADP(+)-dependent malic enzyme
Authors : Klinke, S.; Schneberger, N.; Boehm, J.M.; Willms, S.; Hagelueken, G.; Geyer, M.; Maurino, V.; Alvarez, C.E.
Deposited on : 2024-10-30
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

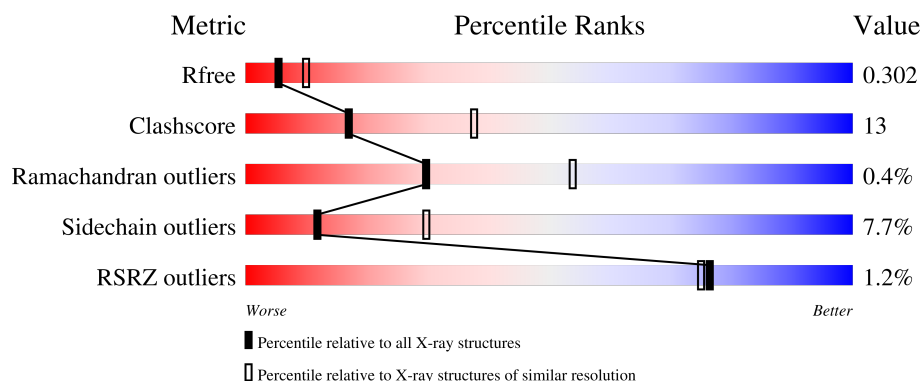
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	576	% 70% 25% ..
1	B	576	2% 69% 24% . .
1	C	576	% 68% 24% . .
1	D	576	% 71% 22% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17498 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.

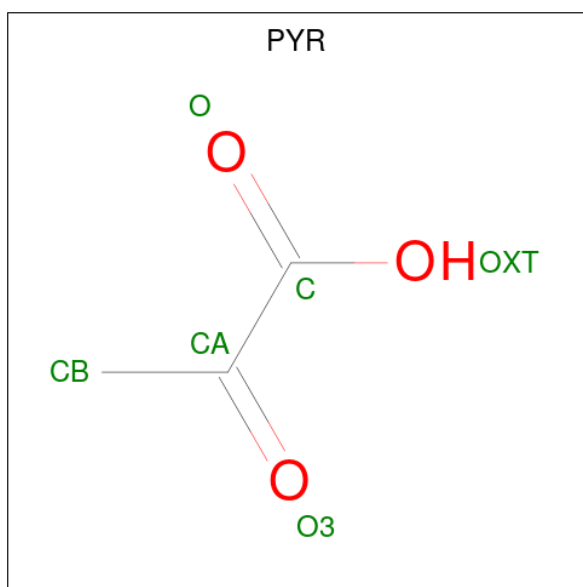
- Molecule 1 is a protein called Malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4405	2819	738	831	17			
1	B	553	Total	C	N	O	S	0	0	0
			4316	2768	724	807	17			
1	C	552	Total	C	N	O	S	0	0	0
			4307	2763	723	804	17			
1	D	565	Total	C	N	O	S	0	0	0
			4405	2819	738	831	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	HIS	-	expression tag	UNP B4F8P6
A	200	ARG	GLY	engineered mutation	UNP B4F8P6
B	61	HIS	-	expression tag	UNP B4F8P6
B	200	ARG	GLY	engineered mutation	UNP B4F8P6
C	61	HIS	-	expression tag	UNP B4F8P6
C	200	ARG	GLY	engineered mutation	UNP B4F8P6
D	61	HIS	-	expression tag	UNP B4F8P6
D	200	ARG	GLY	engineered mutation	UNP B4F8P6

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$) (labeled as "Ligand of Interest" by depositor).



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

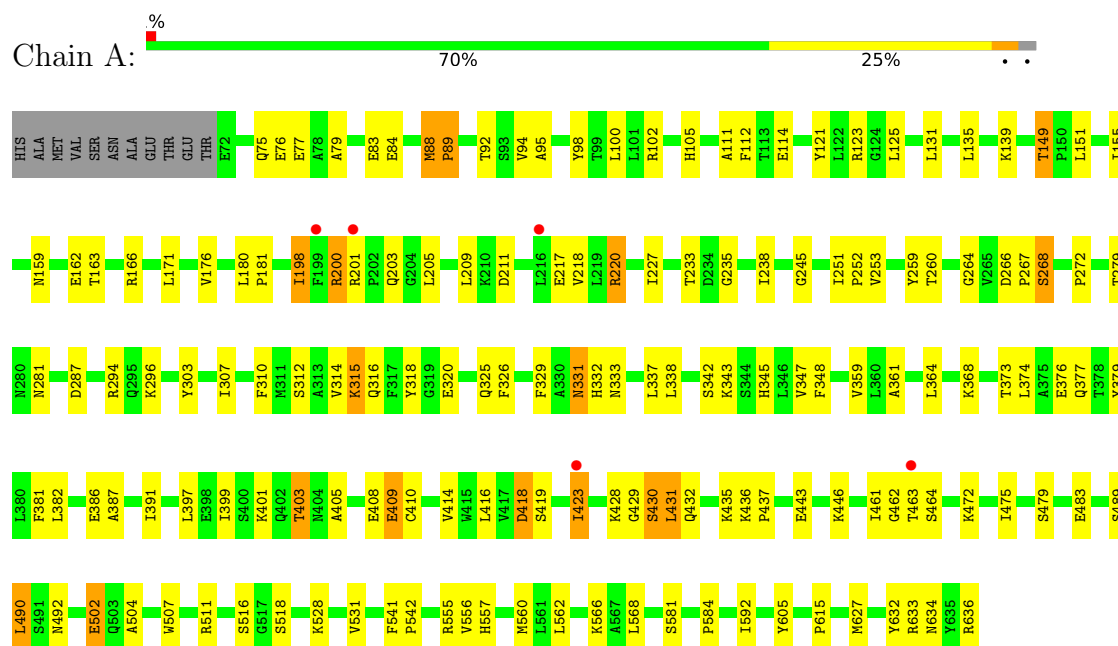
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	4	Total O 4 4	0	0
3	C	7	Total O 7 7	0	0
3	D	10	Total O 10 10	0	0

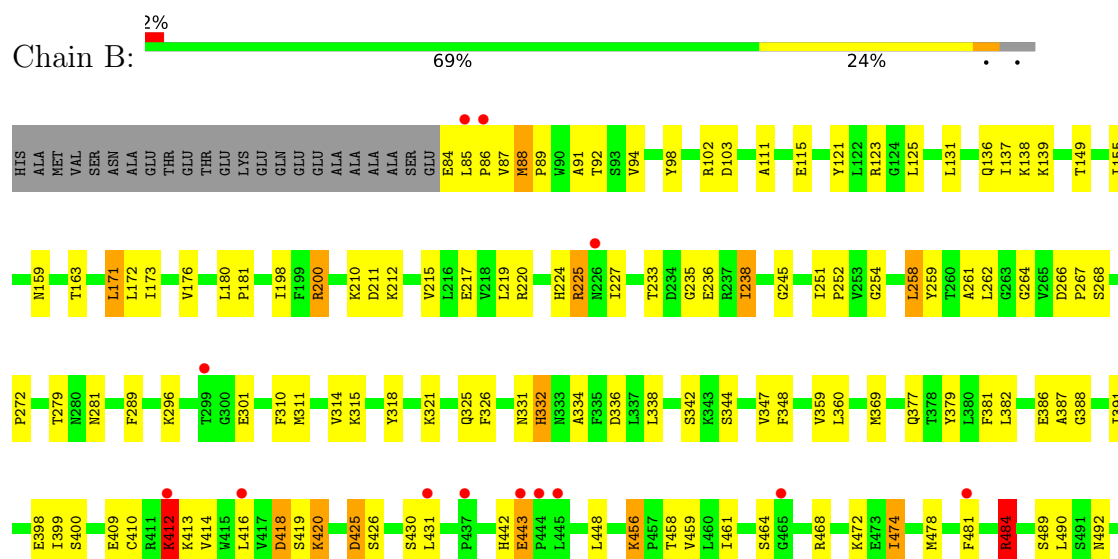
3 Residue-property plots

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: Malic enzyme



• Molecule 1: Malic enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.68Å 124.16Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.70 50.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.01-2.70) 98.7 (50.01-2.70)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.239 , 0.296 0.252 , 0.302	Depositor DCC
R_{free} test set	3227 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17498	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8457e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYR

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	1.13	4/4502 (0.1%)	1.54	11/6105 (0.2%)
1	B	1.12	2/4413 (0.0%)	1.53	13/5986 (0.2%)
1	C	1.12	4/4404 (0.1%)	1.52	10/5974 (0.2%)
1	D	1.14	1/4502 (0.0%)	1.54	9/6105 (0.1%)
All	All	1.13	11/17821 (0.1%)	1.53	43/24170 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	PRO	C-O	-7.48	1.16	1.23
1	C	272	PRO	C-O	-7.29	1.16	1.23
1	A	89	PRO	C-O	-6.98	1.14	1.24
1	D	89	PRO	C-O	-6.78	1.15	1.24
1	B	272	PRO	C-O	-5.86	1.17	1.23
1	A	632	TYR	C-O	5.85	1.30	1.23
1	C	95	ALA	C-O	5.50	1.30	1.24
1	B	89	PRO	C-O	-5.33	1.17	1.24
1	C	203	GLN	C-O	5.20	1.29	1.23
1	A	377	GLN	C-O	5.14	1.30	1.23
1	C	492	ASN	N-CA	5.05	1.50	1.45

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	148	GLN	CB-CA-C	8.64	123.53	109.02
1	A	343	LYS	CB-CA-C	7.25	122.97	110.79
1	C	86	PRO	CA-C-N	7.09	130.49	122.48
1	C	86	PRO	C-N-CA	7.09	130.49	122.48
1	B	236	GLU	CB-CA-C	-6.46	100.06	110.79
1	A	149	THR	CB-CA-C	6.37	118.67	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	GLU	CB-CA-C	6.26	118.27	108.63
1	A	409	GLU	CB-CG-CD	5.97	122.76	112.60
1	C	632	TYR	CA-C-N	5.81	129.52	120.75
1	C	632	TYR	C-N-CA	5.81	129.52	120.75
1	D	103	ASP	CA-C-O	5.67	122.97	119.29
1	D	418	ASP	CA-C-N	5.58	128.02	120.38
1	D	418	ASP	C-N-CA	5.58	128.02	120.38
1	A	114	GLU	CA-C-N	5.54	127.70	120.28
1	A	114	GLU	C-N-CA	5.54	127.70	120.28
1	C	441	GLU	CB-CA-C	5.51	119.23	110.19
1	C	103	ASP	CA-C-O	5.46	122.84	119.29
1	B	418	ASP	CA-C-N	5.43	127.83	120.38
1	B	418	ASP	C-N-CA	5.43	127.83	120.38
1	C	301	GLU	CA-C-O	-5.39	114.84	120.55
1	A	502	GLU	CB-CG-CD	5.37	121.72	112.60
1	B	425	ASP	CA-C-N	5.36	128.20	120.38
1	B	425	ASP	C-N-CA	5.36	128.20	120.38
1	D	468	ARG	CB-CG-CD	5.32	123.54	111.30
1	A	418	ASP	CA-C-N	5.31	127.66	120.38
1	A	418	ASP	C-N-CA	5.31	127.66	120.38
1	B	348	PHE	CA-C-O	-5.30	114.02	120.54
1	D	348	PHE	CA-C-O	-5.30	114.03	120.54
1	B	103	ASP	CA-C-O	5.29	122.73	119.29
1	A	409	GLU	N-CA-C	-5.28	107.00	113.50
1	C	409	GLU	CB-CG-CD	5.26	121.55	112.60
1	D	468	ARG	CB-CA-C	5.24	119.17	111.73
1	B	115	GLU	CB-CG-CD	5.24	121.50	112.60
1	B	149	THR	CB-CA-C	5.22	116.90	108.91
1	D	148	GLN	CB-CG-CD	-5.21	103.73	112.60
1	B	468	ARG	CB-CA-C	5.17	119.07	111.73
1	C	348	PHE	CA-C-O	-5.17	114.18	120.54
1	D	409	GLU	CB-CG-CD	5.15	121.35	112.60
1	A	343	LYS	CA-C-O	-5.14	115.05	120.55
1	B	412	LYS	CA-C-O	-5.08	115.14	120.63
1	A	348	PHE	CA-C-O	-5.08	114.30	120.54
1	B	484	ARG	CG-CD-NE	5.05	123.11	112.00
1	C	87	VAL	N-CA-CB	-5.05	106.59	112.34

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	4405	0	4404	121	0
1	B	4316	0	4328	114	0
1	C	4307	0	4322	117	0
1	D	4405	0	4404	130	0
2	A	12	0	0	0	0
2	B	6	0	0	1	0
2	C	12	0	0	0	0
2	D	6	0	0	0	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
3	C	7	0	0	0	0
3	D	10	0	0	1	0
All	All	17498	0	17458	444	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 13.

All (444) 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:B:377:GLN:OE1	1:B:458:THR:HG21	1.33	1.25
1:A:373:THR:OG1	1:A:376:GLU:OE2	1.63	1.15
1:A:100:LEU:HD11	1:A:112:PHE:CZ	1.83	1.12
1:B:262:LEU:HD12	1:B:589:ILE:HG21	1.46	0.97
1:A:326:PHE:CE1	1:A:347:VAL:HG23	2.03	0.94
1:D:356:ALA:HA	1:D:391:ILE:HD13	1.46	0.94
1:B:409:GLU:O	1:B:412:LYS:HG3	1.68	0.94
1:A:326:PHE:HE1	1:A:347:VAL:HG23	1.32	0.92
1:B:377:GLN:OE1	1:B:458:THR:CG2	2.18	0.90
1:A:211:ASP:OD1	1:B:123:ARG:NH1	2.08	0.85
1:D:98:TYR:HB3	1:D:102:ARG:HH11	1.40	0.84
1:C:425:ASP:HB3	1:C:441:GLU:OE2	1.78	0.84
1:A:100:LEU:HD11	1:A:112:PHE:HZ	1.40	0.82
1:D:356:ALA:CA	1:D:391:ILE:HD13	2.11	0.81
1:C:387:ALA:O	1:C:391:ILE:HG13	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:GLU:OE1	1:D:411:ARG:NH1	2.15	0.80
1:C:311:MET:HE1	1:C:324:ILE:HD13	1.64	0.80
1:C:98:TYR:CE2	1:C:125:LEU:HD12	2.18	0.79
1:B:387:ALA:O	1:B:391:ILE:HG13	1.82	0.78
1:D:280:ASN:OD1	1:D:296:LYS:HG2	1.82	0.78
1:A:205:LEU:HD21	1:A:218:VAL:HG12	1.64	0.78
1:D:157:MET:HE1	1:D:171:LEU:CD2	2.13	0.77
1:C:453:GLN:OE1	1:C:481:PHE:HZ	1.68	0.77
1:C:635:TYR:O	1:C:636:ARG:HG3	1.83	0.77
1:C:110:LEU:HD12	1:D:200:ARG:CZ	2.16	0.76
1:D:72:GLU:HB3	1:D:75:GLN:HE22	1.50	0.75
1:A:387:ALA:O	1:A:391:ILE:HG13	1.86	0.75
1:B:484:ARG:HG2	1:B:484:ARG:HH11	1.50	0.75
1:B:334:ALA:CB	1:B:386:GLU:OE2	2.34	0.75
1:C:161:GLN:OE1	1:C:203:GLN:NE2	2.19	0.75
1:B:259:TYR:OH	1:B:325:GLN:OE1	2.04	0.75
1:C:110:LEU:CD1	1:D:200:ARG:CZ	2.65	0.75
1:A:259:TYR:OH	1:A:325:GLN:OE1	2.04	0.74
1:C:259:TYR:OH	1:C:325:GLN:OE1	2.03	0.74
1:A:636:ARG:CZ	1:C:217:GLU:HG2	2.19	0.73
1:D:387:ALA:O	1:D:391:ILE:HG12	1.89	0.72
1:A:479:SER:O	1:A:511:ARG:NH2	2.23	0.72
1:B:251:ILE:HB	1:B:252:PRO:HD3	1.72	0.72
1:D:98:TYR:HB3	1:D:102:ARG:NH1	2.04	0.72
1:B:456:LYS:HE3	1:B:481:PHE:CG	2.25	0.71
1:D:157:MET:HE1	1:D:171:LEU:HD21	1.70	0.71
1:A:636:ARG:NH2	1:C:217:GLU:HG2	2.05	0.71
1:B:456:LYS:CE	1:B:481:PHE:CD2	2.73	0.71
1:A:556:VAL:HA	1:A:560:MET:HE3	1.72	0.71
1:B:225:ARG:H	1:B:225:ARG:HD3	1.56	0.70
1:C:584:PRO:HG2	1:C:592:ILE:HD11	1.73	0.70
1:D:397:LEU:CD1	1:D:562:LEU:HD11	2.20	0.70
1:A:251:ILE:HB	1:A:252:PRO:HD3	1.73	0.70
1:B:235:GLY:HA2	1:B:238:ILE:CD1	2.22	0.70
1:D:251:ILE:HB	1:D:252:PRO:HD3	1.72	0.70
1:B:359:VAL:HG11	1:B:391:ILE:HG21	1.73	0.69
1:D:259:TYR:OH	1:D:325:GLN:OE1	2.05	0.69
1:D:338:LEU:O	1:D:342:SER:OG	2.10	0.69
1:C:139:LYS:CE	1:D:196:GLY:O	2.40	0.69
1:D:343:LYS:O	1:D:555:ARG:NH1	2.25	0.69
1:B:155:ILE:HD11	1:B:198:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:ARG:O	1:D:431:LEU:HD23	1.93	0.69
1:C:251:ILE:HB	1:C:252:PRO:HD3	1.73	0.69
1:A:359:VAL:HG11	1:A:391:ILE:HG21	1.74	0.69
1:A:531:VAL:O	1:A:581:SER:OG	2.11	0.69
1:D:556:VAL:HA	1:D:560:MET:HE3	1.74	0.69
1:B:492:ASN:HD22	2:B:701:PYR:CB	2.06	0.68
1:A:338:LEU:O	1:A:342:SER:OG	2.09	0.68
1:B:531:VAL:O	1:B:581:SER:OG	2.12	0.68
1:D:287:ASP:O	1:D:294:ARG:NH2	2.26	0.68
1:C:359:VAL:HG11	1:C:391:ILE:HG21	1.74	0.67
1:B:173:ILE:HD11	1:B:261:ALA:HA	1.75	0.67
1:B:381:PHE:HB2	1:B:416:LEU:HG	1.77	0.67
1:C:470:PHE:HB3	1:C:475:ILE:HD11	1.76	0.67
1:C:155:ILE:HD11	1:C:198:ILE:HD12	1.76	0.67
1:D:359:VAL:HG21	1:D:391:ILE:HD12	1.77	0.67
1:D:72:GLU:HB3	1:D:75:GLN:NE2	2.10	0.66
1:B:338:LEU:O	1:B:342:SER:OG	2.09	0.66
1:C:232:VAL:CG2	1:C:275:ILE:CD1	2.74	0.66
1:A:397:LEU:HD23	1:A:562:LEU:HD11	1.77	0.66
1:A:403:THR:CG2	1:A:405:ALA:H	2.08	0.65
1:B:137:ILE:HD12	1:B:171:LEU:HA	1.77	0.65
1:A:326:PHE:CE2	1:A:337:LEU:HD13	2.31	0.65
1:B:217:GLU:HG3	1:D:636:ARG:CZ	2.26	0.65
1:A:94:VAL:HG11	1:D:121:TYR:CE2	2.32	0.65
1:B:261:ALA:O	1:B:590:ARG:NH1	2.30	0.64
1:A:326:PHE:CE1	1:A:347:VAL:CG2	2.80	0.64
1:D:531:VAL:O	1:D:581:SER:OG	2.12	0.64
1:A:266:ASP:OD2	1:A:268:SER:OG	2.16	0.64
1:B:266:ASP:OD1	1:B:267:PRO:HD2	1.98	0.64
1:C:98:TYR:CZ	1:C:125:LEU:HD12	2.33	0.63
1:B:334:ALA:HB3	1:B:386:GLU:OE2	1.98	0.63
1:A:105:HIS:O	1:A:166:ARG:NH1	2.31	0.63
1:D:355:THR:HG22	1:D:391:ILE:HD11	1.80	0.63
1:C:159:ASN:O	1:C:163:THR:HG23	1.99	0.63
1:A:100:LEU:CD1	1:A:112:PHE:CZ	2.73	0.63
1:A:287:ASP:O	1:A:294:ARG:NH2	2.27	0.63
1:D:159:ASN:O	1:D:163:THR:HG23	1.98	0.63
1:C:338:LEU:O	1:C:342:SER:OG	2.09	0.62
1:D:88:MET:CE	1:D:220:ARG:HD3	2.28	0.62
1:A:364:LEU:O	1:A:368:LYS:HG3	2.00	0.62
1:D:266:ASP:OD2	1:D:268:SER:OG	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:MET:HE2	1:D:220:ARG:HD3	1.82	0.62
1:B:409:GLU:O	1:B:412:LYS:CG	2.46	0.62
1:A:200:ARG:HH22	1:B:136:GLN:HG2	1.65	0.62
1:A:431:LEU:HD22	1:A:435:LYS:HB2	1.82	0.62
1:C:261:ALA:O	1:C:590:ARG:NH1	2.34	0.61
1:D:326:PHE:CE2	1:D:337:LEU:HD13	2.35	0.61
1:B:484:ARG:HH11	1:B:484:ARG:CG	2.13	0.61
1:A:159:ASN:O	1:A:163:THR:HG23	2.01	0.61
1:C:176:VAL:O	1:C:180:LEU:HB2	2.01	0.61
1:A:584:PRO:HG2	1:A:592:ILE:HD11	1.82	0.61
1:B:159:ASN:O	1:B:163:THR:HG23	2.00	0.61
1:D:555:ARG:O	1:D:560:MET:HE1	2.00	0.61
1:C:416:LEU:O	1:C:423:ILE:HD12	2.01	0.60
1:A:121:TYR:CE2	1:D:94:VAL:HG11	2.36	0.60
1:A:217:GLU:O	1:A:220:ARG:HG2	2.01	0.60
1:C:110:LEU:HD12	1:D:200:ARG:NH1	2.16	0.60
1:C:379:TYR:CD2	1:C:414:VAL:HG22	2.37	0.60
1:C:281:ASN:OD1	1:C:283:LYS:HG3	2.02	0.60
1:D:584:PRO:HG2	1:D:592:ILE:HD11	1.83	0.59
1:A:203:GLN:OE1	1:A:253:VAL:HG11	2.02	0.59
1:B:258:LEU:HB3	1:B:262:LEU:HD23	1.84	0.59
1:C:338:LEU:HD23	1:C:347:VAL:HG23	1.85	0.59
1:B:258:LEU:CB	1:B:262:LEU:HD23	2.33	0.59
1:B:505:TYR:CD2	1:B:530:PHE:CD2	2.91	0.59
1:B:456:LYS:HE2	1:B:481:PHE:CD2	2.37	0.58
1:A:176:VAL:O	1:A:180:LEU:HB2	2.03	0.58
1:D:281:ASN:HD21	1:D:283:LYS:HB2	1.67	0.58
1:C:389:THR:HG21	1:C:434:PHE:HD1	1.67	0.58
1:D:194:LYS:O	1:D:198:ILE:HG12	2.04	0.58
1:B:225:ARG:H	1:B:225:ARG:HH11	1.51	0.58
1:B:360:LEU:HD11	1:B:398:GLU:HB2	1.86	0.58
1:D:359:VAL:HG11	1:D:391:ILE:HG21	1.85	0.58
1:A:557:HIS:H	1:A:560:MET:HE3	1.68	0.58
1:B:176:VAL:O	1:B:180:LEU:HB2	2.04	0.57
1:A:475:ILE:HD13	1:A:504:ALA:HA	1.86	0.57
1:B:418:ASP:OD1	1:B:420:LYS:HG2	2.02	0.57
1:A:364:LEU:HD12	1:A:374:LEU:HD21	1.86	0.57
1:D:88:MET:HE3	1:D:220:ARG:CD	2.35	0.57
1:A:200:ARG:NH2	1:B:136:GLN:HG2	2.20	0.57
1:A:403:THR:HG23	1:A:405:ALA:H	1.69	0.57
1:C:425:ASP:CB	1:C:441:GLU:OE2	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:THR:HG22	1:B:252:PRO:CG	2.34	0.57
1:B:200:ARG:O	1:B:200:ARG:HG2	2.04	0.57
1:D:233:THR:HG22	1:D:252:PRO:CG	2.35	0.56
1:D:356:ALA:N	1:D:391:ILE:HD13	2.20	0.56
1:D:489:SER:O	1:D:516:SER:HA	2.06	0.56
1:C:233:THR:HG22	1:C:252:PRO:CG	2.36	0.56
1:B:235:GLY:HA2	1:B:238:ILE:HD11	1.87	0.56
1:C:139:LYS:HE3	1:D:196:GLY:O	2.05	0.56
1:A:374:LEU:N	1:A:374:LEU:HD22	2.21	0.56
1:A:131:LEU:HD22	1:A:135:LEU:HB3	1.87	0.56
1:C:590:ARG:NH2	1:C:628:TYR:O	2.39	0.56
1:D:374:LEU:N	1:D:374:LEU:HD22	2.20	0.56
1:D:88:MET:HE3	1:D:220:ARG:HD2	1.86	0.56
1:D:176:VAL:O	1:D:180:LEU:HB2	2.06	0.55
1:B:94:VAL:HG11	1:C:121:TYR:CD2	2.40	0.55
1:C:98:TYR:CE2	1:C:125:LEU:CD1	2.88	0.55
1:C:125:LEU:N	1:C:125:LEU:HD22	2.22	0.55
1:D:137:ILE:HD12	1:D:171:LEU:HA	1.88	0.55
1:A:83:GLU:CD	1:A:84:GLU:HG2	2.30	0.55
1:C:399:ILE:HG22	1:C:410:CYS:SG	2.47	0.55
1:D:180:LEU:N	1:D:181:PRO:CD	2.70	0.55
1:B:310:PHE:O	1:B:314:VAL:HG23	2.07	0.55
1:C:180:LEU:N	1:C:181:PRO:CD	2.69	0.55
1:A:98:TYR:CE2	1:A:125:LEU:HD22	2.42	0.55
1:D:310:PHE:O	1:D:314:VAL:HG23	2.08	0.54
1:B:489:SER:O	1:B:516:SER:HA	2.07	0.54
1:C:136:GLN:HG2	1:D:200:ARG:HH22	1.72	0.54
1:D:281:ASN:C	1:D:281:ASN:HD22	2.15	0.54
1:A:310:PHE:O	1:A:314:VAL:HG23	2.06	0.54
1:B:412:LYS:HD2	1:B:413:LYS:HG2	1.90	0.54
1:B:87:VAL:HG12	1:D:634:ASN:O	2.07	0.54
1:C:111:ALA:HA	1:C:131:LEU:O	2.08	0.54
1:C:139:LYS:HE2	1:D:196:GLY:O	2.07	0.54
1:D:239:LEU:N	1:D:239:LEU:HD23	2.22	0.54
1:A:436:LYS:N	1:A:437:PRO:HD2	2.23	0.54
1:A:303:TYR:CZ	1:A:333:ASN:ND2	2.76	0.54
1:D:393:GLU:CD	1:D:411:ARG:HH12	2.16	0.54
1:B:180:LEU:HD11	1:B:258:LEU:HD21	1.88	0.54
1:A:489:SER:O	1:A:516:SER:HA	2.08	0.53
1:B:111:ALA:HA	1:B:131:LEU:O	2.07	0.53
1:A:180:LEU:N	1:A:181:PRO:CD	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:THR:HG22	1:A:252:PRO:CG	2.38	0.53
1:B:180:LEU:N	1:B:181:PRO:CD	2.71	0.53
1:C:489:SER:O	1:C:516:SER:HA	2.07	0.53
1:C:136:GLN:HG2	1:D:200:ARG:NH2	2.23	0.53
1:D:399:ILE:HG22	1:D:410:CYS:SG	2.49	0.53
1:A:111:ALA:HA	1:A:131:LEU:O	2.08	0.53
1:B:311:MET:HE2	1:B:326:PHE:HZ	1.74	0.53
1:D:556:VAL:HA	1:D:560:MET:CE	2.37	0.53
1:A:401:LYS:HD2	1:A:562:LEU:HD13	1.91	0.53
1:A:403:THR:HG22	1:A:405:ALA:H	1.74	0.53
1:B:173:ILE:CD1	1:B:261:ALA:O	2.57	0.52
1:D:111:ALA:HA	1:D:131:LEU:O	2.09	0.52
1:A:329:PHE:O	1:A:386:GLU:OE1	2.27	0.52
1:D:88:MET:CE	1:D:220:ARG:CD	2.87	0.52
1:A:151:LEU:O	1:A:155:ILE:HG12	2.10	0.52
1:C:359:VAL:HG11	1:C:391:ILE:CG2	2.40	0.52
1:D:472:LYS:HG3	1:D:507:TRP:CD1	2.45	0.52
1:D:359:VAL:HG11	1:D:391:ILE:CG2	2.40	0.52
1:B:98:TYR:CE2	1:B:125:LEU:HD22	2.44	0.52
1:C:359:VAL:CG2	1:C:490:LEU:HD11	2.39	0.52
1:C:453:GLN:OE1	1:C:481:PHE:CZ	2.55	0.52
1:D:131:LEU:HD22	1:D:135:LEU:HB3	1.91	0.52
1:D:557:HIS:HD2	1:D:559:ASP:H	1.56	0.52
1:D:125:LEU:HD12	1:D:125:LEU:N	2.24	0.52
1:A:382:LEU:HG	1:A:464:SER:HB3	1.92	0.51
1:B:399:ILE:HG22	1:B:410:CYS:SG	2.50	0.51
1:D:233:THR:HG22	1:D:252:PRO:HG2	1.91	0.51
1:C:104:PRO:HG2	1:D:102:ARG:HH21	1.74	0.51
1:D:382:LEU:HG	1:D:464:SER:HB3	1.92	0.51
1:A:95:ALA:HB2	1:C:91:ALA:HB2	1.92	0.51
1:C:329:PHE:O	1:C:386:GLU:OE1	2.29	0.51
1:B:121:TYR:CD2	1:C:94:VAL:HG11	2.46	0.51
1:B:359:VAL:CG2	1:B:490:LEU:HD11	2.41	0.51
1:D:364:LEU:O	1:D:368:LYS:HG2	2.11	0.51
1:A:266:ASP:OD1	1:A:267:PRO:HD2	2.11	0.51
1:C:367:LEU:HD12	1:C:374:LEU:CD2	2.42	0.51
1:C:446:LYS:NZ	1:C:450:ASP:OD2	2.41	0.50
1:A:139:LYS:HE3	1:B:200:ARG:HH21	1.74	0.50
1:B:456:LYS:CE	1:B:481:PHE:CG	2.92	0.50
1:C:281:ASN:HD21	1:C:283:LYS:HE3	1.75	0.50
1:C:310:PHE:O	1:C:314:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLU:OE1	1:A:345:HIS:HA	2.10	0.50
1:D:359:VAL:CG2	1:D:391:ILE:HD12	2.41	0.50
1:C:197:SER:HA	1:D:139:LYS:HD2	1.92	0.50
1:D:266:ASP:OD1	1:D:267:PRO:HD2	2.11	0.50
1:C:201:ARG:HH21	1:D:163:THR:HG22	1.76	0.50
1:C:205:LEU:HD12	1:C:271:LEU:HD11	1.94	0.50
1:A:399:ILE:HG22	1:A:410:CYS:SG	2.52	0.50
1:D:492:ASN:OD1	1:D:518:SER:OG	2.21	0.50
1:D:374:LEU:HD22	1:D:374:LEU:H	1.77	0.50
1:A:98:TYR:O	1:A:102:ARG:HG3	2.12	0.49
1:D:360:LEU:O	1:D:364:LEU:HD23	2.11	0.49
1:B:501:ALA:O	1:B:505:TYR:HD1	1.94	0.49
1:A:462:GLY:O	1:A:490:LEU:HB2	2.12	0.49
1:B:412:LYS:HD3	1:B:413:LYS:HD2	1.95	0.49
1:C:424:VAL:HG11	1:C:442:HIS:O	2.12	0.49
1:D:381:PHE:HB2	1:D:416:LEU:HG	1.94	0.49
1:A:359:VAL:HG11	1:A:391:ILE:CG2	2.41	0.49
1:A:364:LEU:CD1	1:A:374:LEU:HD21	2.42	0.49
1:B:359:VAL:HG11	1:B:391:ILE:CG2	2.42	0.49
1:A:162:GLU:CG	1:A:203:GLN:HE21	2.25	0.49
1:A:403:THR:HG23	1:A:405:ALA:N	2.27	0.49
1:D:605:TYR:CE2	1:D:615:PRO:HB3	2.47	0.49
1:B:382:LEU:HG	1:B:464:SER:HB3	1.94	0.49
1:D:544:LEU:O	1:D:548:LEU:HG	2.12	0.49
1:C:281:ASN:OD1	1:C:283:LYS:CG	2.61	0.49
1:A:303:TYR:CE1	1:A:333:ASN:ND2	2.81	0.48
1:A:379:TYR:CD1	1:A:414:VAL:HG22	2.47	0.48
1:B:225:ARG:HD3	1:B:225:ARG:N	2.26	0.48
1:B:233:THR:HG22	1:B:252:PRO:HG2	1.95	0.48
1:B:605:TYR:CE2	1:B:615:PRO:HB3	2.48	0.48
1:D:157:MET:CE	1:D:171:LEU:CD2	2.88	0.48
1:A:123:ARG:NH1	1:B:211:ASP:OD1	2.44	0.48
1:D:461:ILE:HG23	1:D:490:LEU:HD23	1.95	0.48
1:B:484:ARG:HG2	1:B:484:ARG:NH1	2.25	0.48
1:A:555:ARG:O	1:A:560:MET:HE1	2.14	0.48
1:B:225:ARG:H	1:B:225:ARG:CD	2.23	0.48
1:C:462:GLY:O	1:C:490:LEU:HB2	2.14	0.48
1:D:227:ILE:HB	1:D:318:TYR:CD1	2.48	0.48
1:B:94:VAL:HG11	1:C:121:TYR:CE2	2.48	0.48
1:B:635:TYR:O	1:B:636:ARG:NE	2.46	0.48
1:D:137:ILE:HD12	1:D:171:LEU:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:PHE:HB2	1:C:416:LEU:HG	1.96	0.48
1:B:155:ILE:CD1	1:B:198:ILE:HG23	2.44	0.47
1:C:137:ILE:HD11	1:C:170:LYS:HD2	1.96	0.47
1:A:235:GLY:HA2	1:A:238:ILE:HD11	1.96	0.47
1:A:374:LEU:HD22	1:A:374:LEU:H	1.78	0.47
1:D:475:ILE:HD13	1:D:504:ALA:HA	1.96	0.47
1:D:488:PHE:HB3	1:D:490:LEU:HD21	1.96	0.47
1:B:607:LEU:HB3	1:B:609:LEU:CD2	2.44	0.47
1:C:447:THR:HG23	1:C:450:ASP:H	1.79	0.47
1:D:528:LYS:HD3	1:D:529:THR:H	1.79	0.47
1:A:264:GLY:HA3	1:A:627:MET:HG2	1.97	0.47
1:C:251:ILE:HB	1:C:252:PRO:CD	2.44	0.47
1:C:311:MET:HE2	1:C:311:MET:HA	1.95	0.47
1:D:342:SER:O	1:D:555:ARG:HD2	2.14	0.47
1:A:381:PHE:HB2	1:A:416:LEU:HG	1.95	0.47
1:B:264:GLY:HA3	1:B:627:MET:HG2	1.96	0.47
1:C:233:THR:HG22	1:C:252:PRO:HG2	1.97	0.47
1:D:157:MET:HG2	1:D:183:VAL:CG1	2.45	0.47
1:A:75:GLN:OE1	1:A:77:GLU:OE2	2.32	0.47
1:A:326:PHE:HE1	1:A:347:VAL:CG2	2.14	0.47
1:C:235:GLY:HA2	1:C:238:ILE:HD11	1.97	0.47
1:A:403:THR:HG23	1:A:405:ALA:CB	2.45	0.46
1:C:264:GLY:HA3	1:C:627:MET:HG2	1.95	0.46
1:C:382:LEU:HG	1:C:464:SER:HB3	1.97	0.46
1:C:605:TYR:CE2	1:C:615:PRO:HB3	2.50	0.46
1:A:401:LYS:HD2	1:A:562:LEU:CD1	2.45	0.46
1:A:227:ILE:HB	1:A:318:TYR:CD1	2.51	0.46
1:D:397:LEU:HD13	1:D:562:LEU:HD11	1.97	0.46
1:A:634:ASN:O	1:C:86:PRO:HA	2.16	0.46
1:B:251:ILE:HB	1:B:252:PRO:CD	2.44	0.46
1:C:320:GLU:OE2	1:C:554:VAL:HB	2.14	0.46
1:D:155:ILE:HD11	1:D:198:ILE:HD12	1.98	0.46
1:D:528:LYS:HA	1:D:528:LYS:HE2	1.96	0.46
1:B:245:GLY:HA3	1:B:279:THR:HB	1.97	0.46
1:D:205:LEU:HD21	1:D:218:VAL:HG12	1.97	0.46
1:A:245:GLY:HA3	1:A:279:THR:HB	1.98	0.46
1:D:264:GLY:HA3	1:D:627:MET:HG2	1.98	0.46
1:D:397:LEU:HD12	1:D:562:LEU:HD11	1.95	0.46
1:B:91:ALA:HB2	1:D:95:ALA:HB2	1.98	0.46
1:D:541:PHE:CD1	1:D:542:PRO:HD3	2.50	0.46
1:D:101:LEU:HD13	1:D:122:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASN:O	1:D:332:HIS:C	2.59	0.46
1:A:428:LYS:HA	1:A:431:LEU:HB2	1.98	0.45
1:B:86:PRO:O	1:B:220:ARG:CZ	2.64	0.45
1:C:360:LEU:HD23	1:C:360:LEU:O	2.16	0.45
1:D:235:GLY:HA2	1:D:238:ILE:HD11	1.97	0.45
1:D:245:GLY:HA3	1:D:279:THR:HB	1.98	0.45
1:D:619:LEU:HD12	1:D:619:LEU:HA	1.80	0.45
1:A:200:ARG:HH21	1:B:139:LYS:HZ2	1.64	0.45
1:B:254:GLY:O	1:B:258:LEU:HD12	2.17	0.45
1:C:219:LEU:HD22	1:C:318:TYR:CE2	2.52	0.45
1:C:331:ASN:O	1:C:332:HIS:C	2.60	0.45
1:B:262:LEU:CD1	1:B:589:ILE:HG21	2.33	0.45
1:C:381:PHE:HA	1:C:461:ILE:O	2.16	0.45
1:A:374:LEU:H	1:A:374:LEU:CD2	2.30	0.45
1:C:359:VAL:HG22	1:C:490:LEU:HD11	1.98	0.45
1:D:379:TYR:CD1	1:D:414:VAL:HG22	2.52	0.45
1:D:381:PHE:HA	1:D:461:ILE:O	2.17	0.45
1:D:387:ALA:O	1:D:391:ILE:CG1	2.63	0.45
1:A:162:GLU:HG2	1:A:203:GLN:NE2	2.32	0.45
1:A:326:PHE:HE2	1:A:337:LEU:HD13	1.79	0.45
1:A:605:TYR:CE2	1:A:615:PRO:HB3	2.51	0.45
1:C:227:ILE:HB	1:C:318:TYR:CD1	2.51	0.45
1:A:251:ILE:HB	1:A:252:PRO:CD	2.45	0.45
1:A:139:LYS:CE	1:B:200:ARG:HH21	2.30	0.44
1:A:429:GLY:O	1:A:430:SER:OG	2.28	0.44
1:B:381:PHE:HA	1:B:461:ILE:O	2.17	0.44
1:A:423:ILE:CD1	1:A:435:LYS:HD3	2.46	0.44
1:C:360:LEU:HD11	1:C:398:GLU:HB2	1.99	0.44
1:D:106:HIS:HD2	1:D:635:TYR:OH	2.00	0.44
1:A:381:PHE:HA	1:A:461:ILE:O	2.17	0.44
1:B:492:ASN:OD1	1:B:518:SER:OG	2.22	0.44
1:C:201:ARG:HE	1:D:163:THR:HG21	1.81	0.44
1:C:418:ASP:OD1	1:C:418:ASP:C	2.60	0.44
1:C:471:THR:O	1:C:475:ILE:HD13	2.18	0.44
1:C:475:ILE:N	1:C:475:ILE:CD1	2.81	0.44
1:C:541:PHE:CD1	1:C:542:PRO:HD3	2.52	0.44
1:A:162:GLU:CG	1:A:203:GLN:NE2	2.81	0.44
1:A:331:ASN:O	1:A:332:HIS:C	2.61	0.44
1:B:331:ASN:O	1:B:332:HIS:C	2.61	0.44
1:C:245:GLY:HA3	1:C:279:THR:HB	2.00	0.44
1:C:266:ASP:OD1	1:C:267:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:SER:OG	3:D:801:HOH:O	2.20	0.44
1:B:458:THR:HG22	1:B:459:VAL:HG23	2.00	0.44
1:B:478:MET:HE3	1:B:478:MET:HB3	1.89	0.44
1:C:279:THR:O	1:C:296:LYS:HA	2.18	0.44
1:C:425:ASP:C	1:C:425:ASP:OD1	2.60	0.44
1:D:260:THR:HG21	1:D:267:PRO:HG3	2.00	0.44
1:C:232:VAL:HG23	1:C:275:ILE:CD1	2.46	0.43
1:A:541:PHE:CD1	1:A:542:PRO:HD3	2.53	0.43
1:A:220:ARG:HH22	1:C:636:ARG:HB3	1.83	0.43
1:A:233:THR:HG22	1:A:252:PRO:HG2	1.99	0.43
1:A:361:ALA:CB	1:A:568:LEU:HD23	2.49	0.43
1:A:403:THR:CG2	1:A:405:ALA:CB	2.96	0.43
1:A:557:HIS:H	1:A:560:MET:CE	2.31	0.43
1:C:214:LYS:O	1:C:217:GLU:HB2	2.19	0.43
1:A:492:ASN:OD1	1:A:518:SER:OG	2.24	0.43
1:B:359:VAL:HG21	1:B:490:LEU:HD11	1.99	0.43
1:B:505:TYR:CD2	1:B:530:PHE:HD2	2.36	0.43
1:D:541:PHE:CG	1:D:542:PRO:HD3	2.53	0.43
1:C:232:VAL:HG21	1:C:275:ILE:CD1	2.48	0.43
1:C:541:PHE:CG	1:C:542:PRO:HD3	2.53	0.43
1:B:224:HIS:HA	1:B:225:ARG:HH11	1.84	0.43
1:C:311:MET:HE1	1:C:324:ILE:HG21	1.99	0.43
1:A:88:MET:HE3	1:A:88:MET:HA	1.99	0.43
1:A:139:LYS:CE	1:B:200:ARG:NH2	2.82	0.43
1:C:125:LEU:N	1:C:125:LEU:CD2	2.81	0.43
1:D:76:GLU:HG3	1:D:79:ALA:HB3	2.00	0.43
1:A:89:PRO:HD3	1:C:635:TYR:CD1	2.54	0.43
1:B:258:LEU:HD23	1:B:262:LEU:CD2	2.49	0.43
1:B:338:LEU:HD23	1:B:347:VAL:HG23	2.00	0.43
1:B:472:LYS:HG3	1:B:507:TRP:CD1	2.54	0.43
1:A:418:ASP:OD1	1:A:418:ASP:C	2.62	0.43
1:A:541:PHE:CG	1:A:542:PRO:HD3	2.53	0.43
1:D:425:ASP:OD1	1:D:425:ASP:C	2.62	0.43
1:C:472:LYS:HA	1:C:507:TRP:CE3	2.54	0.42
1:B:227:ILE:HB	1:B:318:TYR:CD1	2.55	0.42
1:C:260:THR:HG21	1:C:267:PRO:HG3	2.00	0.42
1:A:139:LYS:HB2	1:B:289:PHE:CE1	2.54	0.42
1:A:260:THR:HG21	1:A:267:PRO:HG3	2.01	0.42
1:B:541:PHE:CD1	1:B:542:PRO:HD3	2.54	0.42
1:C:367:LEU:CD1	1:C:374:LEU:HD22	2.49	0.42
1:D:343:LYS:HA	1:D:555:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:478:MET:HE3	1:D:478:MET:HB3	1.92	0.42
1:A:162:GLU:HG3	1:A:203:GLN:HE21	1.84	0.42
1:B:84:GLU:OE2	1:B:85:LEU:HD12	2.20	0.42
1:B:219:LEU:HD12	1:B:318:TYR:CE2	2.55	0.42
1:B:279:THR:O	1:B:296:LYS:HA	2.18	0.42
1:D:453:GLN:OE1	1:D:477:ALA:HB1	2.19	0.42
1:A:155:ILE:HD12	1:A:198:ILE:HG23	2.01	0.42
1:B:215:VAL:O	1:B:219:LEU:HD23	2.19	0.42
1:B:262:LEU:HD12	1:B:589:ILE:CG2	2.34	0.42
1:B:541:PHE:CG	1:B:542:PRO:HD3	2.54	0.42
1:C:428:LYS:HA	1:C:431:LEU:HB2	2.02	0.42
1:D:621:LYS:HE3	1:D:621:LYS:HB2	1.95	0.42
1:A:279:THR:O	1:A:296:LYS:HA	2.19	0.42
1:C:389:THR:HG21	1:C:434:PHE:CD1	2.52	0.42
1:D:251:ILE:HB	1:D:252:PRO:CD	2.45	0.42
1:A:403:THR:HG23	1:A:405:ALA:HB2	2.01	0.42
1:B:448:LEU:HD23	1:B:474:ILE:HD12	2.01	0.42
1:C:635:TYR:C	1:C:636:ARG:HG3	2.45	0.42
1:D:133:GLN:O	1:D:137:ILE:HG12	2.20	0.42
1:B:360:LEU:C	1:B:360:LEU:HD23	2.45	0.41
1:A:76:GLU:HG3	1:A:79:ALA:HB3	2.01	0.41
1:A:315:LYS:HG2	1:A:316:GLN:N	2.34	0.41
1:B:379:TYR:CD1	1:B:414:VAL:HG22	2.56	0.41
1:D:161:GLN:NE2	1:D:203:GLN:NE2	2.68	0.41
1:D:157:MET:HE1	1:D:171:LEU:HD23	1.99	0.41
1:D:263:GLY:O	1:D:627:MET:HE2	2.20	0.41
1:B:200:ARG:H	1:B:200:ARG:HD3	1.84	0.41
1:C:96:SER:HB3	1:C:120:HIS:O	2.20	0.41
1:C:331:ASN:OD1	1:C:386:GLU:HG3	2.21	0.41
1:D:83:GLU:HG2	1:D:84:GLU:N	2.36	0.41
1:C:259:TYR:HE1	1:C:545:GLY:HA3	1.86	0.41
1:C:619:LEU:HD23	1:C:619:LEU:HA	1.93	0.41
1:D:374:LEU:H	1:D:374:LEU:CD2	2.32	0.41
1:B:590:ARG:HG3	1:B:590:ARG:HH11	1.86	0.41
1:C:113:THR:O	1:C:117:ARG:HG3	2.21	0.41
1:A:139:LYS:HE3	1:B:200:ARG:NH2	2.36	0.41
1:A:326:PHE:CD1	1:A:347:VAL:HG23	2.53	0.41
1:A:472:LYS:HG3	1:A:507:TRP:CD1	2.56	0.41
1:D:418:ASP:C	1:D:418:ASP:OD1	2.63	0.41
1:B:84:GLU:CD	1:B:85:LEU:HD12	2.46	0.41
1:B:574:GLN:HA	1:B:577:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HD22	1:C:318:TYR:HE2	1.86	0.41
1:C:275:ILE:N	1:C:275:ILE:HD12	2.35	0.41
1:C:360:LEU:HD23	1:C:360:LEU:C	2.46	0.41
1:C:541:PHE:N	1:C:542:PRO:CD	2.84	0.41
1:D:214:LYS:O	1:D:217:GLU:HB2	2.20	0.41
1:C:232:VAL:CG2	1:C:275:ILE:HD13	2.48	0.41
1:D:461:ILE:HG23	1:D:490:LEU:CD2	2.50	0.41
1:B:88:MET:HE3	1:B:88:MET:HB2	1.83	0.40
1:B:360:LEU:HD23	1:B:360:LEU:O	2.21	0.40
1:C:359:VAL:HG21	1:C:391:ILE:HD13	2.03	0.40
1:A:303:TYR:CE1	1:A:307:ILE:HG13	2.56	0.40
1:A:636:ARG:HG3	1:C:88:MET:HE3	2.03	0.40
1:B:369:MET:HE3	1:B:577:PHE:HA	2.03	0.40
1:C:148:GLN:HG3	1:D:148:GLN:HG2	2.04	0.40
1:A:431:LEU:HD23	1:A:432:GLN:H	1.86	0.40
1:B:541:PHE:N	1:B:542:PRO:CD	2.84	0.40
1:D:200:ARG:HD3	1:D:200:ARG:H	1.86	0.40
1:D:239:LEU:N	1:D:239:LEU:CD2	2.84	0.40
1:D:239:LEU:HD23	1:D:239:LEU:H	1.85	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	563/576 (98%)	530 (94%)	30 (5%)	3 (0%)	24 48
1	B	551/576 (96%)	519 (94%)	28 (5%)	4 (1%)	18 41
1	C	550/576 (96%)	523 (95%)	26 (5%)	1 (0%)	43 68
1	D	563/576 (98%)	532 (94%)	30 (5%)	1 (0%)	43 68
All	All	2227/2304 (97%)	2104 (94%)	114 (5%)	9 (0%)	30 54

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	A	430	SER
1	B	281	ASN
1	B	301	GLU
1	C	281	ASN
1	D	281	ASN
1	A	331	ASN
1	B	430	SER
1	B	388	GLY

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	472/481 (98%)	445 (94%)	27 (6%)	18	43
1	B	464/481 (96%)	423 (91%)	41 (9%)	9	23
1	C	463/481 (96%)	420 (91%)	43 (9%)	8	21
1	D	472/481 (98%)	439 (93%)	33 (7%)	14	34
All	All	1871/1924 (97%)	1727 (92%)	144 (8%)	12	30

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	MET
1	A	92	THR
1	A	149	THR
1	A	171	LEU
1	A	198	ILE
1	A	200	ARG
1	A	201	ARG
1	A	209	LEU
1	A	220	ARG
1	A	268	SER
1	A	312	SER

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Mol	Chain	Res	Type
1	A	315	LYS
1	A	403	THR
1	A	408	GLU
1	A	409	GLU
1	A	419	SER
1	A	423	ILE
1	A	431	LEU
1	A	443	GLU
1	A	446	LYS
1	A	463	THR
1	A	483	GLU
1	A	490	LEU
1	A	502	GLU
1	A	528	LYS
1	A	566	LYS
1	A	633	ARG
1	B	88	MET
1	B	92	THR
1	B	102	ARG
1	B	138	LYS
1	B	171	LEU
1	B	172	LEU
1	B	200	ARG
1	B	210	LYS
1	B	212	LYS
1	B	225	ARG
1	B	238	ILE
1	B	258	LEU
1	B	268	SER
1	B	315	LYS
1	B	321	LYS
1	B	332	HIS
1	B	336	ASP
1	B	344	SER
1	B	400	SER
1	B	412	LYS
1	B	419	SER
1	B	420	LYS
1	B	425	ASP
1	B	426	SER
1	B	431	LEU
1	B	442	HIS

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Mol	Chain	Res	Type
1	B	443	GLU
1	B	456	LYS
1	B	474	ILE
1	B	484	ARG
1	B	497	SER
1	B	502	GLU
1	B	528	LYS
1	B	555	ARG
1	B	573	THR
1	B	591	LYS
1	B	609	LEU
1	B	617	SER
1	B	619	LEU
1	B	627	MET
1	B	636	ARG
1	C	88	MET
1	C	92	THR
1	C	125	LEU
1	C	131	LEU
1	C	135	LEU
1	C	146	GLN
1	C	170	LYS
1	C	171	LEU
1	C	200	ARG
1	C	205	LEU
1	C	210	LYS
1	C	212	LYS
1	C	225	ARG
1	C	268	SER
1	C	296	LYS
1	C	301	GLU
1	C	312	SER
1	C	315	LYS
1	C	320	GLU
1	C	344	SER
1	C	374	LEU
1	C	400	SER
1	C	408	GLU
1	C	419	SER
1	C	425	ASP
1	C	428	LYS
1	C	445	LEU

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Mol	Chain	Res	Type
1	C	446	LYS
1	C	456	LYS
1	C	475	ILE
1	C	481	PHE
1	C	483	GLU
1	C	490	LEU
1	C	513	ILE
1	C	518	SER
1	C	528	LYS
1	C	555	ARG
1	C	574	GLN
1	C	581	SER
1	C	612	ARG
1	C	629	THR
1	C	633	ARG
1	C	636	ARG
1	D	88	MET
1	D	146	GLN
1	D	148	GLN
1	D	157	MET
1	D	171	LEU
1	D	179	LEU
1	D	200	ARG
1	D	210	LYS
1	D	212	LYS
1	D	220	ARG
1	D	239	LEU
1	D	268	SER
1	D	283	LYS
1	D	296	LYS
1	D	301	GLU
1	D	331	ASN
1	D	338	LEU
1	D	368	LYS
1	D	369	MET
1	D	397	LEU
1	D	401	LYS
1	D	412	LYS
1	D	419	SER
1	D	425	ASP
1	D	431	LEU
1	D	453	GLN

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Mol	Chain	Res	Type
1	D	483	GLU
1	D	490	LEU
1	D	526	GLU
1	D	528	LYS
1	D	555	ARG
1	D	619	LEU
1	D	621	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	136	GLN
1	A	148	GLN
1	A	203	GLN
1	A	404	ASN
1	A	595	HIS
1	B	161	GLN
1	B	402	GLN
1	C	159	ASN
1	C	161	GLN
1	C	203	GLN
1	C	228	GLN
1	C	286	ASN
1	C	534	GLN
1	C	634	ASN
1	D	75	GLN
1	D	159	ASN
1	D	161	GLN
1	D	175	ASN
1	D	247	GLN
1	D	281	ASN
1	D	286	ASN
1	D	404	ASN
1	D	557	HIS
1	D	574	GLN

5.3.3 RNA ⓘ

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](#)

6 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	PYR	B	701	-	5,5,5	3.95	2 (40%)	3,6,6	0.72	0
2	PYR	C	701	-	5,5,5	2.60	1 (20%)	3,6,6	2.23	1 (33%)
2	PYR	D	701	-	5,5,5	3.24	1 (20%)	3,6,6	1.68	1 (33%)
2	PYR	C	702	-	5,5,5	2.64	2 (40%)	3,6,6	2.31	3 (100%)
2	PYR	A	701	-	5,5,5	2.75	2 (40%)	3,6,6	1.97	1 (33%)
2	PYR	A	702	-	5,5,5	2.52	1 (20%)	3,6,6	2.68	2 (66%)

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	PYR	B	701	-	-	1/4/4/4	-
2	PYR	C	701	-	-	3/4/4/4	-
2	PYR	D	701	-	-	3/4/4/4	-
2	PYR	C	702	-	-	0/4/4/4	-
2	PYR	A	701	-	-	0/4/4/4	-
2	PYR	A	702	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	PYR	CA-C	-8.37	1.26	1.54
2	D	701	PYR	CA-C	-6.87	1.31	1.54
2	C	701	PYR	CA-C	-5.47	1.36	1.54
2	A	701	PYR	CA-C	-5.43	1.36	1.54
2	C	702	PYR	CA-C	-5.26	1.36	1.54
2	A	702	PYR	CA-C	-5.24	1.37	1.54
2	A	701	PYR	OXT-C	-2.75	1.23	1.30
2	B	701	PYR	OXT-C	-2.73	1.23	1.30
2	C	702	PYR	OXT-C	-2.53	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	702	PYR	OXT-C-CA	3.35	122.87	113.59
2	C	701	PYR	OXT-C-CA	3.08	122.12	113.59
2	D	701	PYR	OXT-C-CA	2.87	121.56	113.59
2	C	702	PYR	O3-CA-CB	-2.73	113.65	119.77
2	A	702	PYR	O3-CA-CB	-2.53	114.11	119.77
2	A	701	PYR	O3-CA-CB	-2.38	114.44	119.77
2	C	702	PYR	OXT-C-O	-2.09	118.92	123.90
2	C	702	PYR	OXT-C-CA	2.03	119.22	113.59

There are no chirality outliers.

All (7) torsion outliers are listed below:

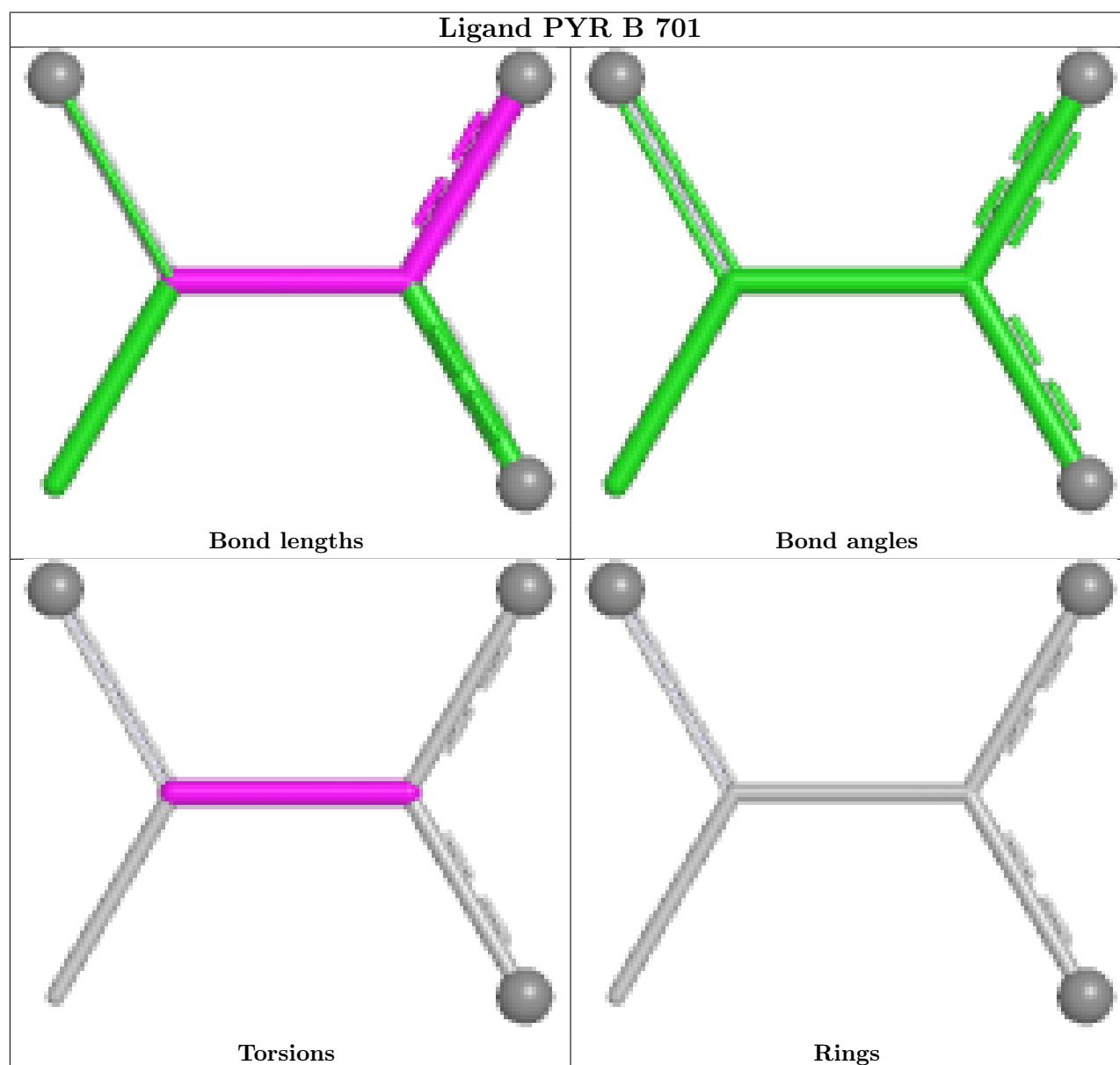
Mol	Chain	Res	Type	Atoms
2	B	701	PYR	OXT-C-CA-CB
2	C	701	PYR	OXT-C-CA-CB
2	D	701	PYR	O-C-CA-CB
2	D	701	PYR	OXT-C-CA-CB
2	C	701	PYR	O-C-CA-CB
2	C	701	PYR	OXT-C-CA-O3
2	D	701	PYR	OXT-C-CA-O3

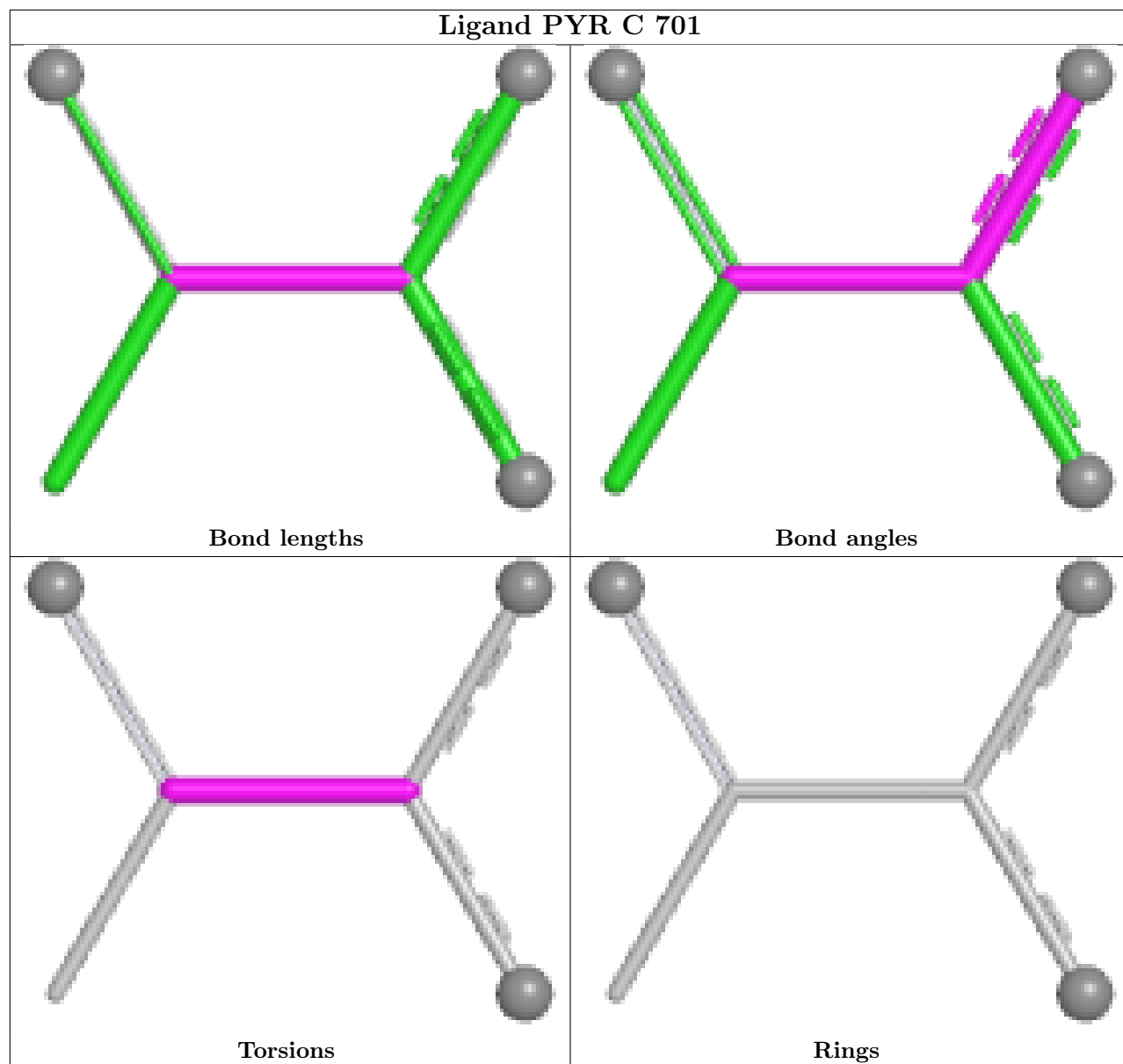
There are no ring outliers.

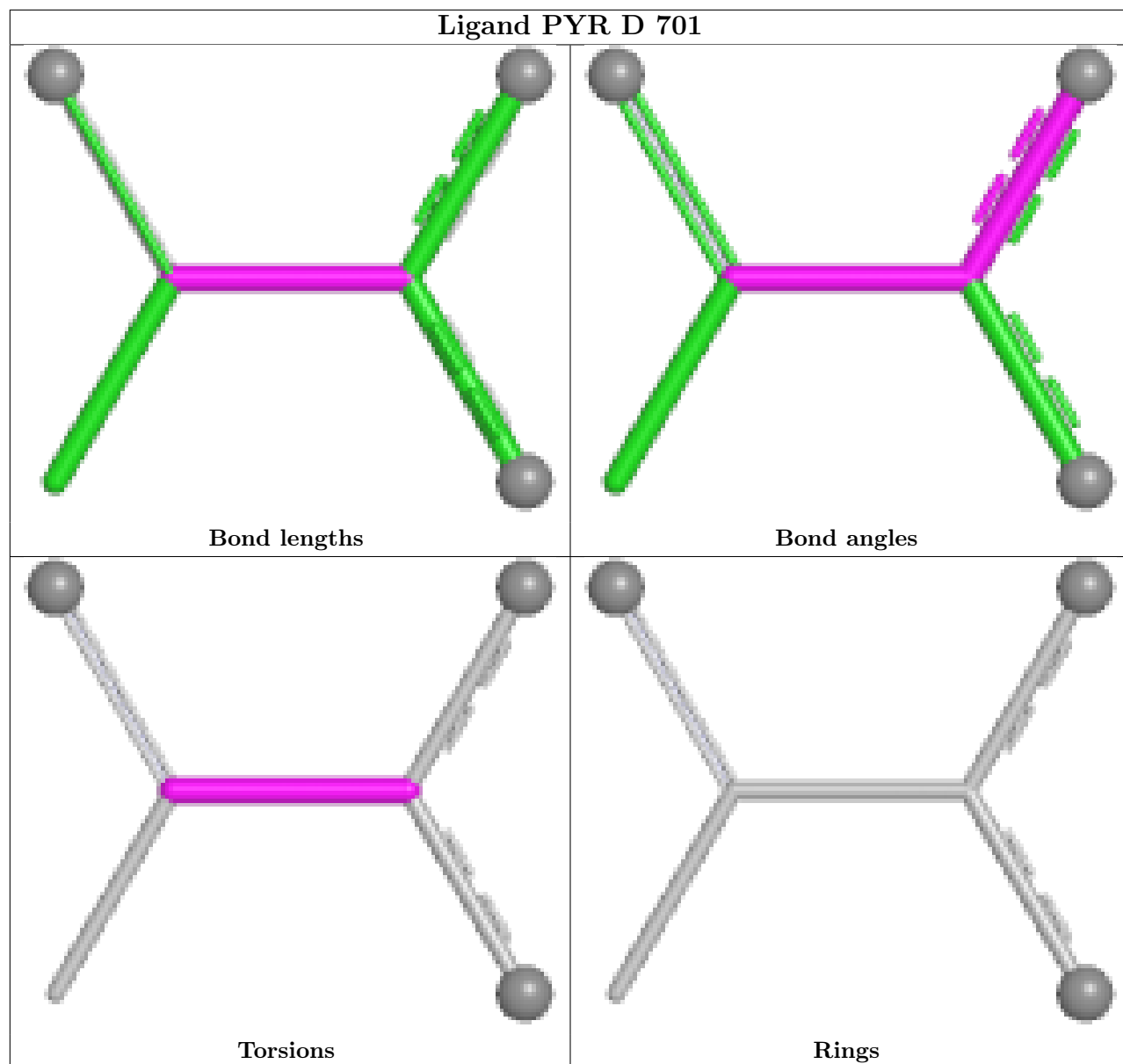
1 monomer is involved in 1 short contact:

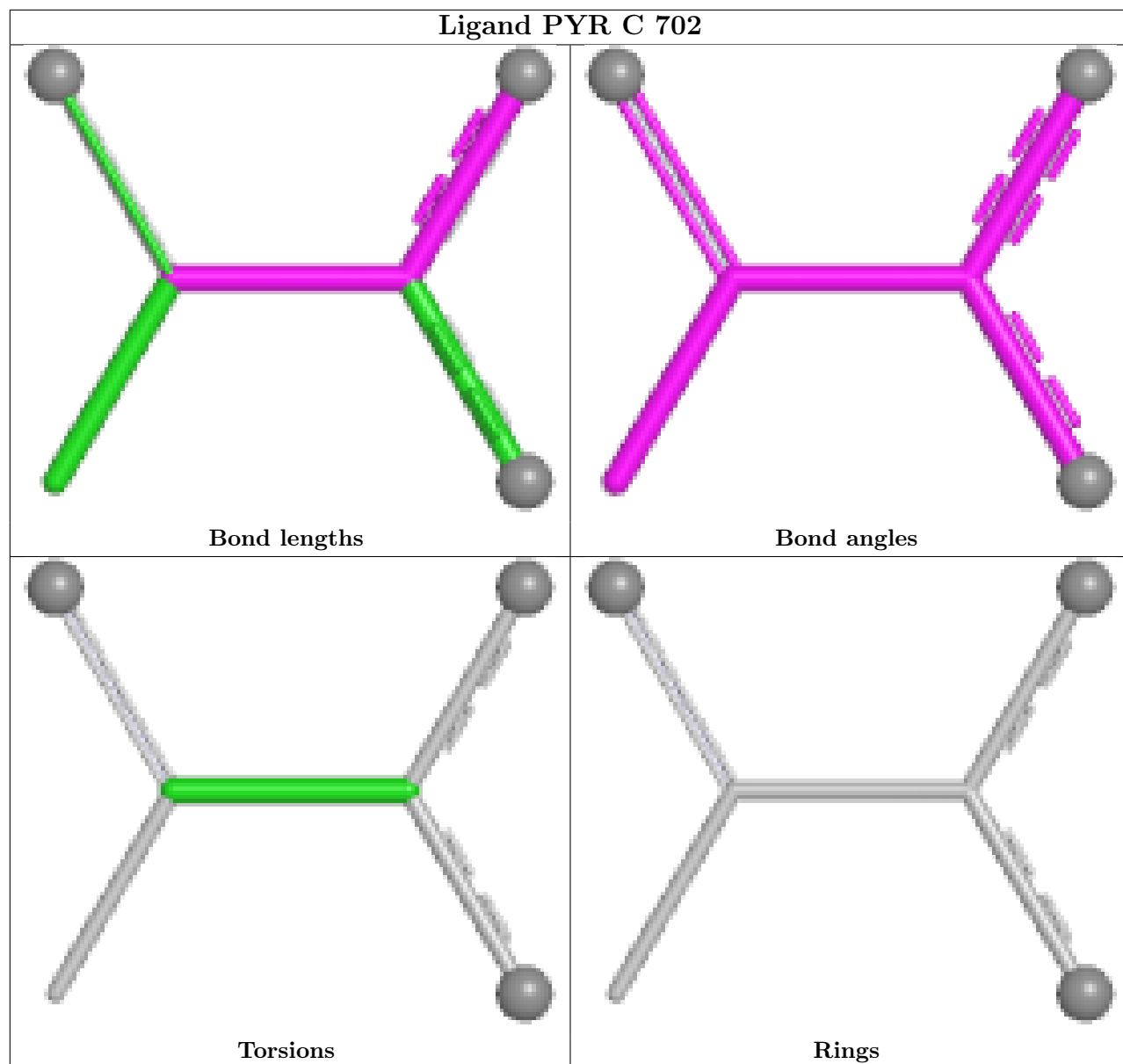
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	PYR	1	0

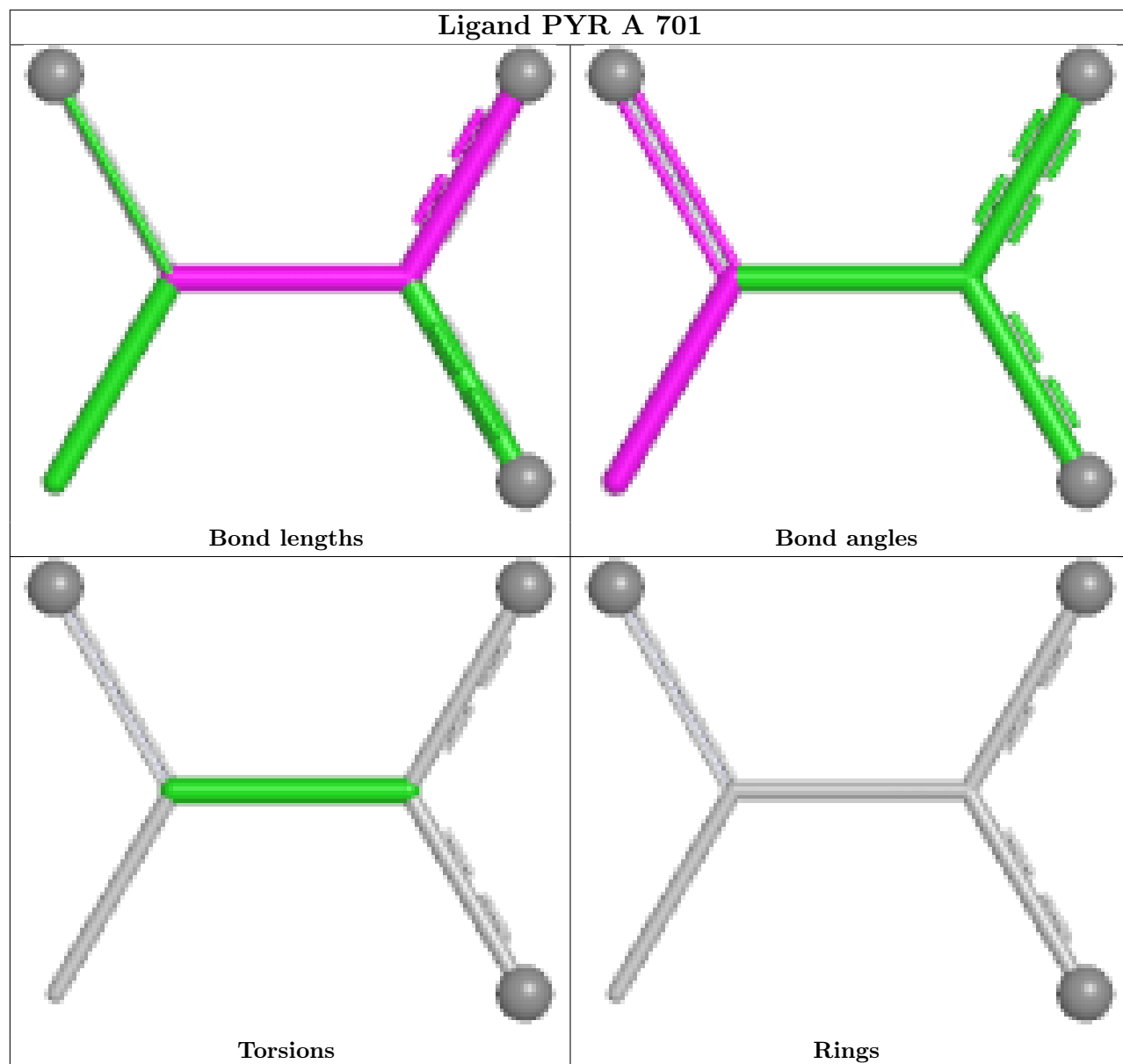
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

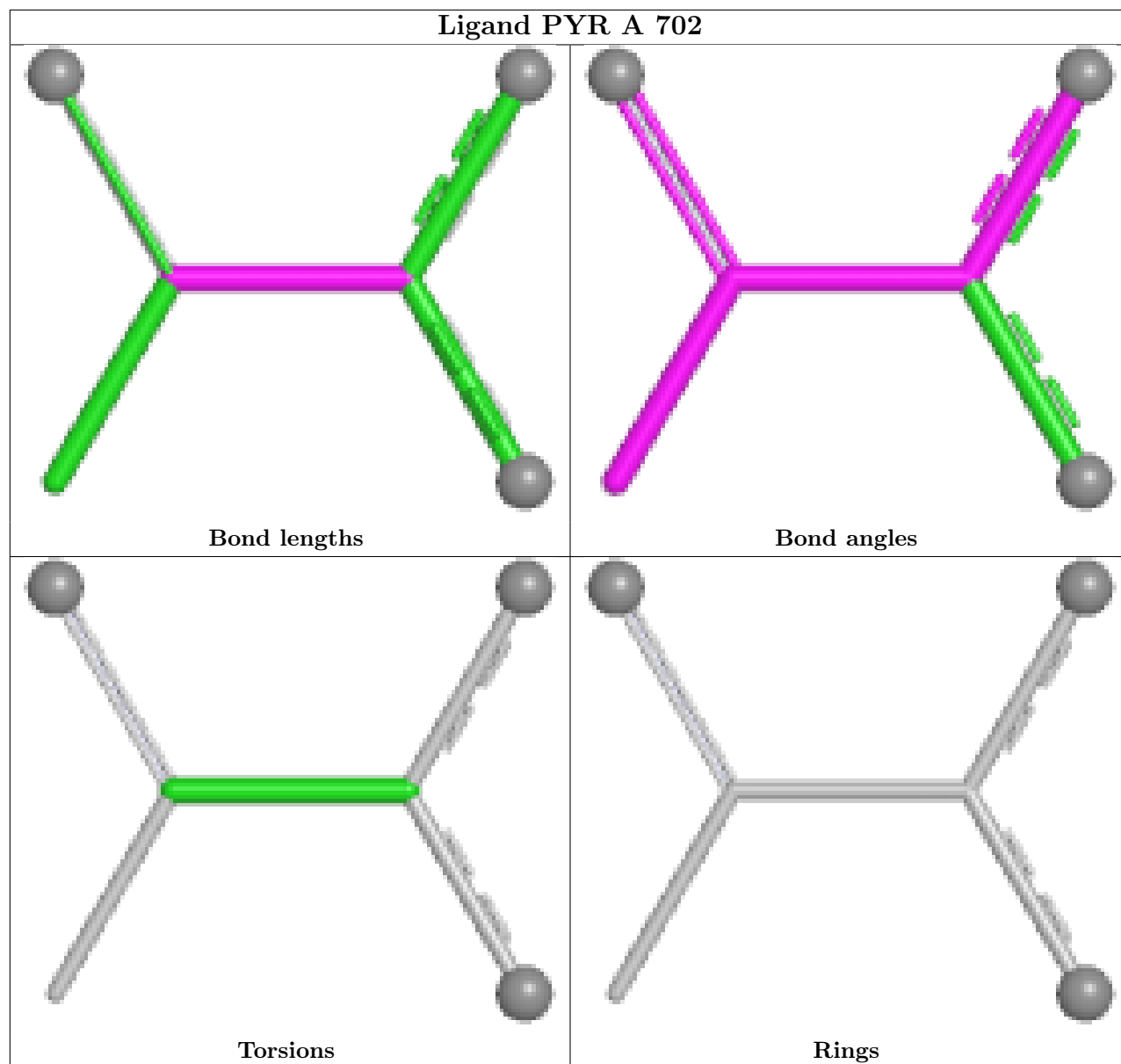












5.7 Other polymers [i](#)

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	565/576 (98%)	0.14	5 (0%) 81 80	40, 60, 97, 146	0
1	B	553/576 (96%)	0.23	14 (2%) 58 55	38, 65, 109, 171	0
1	C	552/576 (95%)	0.15	4 (0%) 84 83	40, 61, 94, 164	0
1	D	565/576 (98%)	0.17	3 (0%) 87 86	38, 60, 97, 136	0
All	All	2235/2304 (97%)	0.17	26 (1%) 76 75	38, 61, 99, 171	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	PRO	3.9
1	B	85	LEU	3.8
1	D	416	LEU	3.3
1	B	445	LEU	3.1
1	B	481	PHE	3.0
1	A	216	LEU	2.7
1	B	416	LEU	2.6
1	B	444	PRO	2.6
1	B	465	GLY	2.6
1	C	85	LEU	2.5
1	A	201	ARG	2.5
1	A	199	PHE	2.5
1	B	633	ARG	2.4
1	B	299	THR	2.4
1	C	86	PRO	2.4
1	B	437	PRO	2.4
1	B	431	LEU	2.3
1	D	528	LYS	2.2
1	B	443	GLU	2.1
1	D	201	ARG	2.1
1	C	446	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	437	PRO	2.1
1	B	226	ASN	2.1
1	A	463	THR	2.1
1	A	423	ILE	2.0
1	B	412	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

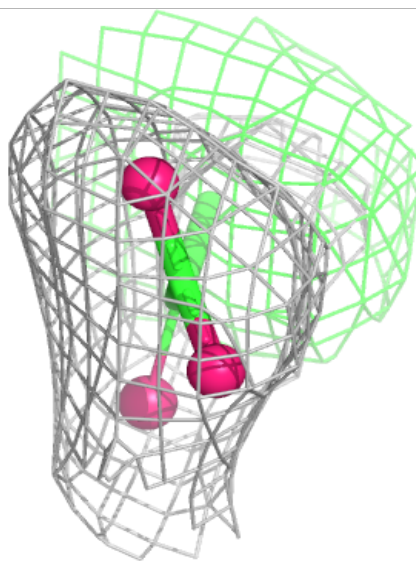
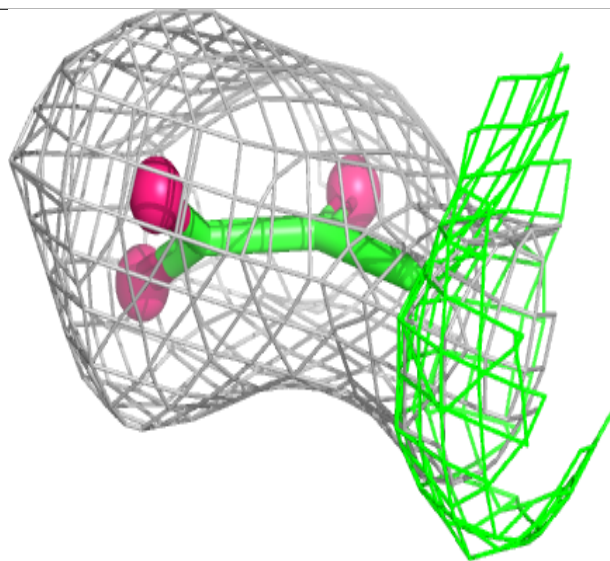
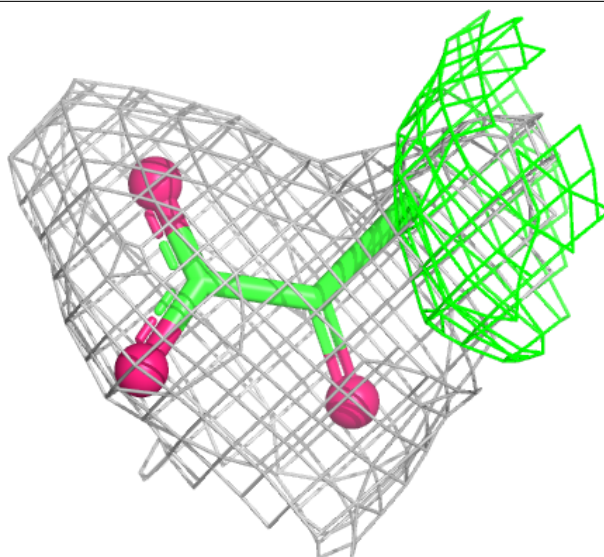
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PYR	D	701	6/6	0.52	0.17	69,84,88,89	0
2	PYR	C	701	6/6	0.59	0.24	71,83,95,96	0
2	PYR	C	702	6/6	0.71	0.28	77,79,90,99	0
2	PYR	A	701	6/6	0.71	0.15	56,69,86,102	0
2	PYR	B	701	6/6	0.75	0.10	67,73,82,89	0
2	PYR	A	702	6/6	0.79	0.22	78,85,94,97	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.

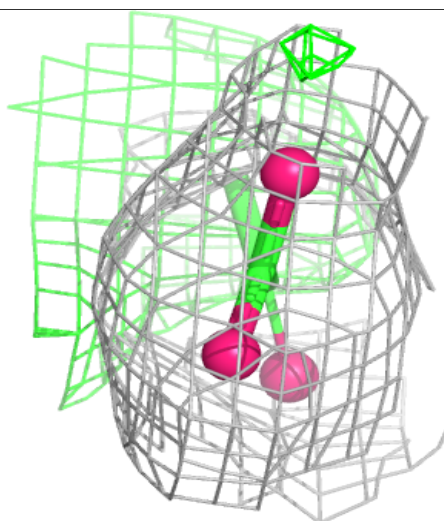
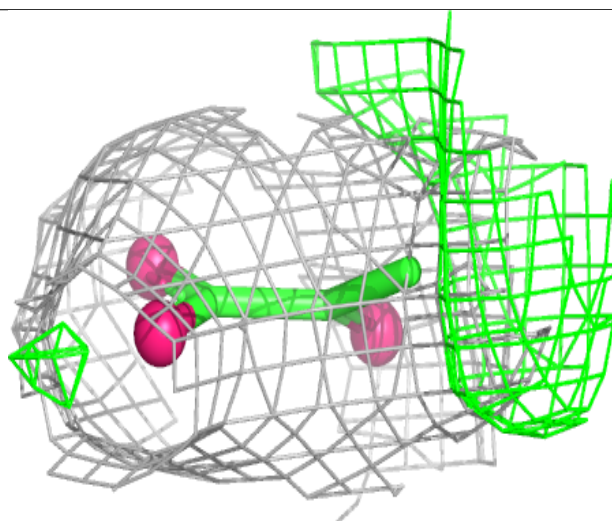
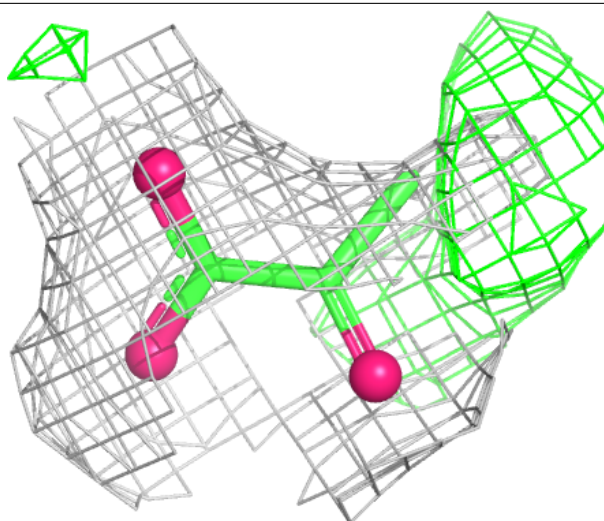
Electron density around PYR D 701:

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



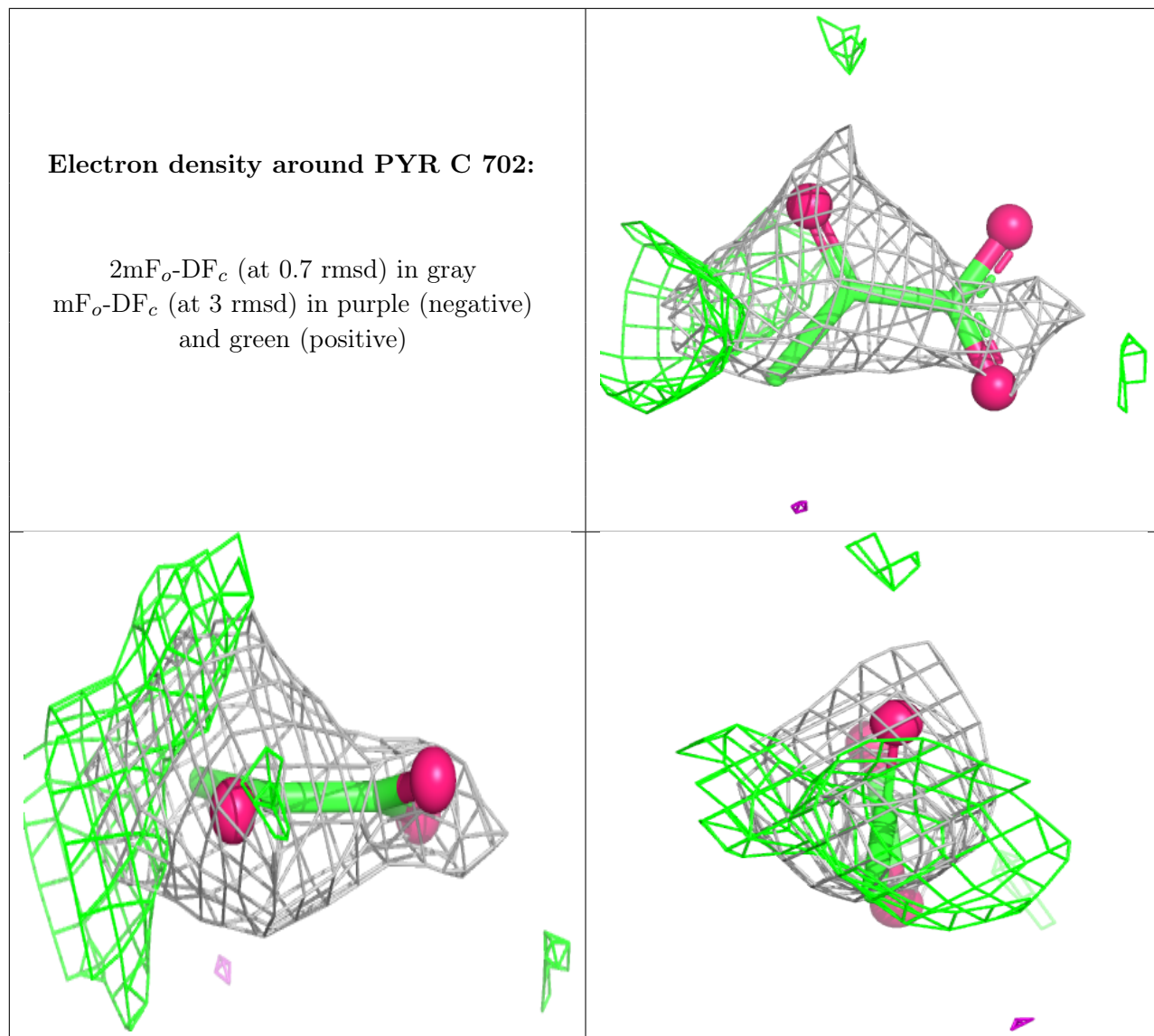
Electron density around PYR C 701:

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



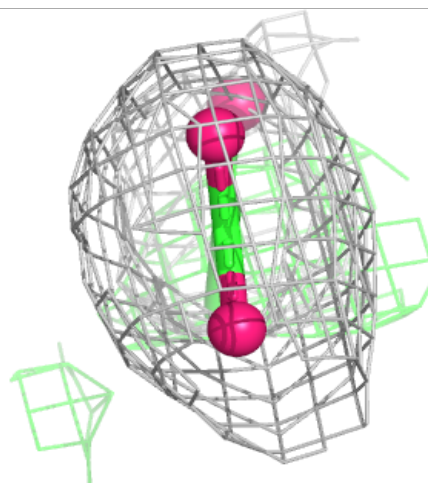
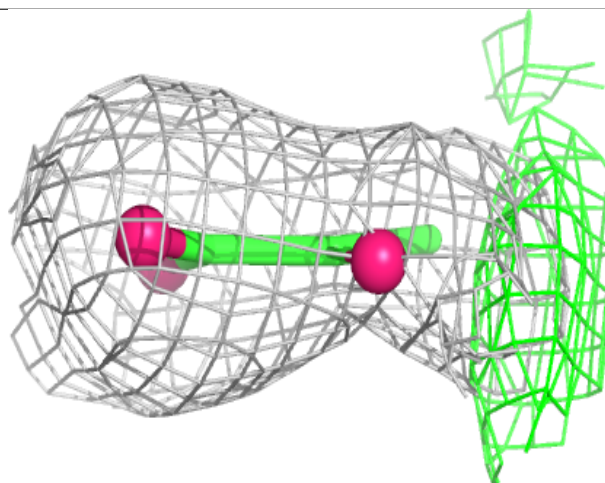
Electron density around PYR C 702:

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



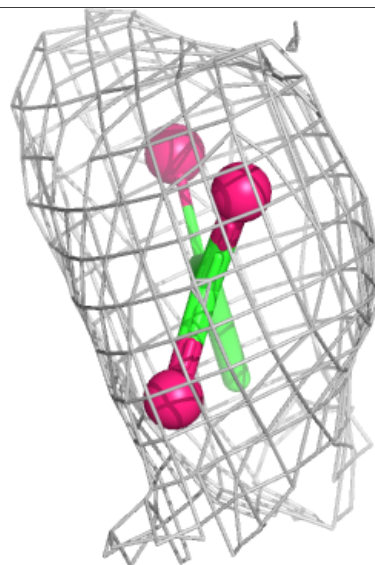
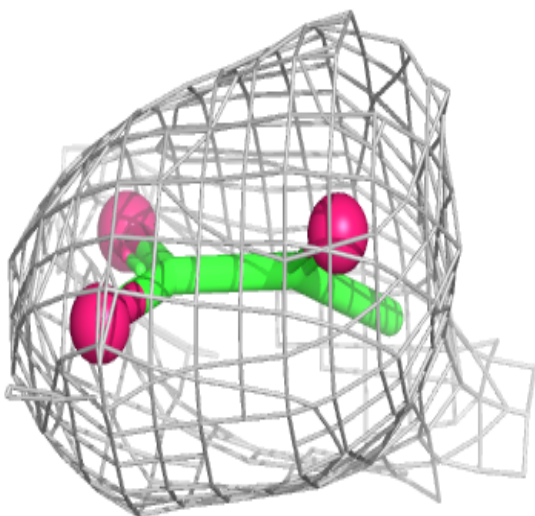
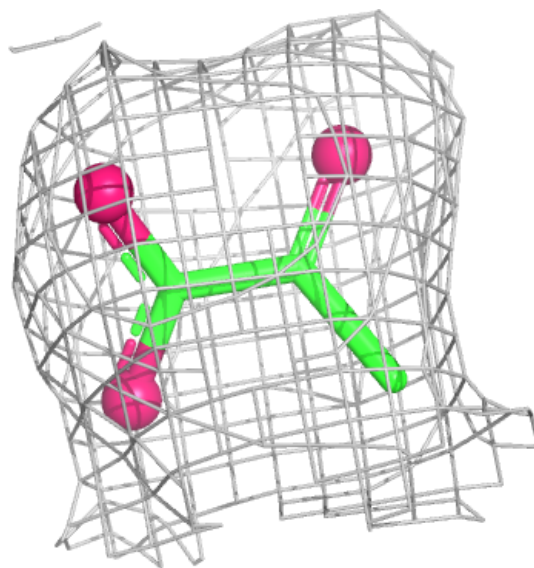
Electron density around PYR A 701:

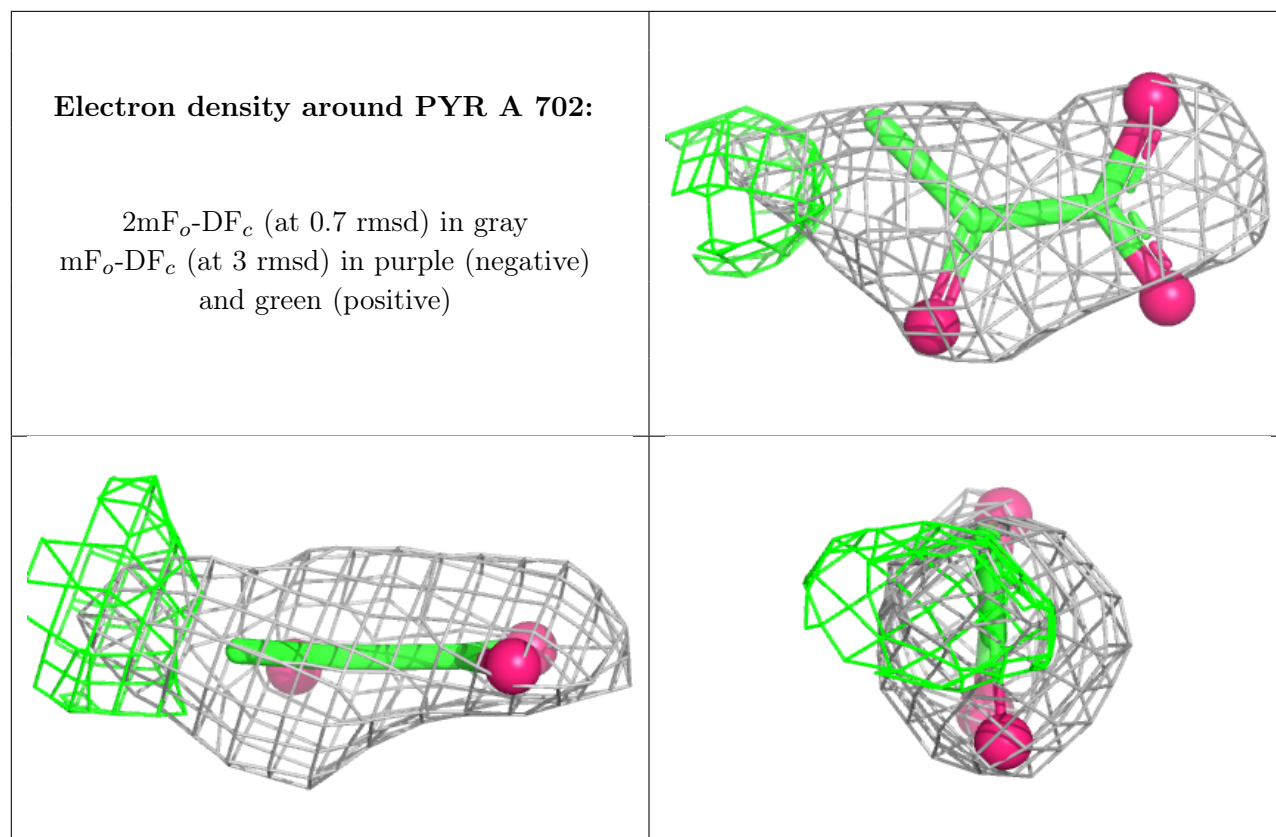
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PYR 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.