



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:20 PM UTC

PDB ID : 5G2Q / pdb_00005g2q
Title : The crystal structure of a S-selective transaminase from *Arthrobacter* sp. with alanine bound
Authors : van Oosterwijk, N.; Willies, S.; Hekelaar, J.; Terwisscha van Scheltinga, A.C.; Turner, N.J.; Dijkstra, B.W.
Deposited on : 2016-04-12
Resolution : 2.30 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

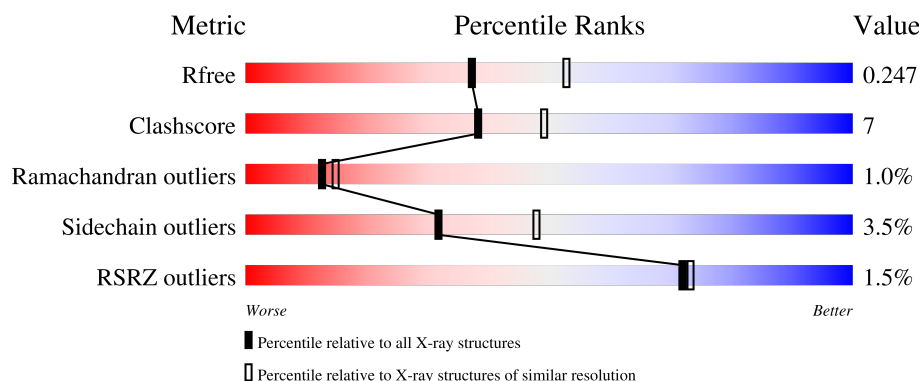
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	485	 80% 14% • 5%
1	B	485	 82% 12% • 5%
1	C	485	 80% 13% • 5%
1	D	485	 82% 12% • •

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Mol	Chain	Length	Quality of chain
1	E	485	78%16%5%
1	F	485	77%17%. .
1	G	485	81%13%5%
1	H	485	79%15%5%
1	I	485	% 75%18%5%
1	J	485	5% 76%18%5%
1	K	485	3% 70%22%5%
1	L	485	6% 71%21%5%

2 Entry composition

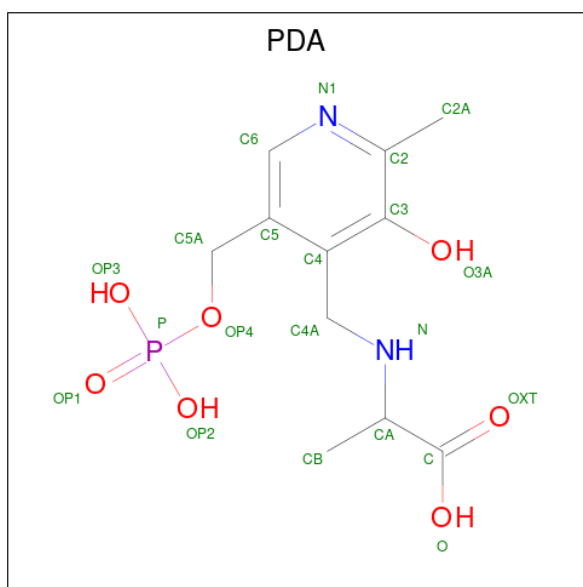
There are 3 unique types of molecules in this entry. The entry contains 44561 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3624	2297	617	692	18			
1	B	461	Total	C	N	O	S	0	0	0
			3624	2297	617	692	18			
1	C	461	Total	C	N	O	S	0	0	0
			3624	2297	617	692	18			
1	D	465	Total	C	N	O	S	0	0	0
			3650	2310	622	700	18			
1	E	461	Total	C	N	O	S	0	0	0
			3624	2297	617	692	18			
1	F	465	Total	C	N	O	S	0	0	0
			3650	2310	622	700	18			
1	G	459	Total	C	N	O	S	0	0	0
			3607	2288	613	688	18			
1	H	462	Total	C	N	O	S	0	0	0
			3629	2300	618	693	18			
1	I	461	Total	C	N	O	S	0	0	0
			3624	2297	617	692	18			
1	J	461	Total	C	N	O	S	0	0	0
			3624	2297	617	692	18			
1	K	461	Total	C	N	O	S	0	0	0
			3624	2297	617	692	18			
1	L	460	Total	C	N	O	S	0	0	0
			3615	2291	615	691	18			

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YLMETHYL)-AMINO]-PROPIONIC ACID (CCD ID: PDA) (formula: C₁₁H₁₇N₂O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	B	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	C	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	D	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	E	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	F	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	G	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	H	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	I	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	J	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	K	1	Total 21	C 11	N 2	O 7	P 1	0	0
2	L	1	Total 21	C 11	N 2	O 7	P 1	0	0

- Molecule 3 is water.

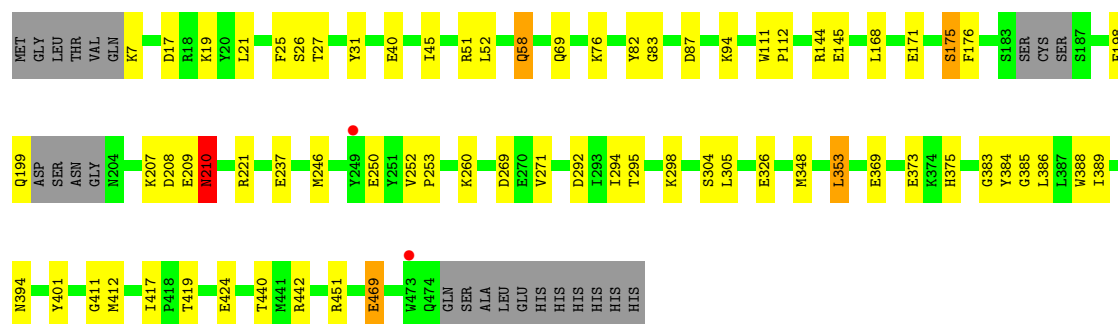
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total 162	O 162	0	0
3	B	110	Total 110	O 110	0	0
3	C	80	Total 80	O 80	0	0
3	D	66	Total 66	O 66	0	0
3	E	63	Total 63	O 63	0	0
3	F	64	Total 64	O 64	0	0
3	G	90	Total 90	O 90	0	0
3	H	74	Total 74	O 74	0	0
3	I	38	Total 38	O 38	0	0
3	J	17	Total 17	O 17	0	0
3	K	12	Total 12	O 12	0	0
3	L	14	Total 14	O 14	0	0

3 Residue-property plots [i](#)

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

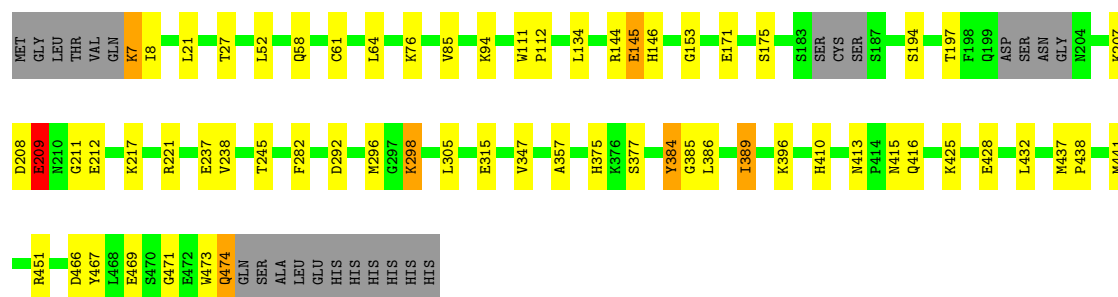
• Molecule 1: TRANSAMINASE

Chain A: 



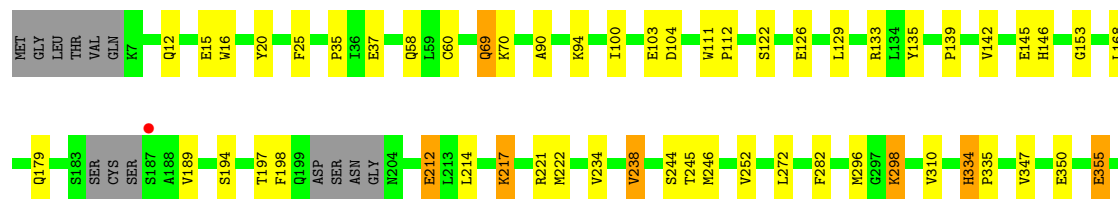
• Molecule 1: TRANSAMINASE

Chain B: 



• Molecule 1: TRANSAMINASE

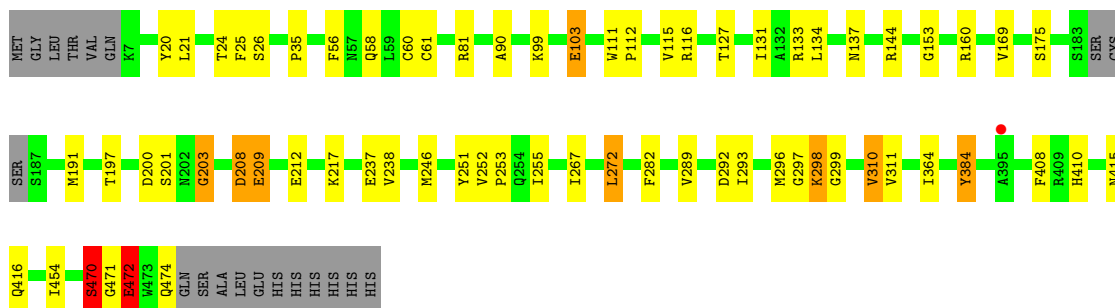
Chain C: 





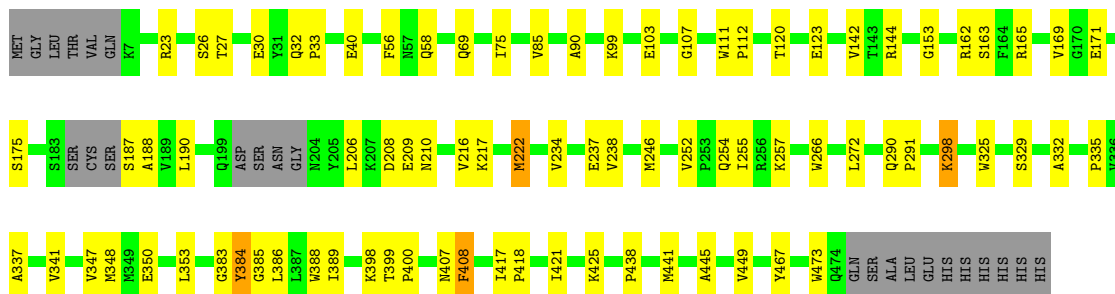
• Molecule 1: TRANSAMINASE

Chain D: 82% 12%



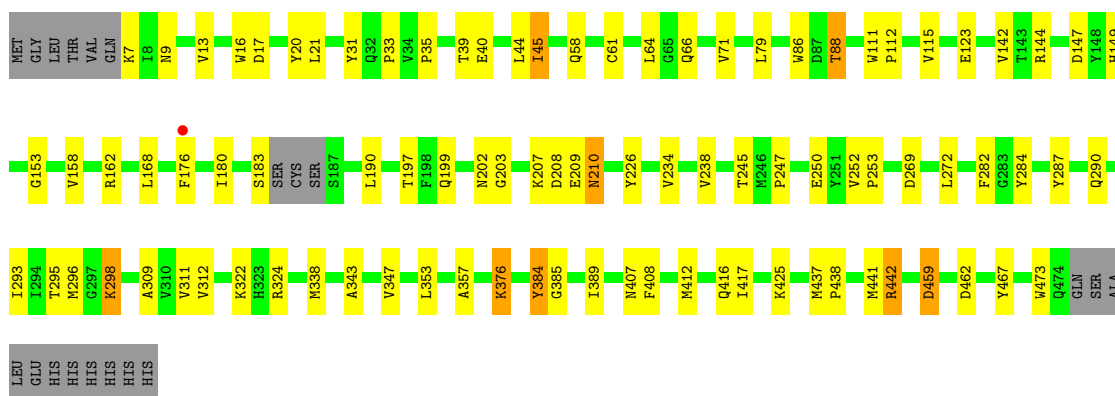
• Molecule 1: TRANSAMINASE

Chain E: 78% 16% 5%



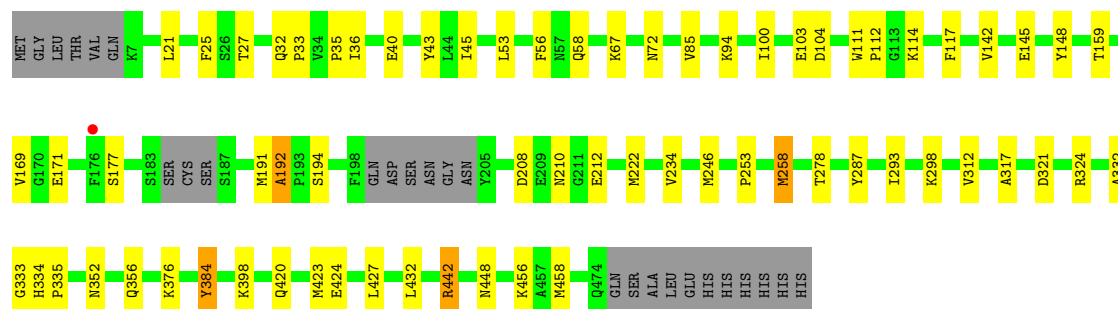
• Molecule 1: TRANSAMINASE

Chain F: 77% 17%



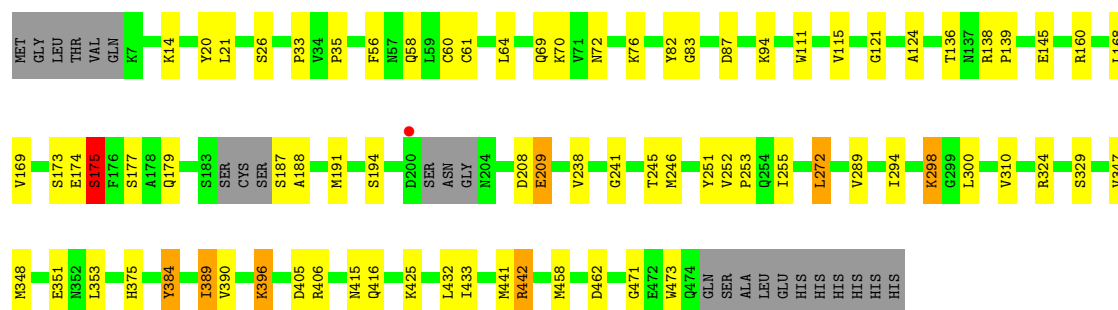
• Molecule 1: TRANSAMINASE

Chain G: 81% 13% 5%



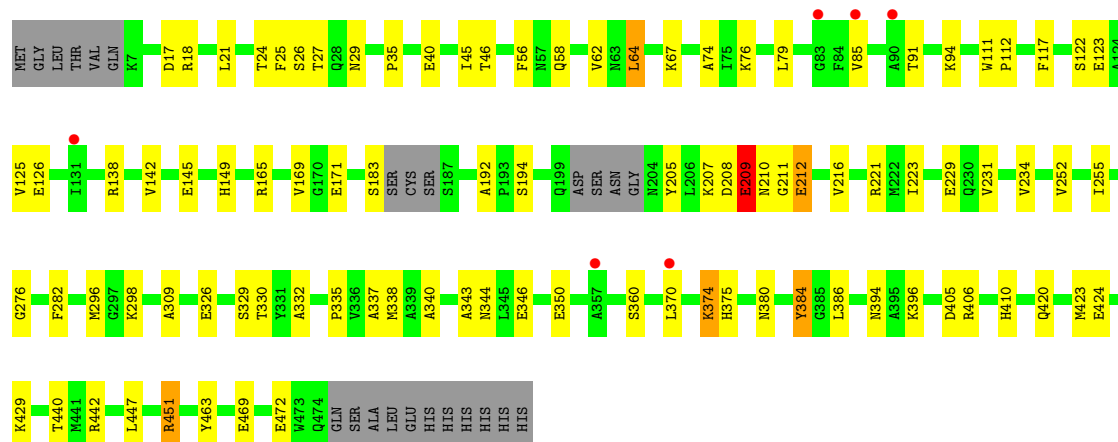
• Molecule 1: TRANSAMINASE

Chain H: 79% 15% 5%



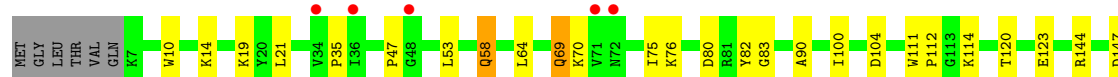
• Molecule 1: TRANSAMINASE

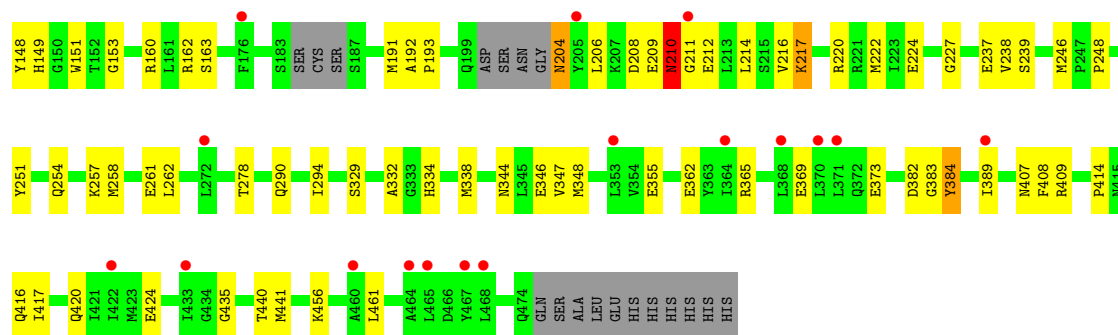
Chain I: 75% 18% 5%



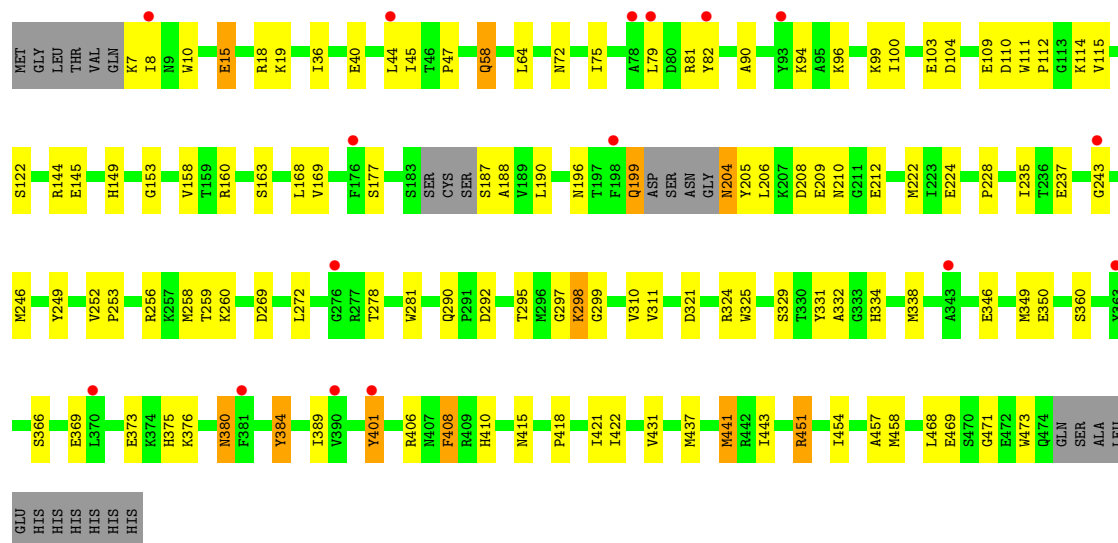
• Molecule 1: TRANSAMINASE

Chain J: 76% 18% 5%

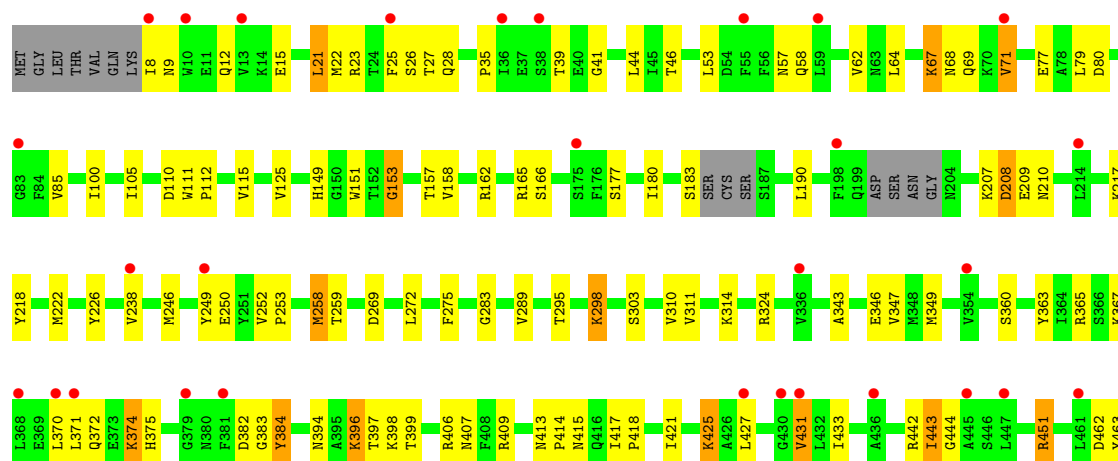




• Molecule 1: TRANSAMINASE



• Molecule 1: TRANSAMINASE



W473
Q474
GLN
SER
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.28Å 99.81Å 217.34Å 81.58° 89.12° 74.49°	Depositor
Resolution (Å)	47.96 – 2.30 47.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.7 (47.96-2.30) 93.8 (47.96-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.192 , 0.249 0.184 , 0.247	Depositor DCC
R_{free} test set	10758 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	44561	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: PDA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.88	0/3700	1.08	9/5009 (0.2%)
1	B	0.90	0/3700	1.08	6/5009 (0.1%)
1	C	0.81	0/3700	1.04	7/5009 (0.1%)
1	D	0.80	0/3727	1.05	6/5047 (0.1%)
1	E	0.77	0/3700	1.05	6/5009 (0.1%)
1	F	0.80	0/3727	1.04	2/5047 (0.0%)
1	G	0.81	0/3683	1.02	5/4986 (0.1%)
1	H	0.87	1/3705 (0.0%)	1.05	3/5016 (0.1%)
1	I	0.70	0/3700	1.02	7/5009 (0.1%)
1	J	0.69	0/3700	1.00	4/5009 (0.1%)
1	K	0.63	1/3700 (0.0%)	0.95	1/5009 (0.0%)
1	L	0.73	5/3691 (0.1%)	1.03	8/4998 (0.2%)
All	All	0.79	7/44433 (0.0%)	1.03	64/60157 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	443	ILE	C-N	10.70	1.47	1.33
1	L	443	ILE	CA-C	8.03	1.62	1.52
1	L	425	LYS	CG-CD	7.63	1.75	1.52
1	L	374	LYS	CB-CG	6.81	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	444	GLY	CA-C	6.79	1.57	1.51
1	K	81	ARG	NE-CZ	6.00	1.39	1.33
1	H	329	SER	CA-C	5.24	1.59	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ASN	N-CA-C	-8.76	102.59	113.28
1	L	443	ILE	CB-CA-C	-8.13	98.45	110.81
1	B	175	SER	N-CA-C	7.59	120.63	111.82
1	E	290	GLN	CA-C-N	7.24	127.16	120.21
1	E	290	GLN	C-N-CA	7.24	127.16	120.21
1	G	192	ALA	CA-C-N	-7.01	112.77	119.85
1	G	192	ALA	C-N-CA	-7.01	112.77	119.85
1	J	227	GLY	CA-C-N	6.69	126.94	119.32
1	J	227	GLY	C-N-CA	6.69	126.94	119.32
1	A	411	GLY	N-CA-C	-6.64	106.62	115.32
1	A	292	ASP	N-CA-C	-6.54	105.43	113.41
1	L	444	GLY	CA-C-O	6.54	126.95	121.06
1	D	175	SER	N-CA-C	6.48	121.20	113.16
1	H	56	PHE	N-CA-C	-6.45	105.57	113.50
1	E	175	SER	N-CA-C	6.44	118.38	111.36
1	B	305	LEU	CA-C-N	-6.39	113.19	119.90
1	B	305	LEU	C-N-CA	-6.39	113.19	119.90
1	A	175	SER	N-CA-C	6.22	118.99	111.40
1	H	175	SER	N-CA-C	6.21	118.13	111.36
1	A	252	VAL	CA-C-N	-6.17	112.49	119.28
1	A	252	VAL	C-N-CA	-6.17	112.49	119.28
1	C	435	GLY	N-CA-C	6.17	120.67	110.55
1	D	292	ASP	N-CA-C	-6.07	106.00	113.41
1	C	244	SER	N-CA-C	6.06	118.00	110.91
1	L	46	THR	CA-C-N	5.85	125.33	119.24
1	L	46	THR	C-N-CA	5.85	125.33	119.24
1	C	179	GLN	N-CA-C	-5.79	101.63	110.14
1	I	46	THR	CA-C-N	5.76	125.23	119.24
1	I	46	THR	C-N-CA	5.76	125.23	119.24
1	E	56	PHE	N-CA-C	-5.74	106.32	113.38
1	A	294	ILE	CB-CA-C	-5.68	102.15	110.62
1	L	383	GLY	N-CA-C	5.68	117.84	110.45
1	I	252	VAL	N-CA-CB	5.66	114.86	110.45
1	A	353	LEU	N-CA-C	5.64	118.20	111.71
1	D	472	GLU	N-CA-C	-5.63	95.24	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	PHE	N-CA-C	-5.62	106.59	113.50
1	F	437	MET	CA-C-N	5.59	125.25	119.05
1	F	437	MET	C-N-CA	5.59	125.25	119.05
1	H	179	GLN	N-CA-C	-5.54	101.56	110.14
1	I	192	ALA	CA-C-N	-5.49	114.27	119.76
1	I	192	ALA	C-N-CA	-5.49	114.27	119.76
1	B	292	ASP	N-CA-C	-5.36	106.88	113.41
1	L	433	ILE	N-CA-C	5.25	114.78	108.06
1	K	292	ASP	N-CA-C	-5.25	107.01	113.41
1	G	210	ASN	N-CA-C	-5.24	106.74	113.02
1	G	43	TYR	N-CA-C	5.23	118.26	109.95
1	I	205	TYR	N-CA-C	5.20	117.70	109.96
1	J	210	ASN	N-CA-C	-5.16	107.01	113.15
1	I	29	ASN	N-CA-C	5.16	116.90	111.28
1	B	413	ASN	CA-C-N	5.11	125.15	119.32
1	B	413	ASN	C-N-CA	5.11	125.15	119.32
1	D	208	ASP	N-CA-C	5.09	117.73	111.82
1	C	334	HIS	CA-C-N	5.09	126.21	119.84
1	C	334	HIS	C-N-CA	5.09	126.21	119.84
1	G	321	ASP	N-CA-C	5.09	118.27	111.75
1	A	469	GLU	N-CA-C	5.09	117.56	111.71
1	C	417	ILE	N-CA-C	5.09	112.59	107.55
1	J	435	GLY	N-CA-C	5.08	118.56	111.19
1	L	431	VAL	N-CA-C	5.07	115.27	108.17
1	E	252	VAL	CA-C-N	-5.05	113.72	119.28
1	E	252	VAL	C-N-CA	-5.05	113.72	119.28
1	L	275	PHE	N-CA-C	5.04	116.81	110.91
1	D	203	GLY	N-CA-C	-5.02	101.33	112.17
1	C	462	ASP	N-CA-C	-5.02	105.70	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	LYS	Peptide
1	F	176	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3624	0	3573	40	0
1	B	3624	0	3573	41	0
1	C	3624	0	3573	46	0
1	D	3650	0	3592	45	0
1	E	3624	0	3573	46	0
1	F	3650	0	3592	67	0
1	G	3607	0	3559	43	0
1	H	3629	0	3575	52	0
1	I	3624	0	3573	62	0
1	J	3624	0	3573	55	0
1	K	3624	0	3573	79	0
1	L	3615	0	3560	73	0
2	A	21	0	13	2	0
2	B	21	0	13	3	0
2	C	21	0	13	3	0
2	D	21	0	14	2	0
2	E	21	0	13	0	0
2	F	21	0	14	4	0
2	G	21	0	14	0	0
2	H	21	0	14	0	0
2	I	21	0	14	2	0
2	J	21	0	13	1	0
2	K	21	0	12	1	0
2	L	21	0	12	1	0
3	A	162	0	0	1	0
3	B	110	0	0	2	0
3	C	80	0	0	2	0
3	D	66	0	0	0	0
3	E	63	0	0	0	0
3	F	64	0	0	0	0
3	G	90	0	0	1	0
3	H	74	0	0	2	0
3	I	38	0	0	1	0
3	J	17	0	0	0	0
3	K	12	0	0	0	0
3	L	14	0	0	2	0
All	All	44561	0	43048	595	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 7.

All (595) 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:L:425:LYS:CD	1:L:425:LYS:CG	1.75	1.58
1:H:208:ASP:O	1:H:209:GLU:HG2	1.41	1.19
1:L:8:ILE:HG22	1:L:9:ASN:H	1.12	1.11
3:A:2078:HOH:O	1:C:221:ARG:HD3	1.64	0.95
1:G:192:ALA:HA	1:G:222:MET:HE1	1.56	0.88
1:J:414:PRO:HA	1:J:417:ILE:HD12	1.59	0.84
1:A:221:ARG:HH21	1:C:145:GLU:CD	1.86	0.83
1:L:64:LEU:HD11	1:L:347:VAL:HG11	1.60	0.81
1:L:8:ILE:HG22	1:L:9:ASN:N	1.95	0.80
1:C:60:CYS:HB2	1:C:272:LEU:HD11	1.65	0.78
1:I:208:ASP:HB3	1:I:211:GLY:H	1.50	0.77
1:A:111:TRP:N	1:A:112:PRO:HD3	2.00	0.77
1:D:282:PHE:CZ	1:D:296:MET:HE2	2.20	0.77
1:F:208:ASP:O	1:F:209:GLU:HB2	1.84	0.75
1:F:282:PHE:CZ	1:F:296:MET:HE2	2.21	0.75
1:J:220:ARG:O	1:J:224:GLU:HG3	1.86	0.74
1:C:246:MET:HE3	1:C:383:GLY:HA2	1.70	0.74
1:I:138:ARG:HD3	1:I:229:GLU:O	1.88	0.74
3:C:2006:HOH:O	1:D:116:ARG:HG3	1.87	0.74
1:F:40:GLU:HG2	1:F:45:ILE:HD11	1.70	0.73
1:F:298:LYS:NZ	2:F:1000:PDA:HA	2.04	0.73
1:D:61:CYS:HB3	1:D:298:LYS:HD3	1.71	0.73
1:J:441:MET:HE1	1:J:461:LEU:HD21	1.70	0.72
1:H:241:GLY:HA3	1:H:272:LEU:HD23	1.72	0.72
1:L:8:ILE:CG2	1:L:9:ASN:H	1.93	0.72
1:F:199:GLN:HE21	1:F:203:GLY:HA2	1.54	0.71
1:I:207:LYS:HE2	1:I:211:GLY:O	1.91	0.71
1:I:142:VAL:HB	1:I:234:VAL:HG22	1.73	0.71
1:L:425:LYS:CD	1:L:425:LYS:CB	2.69	0.71
1:L:272:LEU:HA	1:L:298:LYS:HD2	1.73	0.71
1:G:192:ALA:HA	1:G:222:MET:CE	2.20	0.70
1:L:238:VAL:HG21	1:L:283:GLY:HA3	1.74	0.70
1:B:375:HIS:HE1	1:B:466:ASP:OD1	1.74	0.70
1:B:208:ASP:O	1:B:209:GLU:HB3	1.92	0.69
1:D:115:VAL:HG22	1:D:311:VAL:HG22	1.73	0.69
1:A:111:TRP:N	1:A:112:PRO:CD	2.56	0.68
1:C:94:LYS:HE3	1:D:21:LEU:HD13	1.75	0.68
1:F:282:PHE:HZ	1:F:296:MET:HE2	1.56	0.68
1:I:165:ARG:HH21	1:I:183:SER:HB2	1.59	0.68
1:C:298:LYS:HE2	2:C:1000:PDA:H4A1	1.76	0.68
1:K:441:MET:HE3	1:K:443:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:TRP:N	1:D:112:PRO:HD3	2.09	0.67
1:J:53:LEU:HD22	1:J:456:LYS:HD3	1.76	0.67
1:I:145:GLU:HG2	1:I:194:SER:HB2	1.77	0.67
1:F:115:VAL:HG22	1:F:311:VAL:HG22	1.76	0.67
1:K:376:LYS:H	1:K:376:LYS:HD2	1.59	0.66
1:L:23:ARG:HB3	1:L:26:SER:O	1.95	0.66
1:D:208:ASP:O	1:D:209:GLU:HB2	1.94	0.66
1:A:375:HIS:HB3	1:A:469:GLU:OE2	1.96	0.66
1:H:458:MET:HE2	1:H:458:MET:HA	1.77	0.66
1:J:208:ASP:HB2	1:J:212:GLU:O	1.96	0.66
1:F:207:LYS:NZ	1:F:250:GLU:OE2	2.30	0.65
1:C:298:LYS:CE	2:C:1000:PDA:H4A1	2.26	0.65
1:F:199:GLN:NE2	1:F:203:GLY:HA2	2.11	0.65
1:I:56:PHE:HZ	1:I:423:MET:HE2	1.61	0.65
1:K:115:VAL:HG22	1:K:311:VAL:HG22	1.77	0.65
1:B:245:THR:HA	1:B:389:ILE:HD13	1.78	0.65
1:H:375:HIS:NE2	1:H:462:ASP:OD1	2.26	0.64
1:I:17:ASP:HA	1:I:21:LEU:HD12	1.79	0.64
1:I:429:LYS:HD3	1:I:463:TYR:CD2	2.33	0.64
1:H:208:ASP:C	1:H:209:GLU:HG2	2.22	0.64
1:C:12:GLN:HA	1:C:15:GLU:OE1	1.99	0.63
1:I:276:GLY:HA3	1:I:447:LEU:HD11	1.80	0.63
1:K:329:SER:HB2	1:L:151:TRP:NE1	2.14	0.62
1:F:384:TYR:N	1:F:384:TYR:CD1	2.66	0.62
1:L:365:ARG:NH1	3:L:2010:HOH:O	2.30	0.62
1:E:144:ARG:NH2	1:E:237:GLU:H	1.98	0.62
1:H:145:GLU:HG2	1:H:194:SER:HB2	1.80	0.62
1:L:394:ASN:OD1	1:L:396:LYS:HB2	1.99	0.62
1:K:208:ASP:N	1:K:212:GLU:O	2.32	0.62
1:L:346:GLU:HA	1:L:349:MET:HE2	1.80	0.62
1:C:111:TRP:N	1:C:112:PRO:HD3	2.15	0.62
1:E:348:MET:HG2	1:E:353:LEU:HD12	1.81	0.62
1:I:282:PHE:CZ	1:I:296:MET:HE2	2.35	0.61
1:L:425:LYS:CG	1:L:425:LYS:CE	2.73	0.61
1:K:15:GLU:OE1	1:K:18:ARG:NH1	2.33	0.61
1:K:208:ASP:C	1:K:210:ASN:H	2.06	0.61
1:H:160:ARG:HG3	1:H:191:MET:HG3	1.82	0.61
1:H:384:TYR:N	1:H:384:TYR:CD1	2.67	0.61
1:H:272:LEU:HD12	1:H:272:LEU:O	2.01	0.61
1:I:208:ASP:HB3	1:I:211:GLY:N	2.16	0.61
1:J:144:ARG:O	1:J:147:ASP:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:THR:HG21	1:F:123:GLU:OE2	2.01	0.60
1:L:53:LEU:HD23	1:L:431:VAL:HG22	1.84	0.60
1:L:68:ASN:HB3	1:L:71:VAL:HB	1.83	0.60
1:I:296:MET:HB2	1:I:309:ALA:HB3	1.83	0.60
1:L:153:GLY:O	1:L:157:THR:HG23	2.01	0.60
1:F:298:LYS:HZ3	2:F:1000:PDA:HA	1.66	0.60
1:G:145:GLU:HG2	1:G:194:SER:HB2	1.84	0.60
1:J:144:ARG:HG3	1:J:192:ALA:HB3	1.84	0.59
1:I:165:ARG:NH2	1:I:183:SER:HB2	2.16	0.59
1:K:196:ASN:HA	1:K:205:TYR:HE2	1.68	0.59
1:C:20:TYR:OH	1:D:103:GLU:HG3	2.03	0.59
1:L:208:ASP:C	1:L:210:ASN:H	2.10	0.59
1:A:111:TRP:H	1:A:112:PRO:HD3	1.65	0.59
1:G:56:PHE:CZ	1:G:423:MET:HE2	2.37	0.59
1:I:56:PHE:CZ	1:I:423:MET:HE2	2.37	0.59
1:E:389:ILE:O	1:E:389:ILE:HG13	2.01	0.59
1:K:72:ASN:ND2	1:L:79:LEU:O	2.36	0.59
1:I:138:ARG:HD3	1:I:229:GLU:C	2.28	0.59
1:D:471:GLY:H	1:D:472:GLU:HB2	1.68	0.59
1:H:208:ASP:O	1:H:209:GLU:CG	2.34	0.59
1:G:53:LEU:HD22	1:G:456:LYS:HD3	1.85	0.58
1:K:111:TRP:N	1:K:112:PRO:HD3	2.17	0.58
1:D:144:ARG:HH21	1:D:237:GLU:H	1.51	0.58
1:I:216:VAL:HG13	1:I:255:ILE:HD13	1.86	0.58
1:D:298:LYS:HZ3	2:D:1000:PDA:H4A1	1.69	0.58
1:E:90:ALA:O	1:F:35:PRO:HA	2.03	0.58
1:J:248:PRO:HG2	1:J:251:TYR:HB2	1.84	0.58
1:D:160:ARG:HG3	1:D:191:MET:HG3	1.86	0.58
1:K:40:GLU:HG2	1:K:45:ILE:HD11	1.86	0.58
1:F:111:TRP:HD1	1:F:290:GLN:NE2	2.00	0.58
1:H:389:ILE:HG13	1:H:389:ILE:O	2.04	0.58
1:B:425:LYS:HD2	1:B:428:GLU:OE2	2.03	0.58
1:K:334:HIS:O	1:K:338:MET:HG2	2.04	0.58
1:L:425:LYS:HD2	1:L:463:TYR:CE2	2.39	0.58
1:F:39:THR:OG1	1:F:66:GLN:HB3	2.04	0.57
1:H:70:LYS:HD3	1:H:347:VAL:HG22	1.85	0.57
1:E:386:LEU:HD12	1:E:445:ALA:HB3	1.86	0.57
1:K:256:ARG:NH1	1:K:290:GLN:O	2.31	0.57
1:I:21:LEU:O	1:J:114:LYS:NZ	2.30	0.57
1:I:298:LYS:HE2	2:I:1000:PDA:H4A1	1.86	0.57
1:L:413:ASN:ND2	1:L:415:ASN:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:442:ARG:HH11	1:H:442:ARG:HB3	1.70	0.57
1:B:432:LEU:HA	3:B:2106:HOH:O	2.05	0.57
1:C:282:PHE:CZ	1:C:296:MET:HE2	2.39	0.57
1:K:346:GLU:O	1:K:350:GLU:HG2	2.04	0.57
1:B:389:ILE:O	1:B:389:ILE:HG13	2.03	0.57
1:L:451:ARG:HD2	3:L:2009:HOH:O	2.05	0.56
1:F:343:ALA:O	1:F:347:VAL:HG23	2.05	0.56
1:K:376:LYS:HD2	1:K:376:LYS:N	2.21	0.56
1:I:74:ALA:CB	1:I:343:ALA:HB2	2.35	0.56
1:B:111:TRP:N	1:B:112:PRO:HD3	2.21	0.56
1:L:252:VAL:HG12	1:L:289:VAL:HG21	1.88	0.56
1:B:145:GLU:OE2	1:B:197:THR:OG1	2.24	0.56
1:F:9:ASN:O	1:F:13:VAL:HG23	2.05	0.56
1:A:221:ARG:NH2	1:C:145:GLU:CD	2.62	0.55
1:J:162:ARG:HD3	1:J:407:ASN:O	2.05	0.55
1:B:208:ASP:O	1:B:209:GLU:CB	2.54	0.55
1:C:135:TYR:OH	3:C:2035:HOH:O	2.17	0.55
1:E:266:TRP:CE3	1:E:291:PRO:HA	2.42	0.55
1:D:200:ASP:OD1	1:D:203:GLY:O	2.25	0.55
1:I:111:TRP:N	1:I:112:PRO:HD3	2.21	0.55
1:K:190:LEU:HB3	1:K:222:MET:CE	2.36	0.55
1:I:122:SER:O	1:I:126:GLU:HG2	2.07	0.55
1:K:94:LYS:HG2	1:L:21:LEU:HD11	1.88	0.55
1:K:149:HIS:CE1	1:K:235:ILE:HG12	2.42	0.55
1:H:61:CYS:HB3	1:H:298:LYS:HG2	1.87	0.55
1:J:365:ARG:HG2	1:J:369:GLU:OE2	2.06	0.55
1:L:374:LYS:HE2	1:L:375:HIS:NE2	2.22	0.55
1:B:384:TYR:CD1	1:B:384:TYR:N	2.74	0.55
1:D:111:TRP:N	1:D:112:PRO:CD	2.70	0.55
1:E:473:TRP:CD1	1:E:473:TRP:H	2.25	0.55
1:G:94:LYS:HE3	1:H:21:LEU:HD13	1.89	0.55
1:K:281:TRP:HZ2	1:K:349:MET:HG2	1.72	0.55
1:L:9:ASN:ND2	1:L:12:GLN:HB2	2.22	0.55
1:F:61:CYS:HB3	1:F:298:LYS:HG2	1.89	0.54
1:F:298:LYS:HZ1	2:F:1000:PDA:HA	1.72	0.54
1:H:14:LYS:HG2	1:H:33:PRO:HB2	1.89	0.54
1:A:45:ILE:N	1:A:45:ILE:HD12	2.22	0.54
1:B:298:LYS:HZ1	2:B:1000:PDA:HA	1.72	0.54
1:A:298:LYS:NZ	2:A:1000:PDA:HA	2.22	0.54
1:C:245:THR:HA	1:C:389:ILE:HD13	1.88	0.54
1:A:94:LYS:HE3	1:B:21:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:VAL:HA	1:E:350:GLU:HG2	1.89	0.54
1:F:142:VAL:HB	1:F:234:VAL:HG22	1.89	0.54
1:I:91:THR:HG21	1:I:335:PRO:HB3	1.89	0.54
1:H:390:VAL:HB	1:H:441:MET:HB2	1.90	0.54
1:I:111:TRP:N	1:I:112:PRO:CD	2.71	0.54
1:D:282:PHE:HZ	1:D:296:MET:HE2	1.71	0.54
1:E:399:THR:HB	1:E:400:PRO:CD	2.38	0.54
1:G:191:MET:O	1:G:222:MET:HE1	2.08	0.54
1:G:56:PHE:HZ	1:G:423:MET:HE2	1.72	0.54
1:G:111:TRP:N	1:G:112:PRO:HD3	2.22	0.54
1:K:454:ILE:O	1:K:458:MET:HG2	2.08	0.54
1:E:272:LEU:HA	1:E:298:LYS:HD2	1.90	0.53
1:I:27:THR:HG21	1:I:171:GLU:HB2	1.89	0.53
1:E:27:THR:HG21	1:E:171:GLU:HB2	1.90	0.53
1:C:111:TRP:N	1:C:112:PRO:CD	2.71	0.53
1:F:425:LYS:HG3	1:F:467:TYR:CD2	2.43	0.53
1:F:376:LYS:N	1:F:376:LYS:HD2	2.22	0.53
1:C:142:VAL:HB	1:C:234:VAL:HG22	1.90	0.53
1:E:246:MET:HE2	1:E:383:GLY:HA2	1.90	0.53
1:K:208:ASP:HB2	1:K:212:GLU:O	2.08	0.53
1:K:109:GLU:HB3	1:K:290:GLN:HE21	1.74	0.53
1:L:374:LYS:NZ	1:L:462:ASP:OD1	2.34	0.53
1:B:144:ARG:NH2	1:B:237:GLU:H	2.06	0.53
1:B:437:MET:HB3	1:B:438:PRO:HD2	1.90	0.53
1:K:94:LYS:HE3	1:L:21:LEU:HD13	1.90	0.53
1:I:360:SER:HA	1:I:451:ARG:NH1	2.24	0.53
1:I:298:LYS:CE	2:I:1000:PDA:H4A1	2.39	0.53
1:A:326:GLU:OE2	1:B:410:HIS:ND1	2.35	0.52
1:E:190:LEU:HB3	1:E:222:MET:HE1	1.90	0.52
1:K:208:ASP:C	1:K:210:ASN:N	2.67	0.52
1:L:207:LYS:C	1:L:209:GLU:H	2.17	0.52
1:B:7:LYS:HD3	1:B:8:ILE:N	2.24	0.52
1:J:420:GLN:O	1:J:424:GLU:HG2	2.09	0.52
1:K:36:ILE:HD12	1:K:44:LEU:HB3	1.92	0.52
1:D:272:LEU:HD12	1:D:272:LEU:O	2.09	0.52
1:F:111:TRP:N	1:F:112:PRO:HD3	2.25	0.52
1:F:252:VAL:HB	1:F:253:PRO:HD3	1.90	0.52
1:B:145:GLU:HG3	1:B:194:SER:H	1.74	0.52
1:E:111:TRP:N	1:E:112:PRO:HD3	2.25	0.52
1:J:246:MET:HG3	1:J:382:ASP:HB3	1.91	0.52
1:B:211:GLY:HA2	1:F:202:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HZ3	2:A:1000:PDA:HA	1.75	0.52
1:A:144:ARG:NH2	1:A:237:GLU:H	2.06	0.52
1:D:60:CYS:CB	1:D:272:LEU:HD11	2.40	0.52
1:D:208:ASP:O	1:D:209:GLU:CB	2.58	0.52
1:E:386:LEU:HD11	1:E:449:VAL:HG11	1.91	0.52
1:K:321:ASP:HB3	1:L:28:GLN:HB2	1.91	0.52
1:L:208:ASP:OD1	1:L:210:ASN:HB2	2.10	0.52
1:F:149:HIS:HB2	1:F:158:VAL:HG23	1.92	0.51
1:H:111:TRP:HZ2	1:H:294:ILE:HD11	1.75	0.51
1:I:338:MET:HE2	1:I:338:MET:HA	1.92	0.51
1:K:10:TRP:CD1	1:K:47:PRO:HB3	2.45	0.51
1:D:415:ASN:OD1	1:D:416:GLN:NE2	2.43	0.51
1:E:27:THR:OG1	1:E:30:GLU:HG2	2.10	0.51
1:G:458:MET:HA	1:G:458:MET:HE2	1.92	0.51
1:J:365:ARG:O	1:J:369:GLU:HG3	2.11	0.51
1:K:190:LEU:HB3	1:K:222:MET:HE1	1.92	0.51
1:B:298:LYS:HZ3	2:B:1000:PDA:H4A1	1.75	0.51
1:E:329:SER:HB3	1:E:332:ALA:HB2	1.93	0.51
1:F:338:MET:HE2	1:F:338:MET:HA	1.93	0.51
1:I:326:GLU:HB3	1:J:163:SER:O	2.11	0.51
1:J:257:LYS:O	1:J:261:GLU:HG3	2.10	0.51
1:A:394:ASN:ND2	1:A:401:TYR:CE1	2.78	0.51
1:C:129:LEU:O	1:C:133:ARG:HG3	2.10	0.51
1:G:424:GLU:HA	1:G:424:GLU:OE1	2.11	0.51
1:H:60:CYS:CB	1:H:272:LEU:HD11	2.40	0.51
1:I:76:LYS:HG2	1:J:76:LYS:HG2	1.93	0.51
1:C:414:PRO:HA	1:C:417:ILE:HD12	1.93	0.51
1:E:190:LEU:HB3	1:E:222:MET:CE	2.41	0.51
1:A:76:LYS:HG2	1:B:76:LYS:HG2	1.92	0.51
1:H:64:LEU:HD12	1:H:353:LEU:CD1	2.41	0.51
1:A:419:THR:HG21	1:A:440:THR:O	2.11	0.50
1:I:223:ILE:HG23	1:I:231:VAL:HG21	1.93	0.50
1:A:304:SER:O	1:A:305:LEU:HD23	2.11	0.50
1:I:394:ASN:OD1	1:I:396:LYS:HB2	2.11	0.50
1:I:442:ARG:HD2	3:I:2009:HOH:O	2.12	0.50
1:G:324:ARG:HB2	1:H:169:VAL:HG23	1.94	0.50
1:H:168:LEU:O	1:H:177:SER:HA	2.12	0.50
1:L:397:THR:C	1:L:399:THR:H	2.19	0.50
1:G:117:PHE:O	1:G:332:ALA:HB1	2.12	0.50
1:H:35:PRO:HD2	3:H:2005:HOH:O	2.12	0.50
1:J:208:ASP:C	1:J:210:ASN:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLY:O	1:B:474:GLN:HG3	2.12	0.50
1:A:208:ASP:C	1:A:210:ASN:H	2.20	0.49
1:E:337:ALA:O	1:E:341:VAL:HG23	2.12	0.49
1:F:293:ILE:HG12	1:F:312:VAL:HG12	1.92	0.49
1:G:356:GLN:HE21	1:G:448:ASN:HA	1.77	0.49
1:I:384:TYR:CD1	1:I:384:TYR:N	2.79	0.49
1:J:111:TRP:N	1:J:112:PRO:CD	2.75	0.49
1:A:58:GLN:OE1	1:B:85:VAL:HA	2.13	0.49
1:C:424:GLU:OE1	1:C:424:GLU:HA	2.12	0.49
1:G:111:TRP:N	1:G:112:PRO:CD	2.75	0.49
1:K:451:ARG:HD2	1:K:451:ARG:N	2.28	0.49
1:E:111:TRP:N	1:E:112:PRO:CD	2.75	0.49
1:L:249:TYR:CD1	1:L:249:TYR:C	2.89	0.49
1:K:187:SER:O	1:K:188:ALA:HB3	2.13	0.49
1:F:111:TRP:N	1:F:112:PRO:CD	2.76	0.49
1:K:437:MET:HE2	1:K:437:MET:HA	1.95	0.49
1:H:136:THR:HB	1:H:138:ARG:HD2	1.95	0.49
1:H:208:ASP:C	1:H:208:ASP:OD1	2.56	0.49
1:D:267:ILE:HG12	1:D:293:ILE:HB	1.95	0.49
1:L:367:LYS:O	1:L:371:LEU:HG	2.13	0.49
1:L:394:ASN:OD1	1:L:396:LYS:HD2	2.13	0.49
1:L:64:LEU:HD11	1:L:347:VAL:CG1	2.38	0.49
1:J:100:ILE:O	1:J:104:ASP:HB2	2.13	0.48
1:I:360:SER:HA	1:I:451:ARG:HH12	1.77	0.48
1:I:386:LEU:HD13	1:I:447:LEU:HA	1.95	0.48
1:K:100:ILE:HA	1:K:104:ASP:HB2	1.95	0.48
1:L:208:ASP:O	1:L:209:GLU:HB2	2.13	0.48
1:I:276:GLY:HA3	1:I:447:LEU:CD1	2.43	0.48
1:J:258:MET:HG2	1:J:262:LEU:HD12	1.93	0.48
1:J:334:HIS:O	1:J:338:MET:HG2	2.14	0.48
1:G:420:GLN:O	1:G:424:GLU:HG2	2.12	0.48
1:A:424:GLU:OE1	1:A:424:GLU:HA	2.14	0.48
1:B:282:PHE:CZ	1:B:296:MET:HE2	2.49	0.48
1:G:40:GLU:HG2	1:G:45:ILE:HD11	1.95	0.48
1:G:169:VAL:HG23	1:H:324:ARG:HB2	1.95	0.48
1:I:337:ALA:O	1:I:340:ALA:HB3	2.14	0.48
1:K:415:ASN:O	1:K:421:ILE:HD11	2.13	0.48
1:L:222:MET:O	1:L:226:TYR:HD1	1.96	0.48
1:D:252:VAL:HB	1:D:253:PRO:HD3	1.95	0.48
1:D:470:SER:HB3	1:D:472:GLU:HB2	1.96	0.48
1:E:23:ARG:HB3	1:E:26:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:ILE:HB	1:F:183:SER:OG	2.13	0.48
1:K:111:TRP:N	1:K:112:PRO:CD	2.77	0.48
1:B:425:LYS:HG3	1:B:467:TYR:CD2	2.48	0.48
1:E:425:LYS:HG3	1:E:467:TYR:CD2	2.49	0.48
1:L:269:ASP:HA	1:L:295:THR:OG1	2.14	0.48
1:F:144:ARG:NH2	1:F:147:ASP:OD1	2.46	0.47
1:E:142:VAL:HB	1:E:234:VAL:HG22	1.96	0.47
1:J:120:THR:OG1	1:J:123:GLU:HG3	2.14	0.47
1:D:127:THR:O	1:D:131:ILE:HG13	2.13	0.47
1:F:298:LYS:HE2	2:F:1000:PDA:H4A1	1.96	0.47
1:L:343:ALA:O	1:L:347:VAL:HG23	2.14	0.47
1:F:384:TYR:N	1:F:384:TYR:HD1	2.11	0.47
1:J:216:VAL:HG11	1:J:254:GLN:HB3	1.95	0.47
1:F:412:MET:HG3	1:F:417:ILE:HD11	1.95	0.47
1:I:208:ASP:HB2	1:I:212:GLU:O	2.14	0.47
1:A:250:GLU:C	1:A:253:PRO:HD2	2.40	0.47
1:E:103:GLU:OE2	1:F:20:TYR:OH	2.26	0.47
1:E:325:TRP:HA	1:F:168:LEU:HD23	1.97	0.47
1:F:357:ALA:O	1:F:385:GLY:HA2	2.15	0.47
1:G:148:TYR:HA	1:G:159:THR:HG23	1.97	0.47
1:J:162:ARG:NH1	1:J:409:ARG:HG3	2.30	0.47
1:A:348:MET:HA	1:A:353:LEU:HD12	1.97	0.47
1:C:103:GLU:OE2	1:D:20:TYR:OH	2.25	0.47
1:G:27:THR:HG21	1:G:171:GLU:HB2	1.97	0.47
1:J:69:GLN:HG3	1:J:70:LYS:N	2.30	0.47
2:L:1000:PDA:O3A	2:L:1000:PDA:N	2.46	0.47
1:A:27:THR:HG21	1:A:171:GLU:HB2	1.95	0.47
1:A:246:MET:HG2	1:A:389:ILE:HG12	1.97	0.47
1:A:40:GLU:HG2	1:A:45:ILE:HD11	1.97	0.46
1:E:417:ILE:O	1:E:421:ILE:HG12	2.15	0.46
1:H:187:SER:O	1:H:188:ALA:HB3	2.15	0.46
1:C:37:GLU:O	1:D:81:ARG:HD2	2.15	0.46
1:D:169:VAL:HG21	1:D:410:HIS:C	2.40	0.46
1:G:427:LEU:HD13	1:G:432:LEU:HD23	1.97	0.46
1:I:375:HIS:HB3	1:I:469:GLU:OE2	2.14	0.46
1:K:90:ALA:O	1:L:35:PRO:HA	2.15	0.46
1:C:378:ILE:O	1:C:378:ILE:HG22	2.15	0.46
1:G:103:GLU:OE2	1:H:20:TYR:OH	2.18	0.46
1:K:169:VAL:HG21	1:K:410:HIS:C	2.41	0.46
1:G:376:LYS:HE2	1:G:398:LYS:HZ1	1.80	0.46
1:I:405:ASP:CG	1:I:406:ARG:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:246:MET:HE1	1:K:384:TYR:CZ	2.51	0.46
1:K:473:TRP:O	1:K:473:TRP:CE3	2.68	0.46
1:C:272:LEU:HA	1:C:298:LYS:HD2	1.96	0.46
1:C:366:SER:HA	1:C:369:GLU:HB2	1.98	0.46
1:H:238:VAL:HG13	1:H:252:VAL:HG21	1.97	0.46
1:H:433:ILE:HG12	1:H:441:MET:HE1	1.96	0.46
1:F:111:TRP:CD1	1:F:290:GLN:NE2	2.83	0.46
1:F:208:ASP:C	1:F:210:ASN:H	2.24	0.46
1:J:163:SER:HB3	1:J:408:PHE:O	2.15	0.46
1:A:269:ASP:OD1	1:A:271:VAL:HG23	2.16	0.46
1:D:246:MET:HE1	1:D:384:TYR:CZ	2.51	0.46
1:D:251:TYR:CZ	1:D:255:ILE:HG13	2.50	0.46
1:J:278:THR:HB	1:J:384:TYR:CD1	2.51	0.46
1:K:144:ARG:NH2	1:K:237:GLU:H	2.14	0.46
1:L:115:VAL:HG22	1:L:311:VAL:HG22	1.97	0.46
1:L:162:ARG:HD3	1:L:407:ASN:O	2.16	0.46
1:A:21:LEU:HD13	1:B:94:LYS:HE3	1.98	0.46
1:E:99:LYS:HG3	1:F:16:TRP:CE2	2.50	0.46
1:E:246:MET:HE2	1:E:383:GLY:CA	2.46	0.46
1:G:208:ASP:HB2	1:G:212:GLU:O	2.16	0.46
1:L:111:TRP:N	1:L:112:PRO:CD	2.79	0.46
1:E:169:VAL:HG23	1:F:324:ARG:HB2	1.98	0.46
1:G:21:LEU:HD13	1:H:94:LYS:HE3	1.98	0.46
1:K:79:LEU:HA	1:K:82:TYR:O	2.16	0.46
1:K:111:TRP:H	1:K:112:PRO:HD3	1.81	0.46
1:B:111:TRP:N	1:B:112:PRO:CD	2.78	0.45
1:B:208:ASP:HB2	1:B:212:GLU:O	2.14	0.45
1:C:69:GLN:HG3	1:C:70:LYS:N	2.27	0.45
1:D:99:LYS:C	1:D:99:LYS:HD3	2.41	0.45
1:J:111:TRP:HZ2	1:J:294:ILE:HD11	1.80	0.45
1:J:278:THR:HB	1:J:384:TYR:CE1	2.51	0.45
1:G:432:LEU:HA	3:G:2087:HOH:O	2.16	0.45
1:H:64:LEU:HD12	1:H:353:LEU:HD11	1.97	0.45
1:J:344:ASN:O	1:J:348:MET:HG3	2.16	0.45
1:B:145:GLU:O	1:B:146:HIS:HB2	2.16	0.45
1:C:212:GLU:OE2	1:C:217:LYS:HA	2.17	0.45
1:J:14:LYS:HD3	1:J:35:PRO:HG3	1.98	0.45
1:K:144:ARG:HH21	1:K:237:GLU:H	1.63	0.45
1:F:208:ASP:HB3	1:F:210:ASN:H	1.81	0.45
1:I:208:ASP:CG	1:I:210:ASN:HB2	2.42	0.45
1:C:334:HIS:HA	1:C:335:PRO:HD2	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:VAL:HA	1:C:350:GLU:HG2	1.98	0.45
1:D:470:SER:HB3	1:D:471:GLY:H	1.47	0.45
1:K:249:TYR:CD1	1:K:249:TYR:C	2.94	0.45
1:K:269:ASP:HA	1:K:295:THR:OG1	2.16	0.45
1:K:360:SER:OG	1:K:451:ARG:NH2	2.49	0.45
1:A:82:TYR:HA	1:A:83:GLY:HA3	1.83	0.45
1:C:122:SER:O	1:C:126:GLU:HG2	2.17	0.45
1:G:442:ARG:HE	1:G:442:ARG:HB3	1.56	0.45
1:L:165:ARG:HH21	1:L:183:SER:HB2	1.82	0.45
1:C:145:GLU:HG2	1:C:194:SER:HB3	1.97	0.45
1:F:31:TYR:CE2	1:F:33:PRO:HG3	2.52	0.45
1:F:190:LEU:HD11	1:F:226:TYR:CD1	2.52	0.45
1:H:396:LYS:HB2	1:H:396:LYS:NZ	2.32	0.45
1:B:298:LYS:NZ	2:B:1000:PDA:H4A1	2.32	0.45
1:F:149:HIS:HD2	1:F:158:VAL:O	1.99	0.45
1:J:329:SER:HB3	1:J:332:ALA:HB2	1.98	0.45
1:K:451:ARG:HD2	1:K:451:ARG:H	1.82	0.45
1:F:147:ASP:OD2	1:F:149:HIS:NE2	2.42	0.45
1:H:390:VAL:HB	1:H:441:MET:HG3	1.98	0.45
1:J:160:ARG:HG3	1:J:191:MET:HG3	1.99	0.45
1:K:473:TRP:O	1:K:473:TRP:HE3	2.00	0.45
1:F:272:LEU:HD11	1:F:442:ARG:NH1	2.32	0.45
1:I:85:VAL:HA	1:J:58:GLN:OE1	2.17	0.45
1:K:169:VAL:CG2	1:L:324:ARG:HB2	2.47	0.45
1:D:24:THR:C	1:D:26:SER:H	2.25	0.44
1:H:415:ASN:O	1:H:416:GLN:NE2	2.50	0.44
1:I:40:GLU:HG2	1:I:45:ILE:HD11	1.99	0.44
1:F:86:TRP:CZ2	1:F:88:THR:HB	2.53	0.44
1:F:111:TRP:CD1	1:F:112:PRO:HD3	2.51	0.44
1:F:269:ASP:HA	1:F:295:THR:OG1	2.16	0.44
1:F:412:MET:HE3	1:F:412:MET:HB2	1.83	0.44
1:H:72:ASN:O	1:H:76:LYS:HG3	2.17	0.44
1:I:24:THR:C	1:I:26:SER:H	2.24	0.44
1:K:252:VAL:HB	1:K:253:PRO:HD3	1.98	0.44
1:K:331:TYR:HE1	1:L:303:SER:HA	1.83	0.44
1:L:190:LEU:HD21	1:L:226:TYR:CZ	2.53	0.44
1:C:168:LEU:HG	1:D:134:LEU:HD13	2.00	0.44
1:G:100:ILE:O	1:G:104:ASP:HB2	2.18	0.44
1:H:173:SER:OG	1:H:175:SER:HB2	2.17	0.44
1:I:79:LEU:HD11	1:J:75:ILE:HG21	1.99	0.44
1:I:111:TRP:H	1:I:112:PRO:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:LEU:HD11	1:J:347:VAL:HG11	1.98	0.44
1:L:252:VAL:HB	1:L:253:PRO:HD3	1.99	0.44
1:L:417:ILE:O	1:L:421:ILE:HG12	2.17	0.44
1:E:449:VAL:O	1:E:449:VAL:HG13	2.17	0.44
1:G:94:LYS:CE	1:H:21:LEU:HD13	2.48	0.44
1:I:64:LEU:HD13	1:I:344:ASN:OD1	2.17	0.44
1:K:58:GLN:OE1	1:L:85:VAL:HA	2.17	0.44
1:K:163:SER:HB3	1:K:408:PHE:O	2.18	0.44
1:C:60:CYS:CB	1:C:272:LEU:HD11	2.41	0.44
1:C:100:ILE:O	1:C:104:ASP:HB2	2.17	0.44
1:C:212:GLU:HG2	1:C:217:LYS:HG2	1.99	0.44
1:D:298:LYS:CE	2:D:1000:PDA:H4A1	2.48	0.44
1:L:208:ASP:C	1:L:210:ASN:N	2.72	0.44
1:L:360:SER:O	1:L:363:TYR:HB3	2.17	0.44
1:L:372:GLN:C	1:L:374:LYS:N	2.75	0.44
1:A:207:LYS:NZ	1:A:250:GLU:OE2	2.44	0.44
1:H:253:PRO:HA	1:H:289:VAL:HG11	1.99	0.44
1:I:169:VAL:HG21	1:I:410:HIS:C	2.43	0.44
1:K:72:ASN:HA	1:K:75:ILE:HD12	2.00	0.44
1:L:258:MET:HE3	1:L:259:THR:HG23	2.00	0.44
1:A:221:ARG:NH2	1:C:145:GLU:OE1	2.47	0.44
1:B:27:THR:HG21	1:B:171:GLU:HB2	1.98	0.44
1:B:245:THR:CA	1:B:389:ILE:HD13	2.48	0.44
1:F:238:VAL:O	1:F:247:PRO:HG3	2.18	0.44
1:K:325:TRP:NE1	1:L:166:SER:O	2.51	0.44
1:L:77:GLU:O	1:L:80:ASP:HB2	2.18	0.44
1:A:412:MET:HG3	1:A:417:ILE:HD11	2.00	0.43
1:J:111:TRP:N	1:J:112:PRO:HD3	2.32	0.43
1:H:251:TYR:CZ	1:H:255:ILE:HG13	2.53	0.43
1:I:94:LYS:HG2	1:J:21:LEU:HD11	2.00	0.43
1:L:39:THR:O	1:L:67:LYS:NZ	2.42	0.43
1:L:57:ASN:HD21	1:L:62:VAL:HB	1.82	0.43
1:B:473:TRP:H	1:B:473:TRP:CD1	2.36	0.43
1:C:426:ALA:CB	1:C:433:ILE:HG22	2.48	0.43
1:I:117:PHE:O	1:I:332:ALA:HB1	2.18	0.43
1:K:96:LYS:HE2	1:K:100:ILE:HD11	2.00	0.43
1:K:258:MET:HE2	1:K:259:THR:HG23	1.99	0.43
1:K:380:ASN:HD22	1:K:380:ASN:HA	1.54	0.43
1:E:222:MET:HE2	1:E:222:MET:HB3	1.83	0.43
1:J:214:LEU:HA	1:J:217:LYS:HB2	1.99	0.43
1:K:431:VAL:HG11	1:K:457:ALA:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:LEU:C	1:F:45:ILE:HG13	2.43	0.43
1:F:162:ARG:HD3	1:F:407:ASN:O	2.17	0.43
1:L:100:ILE:HG22	1:L:105:ILE:HD12	2.01	0.43
1:G:253:PRO:HD3	1:G:287:TYR:HB3	2.00	0.43
1:H:60:CYS:HB3	1:H:272:LEU:HD11	2.01	0.43
1:H:246:MET:HE3	1:H:246:MET:HB3	1.90	0.43
1:J:144:ARG:HH21	1:J:237:GLU:H	1.65	0.43
1:C:197:THR:HG22	1:C:198:PHE:N	2.33	0.43
1:H:145:GLU:HG2	1:H:194:SER:CB	2.48	0.43
1:B:7:LYS:HD3	1:B:7:LYS:C	2.44	0.43
1:B:217:LYS:O	1:B:221:ARG:HG2	2.18	0.43
1:G:258:MET:HE2	1:G:258:MET:HB3	1.97	0.43
1:F:296:MET:HB2	1:F:309:ALA:HB3	2.00	0.43
1:H:272:LEU:HD12	1:H:272:LEU:C	2.43	0.43
1:F:17:ASP:OD1	1:F:31:TYR:OH	2.33	0.43
1:H:82:TYR:HA	1:H:83:GLY:HA3	1.69	0.43
1:K:297:GLY:O	1:K:299:GLY:N	2.52	0.42
1:A:369:GLU:O	1:A:373:GLU:HG3	2.18	0.42
1:F:459:ASP:O	1:F:462:ASP:HB3	2.19	0.42
1:F:473:TRP:CD1	1:F:473:TRP:H	2.35	0.42
1:G:85:VAL:HG22	1:G:335:PRO:HG3	2.01	0.42
1:I:346:GLU:O	1:I:350:GLU:HG2	2.19	0.42
1:K:149:HIS:HB2	1:K:158:VAL:HG23	2.01	0.42
1:A:17:ASP:OD2	1:A:31:TYR:OH	2.33	0.42
1:F:64:LEU:HD23	1:F:71:VAL:HG21	2.00	0.42
1:F:284:TYR:CD1	1:F:284:TYR:C	2.97	0.42
1:F:322:LYS:HB3	1:F:322:LYS:HE2	1.85	0.42
1:H:121:GLY:O	1:H:124:ALA:HB3	2.19	0.42
1:E:187:SER:O	1:E:188:ALA:HB3	2.19	0.42
1:H:405:ASP:CG	1:H:406:ARG:H	2.27	0.42
1:J:209:GLU:C	1:J:211:GLY:H	2.27	0.42
1:C:298:LYS:NZ	2:C:1000:PDA:H4A1	2.34	0.42
1:D:61:CYS:HB3	1:D:298:LYS:CD	2.46	0.42
1:G:208:ASP:N	1:G:212:GLU:O	2.53	0.42
1:K:243:GLY:O	1:K:406:ARG:NE	2.49	0.42
1:E:32:GLN:HA	1:E:33:PRO:HD3	1.93	0.42
1:F:238:VAL:CG1	1:F:287:TYR:HE2	2.32	0.42
1:J:148:TYR:HE2	2:J:1000:PDA:H4A2	1.83	0.42
1:A:383:GLY:HA3	1:A:388:TRP:CE3	2.54	0.42
1:G:278:THR:HB	1:G:384:TYR:CD1	2.54	0.42
1:D:127:THR:CG2	1:D:310:VAL:HG11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:385:GLY:O	1:E:388:TRP:NE1	2.50	0.42
1:H:390:VAL:HB	1:H:441:MET:CG	2.50	0.42
1:K:366:SER:HA	1:K:369:GLU:HG3	2.02	0.42
1:K:401:TYR:HB2	1:K:418:PRO:HG3	2.01	0.42
1:D:208:ASP:N	1:D:212:GLU:O	2.52	0.42
1:I:221:ARG:HH21	1:K:145:GLU:CD	2.28	0.42
1:I:429:LYS:HD3	1:I:463:TYR:CE2	2.54	0.42
1:K:471:GLY:C	1:K:473:TRP:H	2.28	0.42
1:L:57:ASN:ND2	1:L:62:VAL:HB	2.35	0.42
1:A:385:GLY:C	1:A:386:LEU:HD22	2.44	0.42
1:F:417:ILE:HG23	1:F:438:PRO:HA	2.01	0.42
1:L:177:SER:HB2	1:L:409:ARG:NH1	2.35	0.42
1:C:363:TYR:CE2	1:C:367:LYS:HD2	2.55	0.41
1:D:252:VAL:HG12	1:D:289:VAL:HG21	2.01	0.41
1:H:432:LEU:HA	3:H:2073:HOH:O	2.19	0.41
1:H:471:GLY:C	1:H:473:TRP:H	2.28	0.41
1:L:111:TRP:N	1:L:112:PRO:HD3	2.34	0.41
1:A:198:PHE:HD1	1:C:214:LEU:HD13	1.85	0.41
1:C:35:PRO:HA	1:D:90:ALA:O	2.20	0.41
1:D:364:ILE:HG13	1:D:454:ILE:HD13	2.01	0.41
1:E:120:THR:OG1	1:E:123:GLU:HG3	2.20	0.41
1:G:145:GLU:CG	1:G:194:SER:HB2	2.49	0.41
1:B:64:LEU:HD11	1:B:347:VAL:HG12	2.01	0.41
1:D:133:ARG:O	1:D:137:ASN:N	2.53	0.41
1:E:85:VAL:HG22	1:E:335:PRO:HG3	2.03	0.41
1:F:245:THR:HA	1:F:389:ILE:HD13	2.01	0.41
1:J:193:PRO:HB3	1:L:218:TYR:CE1	2.55	0.41
1:J:204:ASN:OD1	1:J:204:ASN:N	2.54	0.41
1:J:246:MET:HE2	1:J:383:GLY:HA2	2.02	0.41
1:B:377:SER:HB3	1:B:469:GLU:HG3	2.02	0.41
1:F:272:LEU:HD12	1:F:298:LYS:HE3	2.03	0.41
1:C:90:ALA:O	1:D:35:PRO:HA	2.20	0.41
1:E:103:GLU:O	1:E:107:GLY:HA3	2.20	0.41
1:G:32:GLN:HA	1:G:33:PRO:HD3	1.88	0.41
1:G:142:VAL:HB	1:G:234:VAL:HG22	2.02	0.41
1:I:329:SER:O	1:I:330:THR:C	2.63	0.41
1:I:370:LEU:O	1:I:374:LYS:HB2	2.20	0.41
1:K:114:LYS:HD3	1:L:22:MET:HA	2.01	0.41
1:K:324:ARG:HG3	1:L:27:THR:HG23	2.02	0.41
1:B:52:LEU:HD13	1:B:432:LEU:HD21	2.03	0.41
1:C:145:GLU:O	1:C:146:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ARG:NH2	1:D:237:GLU:H	2.14	0.41
1:E:162:ARG:HD3	1:E:407:ASN:O	2.20	0.41
1:E:165:ARG:HA	1:E:165:ARG:HD2	1.85	0.41
1:E:208:ASP:C	1:E:210:ASN:N	2.78	0.41
1:G:293:ILE:HG12	1:G:312:VAL:HG12	2.02	0.41
1:I:420:GLN:O	1:I:424:GLU:HG2	2.21	0.41
1:L:246:MET:HE1	1:L:384:TYR:CZ	2.56	0.41
1:L:252:VAL:N	1:L:253:PRO:HD2	2.35	0.41
1:A:144:ARG:HH21	1:A:237:GLU:H	1.67	0.41
1:D:60:CYS:HB3	1:D:272:LEU:HD11	2.02	0.41
1:I:123:GLU:HB3	1:J:151:TRP:HZ2	1.85	0.41
1:I:125:VAL:HG21	1:I:149:HIS:O	2.20	0.41
1:J:147:ASP:OD2	1:J:149:HIS:NE2	2.41	0.41
1:K:99:LYS:HE2	1:K:103:GLU:OE1	2.21	0.41
1:L:149:HIS:HB2	1:L:158:VAL:HG23	2.03	0.41
1:L:413:ASN:HA	1:L:414:PRO:HD2	1.83	0.41
1:B:357:ALA:O	1:B:385:GLY:HA2	2.20	0.41
1:E:75:ILE:HG21	1:F:79:LEU:HD11	2.02	0.41
1:E:216:VAL:HG11	1:E:254:GLN:HB3	2.03	0.41
1:G:114:LYS:HD2	1:G:317:ALA:HB1	2.02	0.41
1:G:246:MET:HE3	1:G:246:MET:HB3	1.94	0.41
1:H:348:MET:HG2	1:H:353:LEU:HD12	2.02	0.41
1:I:35:PRO:HA	1:J:90:ALA:O	2.21	0.41
1:J:10:TRP:CD1	1:J:47:PRO:HB3	2.56	0.41
1:J:82:TYR:HA	1:J:83:GLY:HA3	1.83	0.41
1:B:415:ASN:OD1	1:B:416:GLN:HG2	2.21	0.41
1:C:238:VAL:HG22	1:C:252:VAL:HG21	2.03	0.41
1:G:333:GLY:O	1:G:334:HIS:C	2.64	0.41
1:J:206:LEU:HB3	1:J:214:LEU:CD1	2.51	0.41
1:K:79:LEU:HD23	1:K:82:TYR:O	2.21	0.41
1:K:422:ILE:HD11	1:K:468:LEU:HD22	2.03	0.41
1:L:125:VAL:HG21	1:L:149:HIS:O	2.21	0.41
1:L:166:SER:HB2	1:L:180:ILE:HD11	2.02	0.41
1:I:208:ASP:O	1:I:209:GLU:CB	2.68	0.40
1:A:269:ASP:HA	1:A:295:THR:OG1	2.20	0.40
1:C:16:TRP:CE2	1:D:99:LYS:HG3	2.57	0.40
1:D:297:GLY:O	1:D:299:GLY:N	2.54	0.40
1:E:163:SER:HB3	1:E:408:PHE:O	2.21	0.40
1:E:347:VAL:O	1:E:350:GLU:HG2	2.22	0.40
1:K:122:SER:N	2:K:1000:PDA:OP1	2.49	0.40
1:K:278:THR:O	1:K:384:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:PRO:O	1:G:36:ILE:HD13	2.21	0.40
1:G:67:LYS:HG3	1:G:72:ASN:HD21	1.86	0.40
1:H:245:THR:HA	1:H:389:ILE:HD13	2.03	0.40
1:I:67:LYS:HE2	1:J:80:ASP:O	2.20	0.40
1:J:384:TYR:CD1	1:J:384:TYR:N	2.89	0.40
1:L:110:ASP:O	1:L:314:LYS:HD2	2.22	0.40
1:A:40:GLU:OE2	1:A:51:ARG:NH1	2.49	0.40
1:B:61:CYS:HB3	1:B:298:LYS:HD3	2.03	0.40
1:C:355:GLU:OE1	1:C:355:GLU:HA	2.20	0.40
1:E:418:PRO:HD2	1:E:438:PRO:O	2.22	0.40
1:F:272:LEU:HA	1:F:298:LYS:HD2	2.03	0.40
1:J:160:ARG:NE	1:J:160:ARG:HA	2.37	0.40
1:K:160:ARG:NE	1:K:160:ARG:HA	2.36	0.40
1:K:168:LEU:O	1:K:177:SER:HA	2.22	0.40
1:K:199:GLN:HA	1:K:204:ASN:O	2.22	0.40
1:K:224:GLU:HA	1:K:228:PRO:HD3	2.03	0.40
1:K:375:HIS:ND1	1:K:469:GLU:OE1	2.54	0.40
1:A:168:LEU:HG	1:B:134:LEU:HD22	2.04	0.40
1:A:176:PHE:HB3	3:B:2088:HOH:O	2.21	0.40
1:K:111:TRP:CE2	1:K:112:PRO:HG3	2.56	0.40
1:K:272:LEU:HD12	1:K:298:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/485 (94%)	429 (94%)	22 (5%)	4 (1%)	14	17
1	B	455/485 (94%)	429 (94%)	22 (5%)	4 (1%)	14	17
1	C	455/485 (94%)	428 (94%)	22 (5%)	5 (1%)	11	13
1	D	461/485 (95%)	429 (93%)	26 (6%)	6 (1%)	9	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	455/485 (94%)	430 (94%)	21 (5%)	4 (1%)	14	17
1	F	461/485 (95%)	435 (94%)	23 (5%)	3 (1%)	18	23
1	G	453/485 (93%)	430 (95%)	20 (4%)	3 (1%)	18	23
1	H	456/485 (94%)	434 (95%)	18 (4%)	4 (1%)	14	17
1	I	455/485 (94%)	421 (92%)	30 (7%)	4 (1%)	14	17
1	J	455/485 (94%)	422 (93%)	31 (7%)	2 (0%)	30	38
1	K	455/485 (94%)	420 (92%)	30 (7%)	5 (1%)	11	13
1	L	454/485 (94%)	419 (92%)	27 (6%)	8 (2%)	6	6
All	All	5470/5820 (94%)	5126 (94%)	292 (5%)	52 (1%)	12	15

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	153	GLY
1	K	209	GLU
1	A	87	ASP
1	B	209	GLU
1	D	153	GLY
1	D	298	LYS
1	E	153	GLY
1	G	25	PHE
1	G	58	GLN
1	J	153	GLY
1	K	58	GLN
1	L	153	GLY
1	L	208	ASP
1	L	298	LYS
1	A	58	GLN
1	B	298	LYS
1	C	298	LYS
1	D	470	SER
1	E	58	GLN
1	F	153	GLY
1	F	298	LYS
1	G	298	LYS
1	H	298	LYS
1	I	25	PHE
1	I	472	GLU
1	J	58	GLN

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Mol	Chain	Res	Type
1	L	58	GLN
1	B	58	GLN
1	C	58	GLN
1	C	153	GLY
1	D	58	GLN
1	E	298	LYS
1	F	58	GLN
1	H	58	GLN
1	H	87	ASP
1	K	298	LYS
1	K	332	ALA
1	L	398	LYS
1	A	25	PHE
1	A	209	GLU
1	D	25	PHE
1	D	209	GLU
1	I	58	GLN
1	I	209	GLU
1	C	25	PHE
1	E	384	TYR
1	L	25	PHE
1	L	41	GLY
1	L	406	ARG
1	B	153	GLY
1	C	139	PRO
1	H	139	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	388/409 (95%)	375 (97%)	13 (3%)	32	49
1	B	388/409 (95%)	376 (97%)	12 (3%)	35	52
1	C	388/409 (95%)	373 (96%)	15 (4%)	28	43
1	D	391/409 (96%)	379 (97%)	12 (3%)	35	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	388/409 (95%)	375 (97%)	13 (3%)	32	49
1	F	391/409 (96%)	377 (96%)	14 (4%)	31	47
1	G	386/409 (94%)	381 (99%)	5 (1%)	61	77
1	H	388/409 (95%)	373 (96%)	15 (4%)	28	43
1	I	388/409 (95%)	378 (97%)	10 (3%)	40	59
1	J	388/409 (95%)	371 (96%)	17 (4%)	25	38
1	K	388/409 (95%)	369 (95%)	19 (5%)	22	34
1	L	387/409 (95%)	368 (95%)	19 (5%)	22	34
All	All	4659/4908 (95%)	4495 (96%)	164 (4%)	32	48

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	19	LYS
1	A	26	SER
1	A	52	LEU
1	A	69	GLN
1	A	145	GLU
1	A	175	SER
1	A	199	GLN
1	A	210	ASN
1	A	260	LYS
1	A	384	TYR
1	A	442	ARG
1	A	451	ARG
1	B	7	LYS
1	B	145	GLU
1	B	209	GLU
1	B	238	VAL
1	B	315	GLU
1	B	384	TYR
1	B	386	LEU
1	B	389	ILE
1	B	396	LYS
1	B	441	MET
1	B	451	ARG
1	B	474	GLN
1	C	69	GLN

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Mol	Chain	Res	Type
1	C	189	VAL
1	C	212	GLU
1	C	217	LYS
1	C	222	MET
1	C	238	VAL
1	C	310	VAL
1	C	355	GLU
1	C	367	LYS
1	C	384	TYR
1	C	386	LEU
1	C	389	ILE
1	C	427	LEU
1	C	442	ARG
1	C	474	GLN
1	D	103	GLU
1	D	197	THR
1	D	201	SER
1	D	217	LYS
1	D	238	VAL
1	D	272	LEU
1	D	310	VAL
1	D	384	TYR
1	D	408	PHE
1	D	470	SER
1	D	472	GLU
1	D	474	GLN
1	E	40	GLU
1	E	69	GLN
1	E	206	LEU
1	E	209	GLU
1	E	217	LYS
1	E	222	MET
1	E	238	VAL
1	E	255	ILE
1	E	257	LYS
1	E	384	TYR
1	E	398	LYS
1	E	408	PHE
1	E	441	MET
1	F	7	LYS
1	F	21	LEU
1	F	45	ILE

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Mol	Chain	Res	Type
1	F	88	THR
1	F	197	THR
1	F	210	ASN
1	F	353	LEU
1	F	376	LYS
1	F	384	TYR
1	F	408	PHE
1	F	416	GLN
1	F	441	MET
1	F	442	ARG
1	F	459	ASP
1	G	177	SER
1	G	258	MET
1	G	352	ASN
1	G	384	TYR
1	G	442	ARG
1	H	26	SER
1	H	69	GLN
1	H	115	VAL
1	H	174	GLU
1	H	175	SER
1	H	209	GLU
1	H	272	LEU
1	H	300	LEU
1	H	310	VAL
1	H	351	GLU
1	H	384	TYR
1	H	389	ILE
1	H	396	LYS
1	H	425	LYS
1	H	442	ARG
1	I	18	ARG
1	I	62	VAL
1	I	64	LEU
1	I	209	GLU
1	I	212	GLU
1	I	374	LYS
1	I	380	ASN
1	I	384	TYR
1	I	440	THR
1	I	451	ARG
1	J	19	LYS

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Mol	Chain	Res	Type
1	J	69	GLN
1	J	204	ASN
1	J	210	ASN
1	J	217	LYS
1	J	222	MET
1	J	238	VAL
1	J	239	SER
1	J	290	GLN
1	J	346	GLU
1	J	355	GLU
1	J	362	GLU
1	J	373	GLU
1	J	384	TYR
1	J	389	ILE
1	J	416	GLN
1	J	440	THR
1	K	7	LYS
1	K	8	ILE
1	K	15	GLU
1	K	19	LYS
1	K	64	LEU
1	K	110	ASP
1	K	199	GLN
1	K	204	ASN
1	K	206	LEU
1	K	260	LYS
1	K	310	VAL
1	K	373	GLU
1	K	380	ASN
1	K	384	TYR
1	K	389	ILE
1	K	401	TYR
1	K	408	PHE
1	K	441	MET
1	K	451	ARG
1	L	15	GLU
1	L	21	LEU
1	L	44	LEU
1	L	67	LYS
1	L	69	GLN
1	L	71	VAL
1	L	217	LYS

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Mol	Chain	Res	Type
1	L	250	GLU
1	L	258	MET
1	L	310	VAL
1	L	370	LEU
1	L	382	ASP
1	L	384	TYR
1	L	396	LYS
1	L	418	PRO
1	L	427	LEU
1	L	442	ARG
1	L	443	ILE
1	L	451	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	GLN
1	A	372	GLN
1	B	196	ASN
1	B	356	GLN
1	C	474	GLN
1	D	72	ASN
1	D	202	ASN
1	D	356	GLN
1	D	416	GLN
1	E	372	GLN
1	E	474	GLN
1	F	196	ASN
1	F	199	GLN
1	F	202	ASN
1	F	290	GLN
1	G	69	GLN
1	G	356	GLN
1	G	372	GLN
1	G	474	GLN
1	H	204	ASN
1	H	344	ASN
1	H	356	GLN
1	H	372	GLN
1	H	413	ASN
1	H	415	ASN
1	I	9	ASN

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Mol	Chain	Res	Type
1	I	372	GLN
1	J	199	GLN
1	J	290	GLN
1	J	359	ASN
1	J	474	GLN
1	K	196	ASN
1	K	372	GLN
1	K	380	ASN
1	L	9	ASN
1	L	12	GLN
1	L	204	ASN
1	L	372	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	PDA	J	1000	-	20,21,21	2.26	2 (10%)	26,30,30	1.12	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PDA	I	1000	-	20,21,21	2.36	2 (10%)	26,30,30	1.48	7 (26%)
2	PDA	C	1000	-	20,21,21	2.34	3 (15%)	26,30,30	1.38	3 (11%)
2	PDA	A	1000	-	20,21,21	2.31	2 (10%)	26,30,30	1.14	2 (7%)
2	PDA	L	1000	-	20,21,21	2.57	3 (15%)	26,30,30	1.55	4 (15%)
2	PDA	F	1000	-	20,21,21	2.54	2 (10%)	26,30,30	1.28	2 (7%)
2	PDA	H	1000	-	20,21,21	2.52	2 (10%)	26,30,30	1.55	3 (11%)
2	PDA	D	1000	-	20,21,21	2.17	3 (15%)	26,30,30	1.59	6 (23%)
2	PDA	G	1000	-	20,21,21	2.23	3 (15%)	26,30,30	1.34	4 (15%)
2	PDA	E	1000	-	20,21,21	2.43	2 (10%)	26,30,30	1.38	2 (7%)
2	PDA	K	1000	-	20,21,21	2.26	2 (10%)	26,30,30	1.36	3 (11%)
2	PDA	B	1000	-	20,21,21	2.18	3 (15%)	26,30,30	1.55	6 (23%)

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	PDA	J	1000	-	-	5/15/15/15	0/1/1/1
2	PDA	I	1000	-	-	8/15/15/15	0/1/1/1
2	PDA	C	1000	-	-	5/15/15/15	0/1/1/1
2	PDA	A	1000	-	-	5/15/15/15	0/1/1/1
2	PDA	L	1000	-	-	5/15/15/15	0/1/1/1
2	PDA	F	1000	-	-	5/15/15/15	0/1/1/1
2	PDA	H	1000	-	-	5/15/15/15	0/1/1/1
2	PDA	D	1000	-	-	4/15/15/15	0/1/1/1
2	PDA	G	1000	-	-	6/15/15/15	0/1/1/1
2	PDA	E	1000	-	-	8/15/15/15	0/1/1/1
2	PDA	K	1000	-	-	5/15/15/15	0/1/1/1
2	PDA	B	1000	-	-	5/15/15/15	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1000	PDA	C3-C2	8.73	1.50	1.41
2	H	1000	PDA	C3-C2	8.28	1.49	1.41
2	E	1000	PDA	C3-C2	7.94	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1000	PDA	C3-C2	7.42	1.48	1.41
2	L	1000	PDA	C4A-N	-7.38	1.25	1.46
2	L	1000	PDA	C3-C2	7.37	1.48	1.41
2	J	1000	PDA	C3-C2	7.24	1.48	1.41
2	C	1000	PDA	C3-C2	7.22	1.48	1.41
2	A	1000	PDA	C3-C2	7.03	1.48	1.41
2	K	1000	PDA	C4A-N	-6.87	1.26	1.46
2	G	1000	PDA	C4A-N	-6.81	1.26	1.46
2	I	1000	PDA	C4A-N	-6.74	1.27	1.46
2	C	1000	PDA	C4A-N	-6.65	1.27	1.46
2	D	1000	PDA	C4A-N	-6.59	1.27	1.46
2	K	1000	PDA	C3-C2	6.46	1.47	1.41
2	B	1000	PDA	C3-C2	6.43	1.47	1.41
2	E	1000	PDA	C4A-N	-6.40	1.28	1.46
2	H	1000	PDA	C4A-N	-6.29	1.28	1.46
2	A	1000	PDA	C4A-N	-6.27	1.28	1.46
2	J	1000	PDA	C4A-N	-6.21	1.28	1.46
2	F	1000	PDA	C4A-N	-6.20	1.28	1.46
2	G	1000	PDA	C3-C2	6.16	1.47	1.41
2	B	1000	PDA	C4A-N	-6.00	1.29	1.46
2	D	1000	PDA	C3-C2	5.90	1.47	1.41
2	L	1000	PDA	C4A-C4	-3.10	1.47	1.52
2	D	1000	PDA	C4A-C4	-2.39	1.48	1.52
2	G	1000	PDA	C4A-C4	-2.31	1.48	1.52
2	B	1000	PDA	C4A-C4	-2.26	1.48	1.52
2	C	1000	PDA	OXT-C	2.08	1.28	1.22

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1000	PDA	C6-C5-C4	4.77	121.67	118.06
2	L	1000	PDA	OP4-C5A-C5	4.04	116.93	109.36
2	D	1000	PDA	C4A-C4-C5	3.55	123.62	119.75
2	B	1000	PDA	C4A-C4-C5	3.54	123.60	119.75
2	E	1000	PDA	C4A-C4-C5	3.21	123.24	119.75
2	G	1000	PDA	C6-C5-C4	3.02	120.35	118.06
2	D	1000	PDA	C2A-C2-N1	2.95	123.19	117.64
2	C	1000	PDA	C6-C5-C4	2.90	120.25	118.06
2	F	1000	PDA	C6-C5-C4	2.85	120.22	118.06
2	B	1000	PDA	C2A-C2-N1	2.85	123.01	117.64
2	B	1000	PDA	OXT-C-CA	-2.77	113.74	122.14
2	B	1000	PDA	O-C-CA	2.72	122.80	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1000	PDA	C5A-C5-C6	-2.70	114.95	119.36
2	D	1000	PDA	C2A-C2-C3	-2.69	117.65	120.80
2	C	1000	PDA	C4A-C4-C5	2.67	122.66	119.75
2	L	1000	PDA	C2A-C2-N1	2.62	122.57	117.64
2	I	1000	PDA	O-C-CA	2.60	122.40	113.84
2	A	1000	PDA	C4A-C4-C5	2.59	122.57	119.75
2	C	1000	PDA	OP3-P-OP2	2.58	117.48	107.80
2	K	1000	PDA	C4A-C4-C3	2.54	123.36	119.98
2	I	1000	PDA	CB-CA-C	2.54	115.79	110.23
2	L	1000	PDA	OP2-P-OP4	2.50	113.19	106.67
2	A	1000	PDA	C6-C5-C4	2.49	119.95	118.06
2	I	1000	PDA	OP4-C5A-C5	2.48	114.00	109.36
2	E	1000	PDA	C6-C5-C4	2.47	119.93	118.06
2	L	1000	PDA	C3-C2-N1	-2.41	117.92	120.96
2	H	1000	PDA	OP3-P-OP2	2.39	116.77	107.80
2	I	1000	PDA	C2A-C2-N1	2.34	122.05	117.64
2	K	1000	PDA	C2A-C2-N1	2.33	122.03	117.64
2	B	1000	PDA	OP3-P-OP4	2.29	112.64	106.67
2	D	1000	PDA	C6-C5-C4	2.28	119.78	118.06
2	D	1000	PDA	C4A-C4-C3	-2.20	117.06	119.98
2	I	1000	PDA	C3-C2-N1	-2.18	118.20	120.96
2	D	1000	PDA	O-C-CA	2.16	120.97	113.84
2	B	1000	PDA	C4A-C4-C3	-2.16	117.11	119.98
2	I	1000	PDA	C6-C5-C4	2.15	119.69	118.06
2	G	1000	PDA	O3A-C3-C4	2.14	124.40	118.18
2	G	1000	PDA	C5-C6-N1	-2.10	120.42	123.83
2	K	1000	PDA	OP2-P-OP4	2.09	112.12	106.67
2	G	1000	PDA	C6-N1-C2	2.09	122.98	119.20
2	F	1000	PDA	C2A-C2-C3	2.08	123.23	120.80
2	J	1000	PDA	O-C-CA	2.07	120.67	113.84
2	I	1000	PDA	OXT-C-CA	-2.06	115.91	122.14

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	PDA	C5-C4-C4A-N
2	B	1000	PDA	C-CA-N-C4A
2	C	1000	PDA	CB-CA-N-C4A
2	C	1000	PDA	C-CA-N-C4A
2	D	1000	PDA	CB-CA-N-C4A
2	E	1000	PDA	C-CA-N-C4A

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Mol	Chain	Res	Type	Atoms
2	E	1000	PDA	O-C-CA-N
2	E	1000	PDA	OXT-C-CA-N
2	F	1000	PDA	C-CA-N-C4A
2	G	1000	PDA	C-CA-N-C4A
2	H	1000	PDA	C-CA-N-C4A
2	H	1000	PDA	C3-C4-C4A-N
2	H	1000	PDA	C5-C4-C4A-N
2	I	1000	PDA	CB-CA-N-C4A
2	I	1000	PDA	C-CA-N-C4A
2	I	1000	PDA	C5-C4-C4A-N
2	I	1000	PDA	O-C-CA-N
2	I	1000	PDA	OXT-C-CA-N
2	J	1000	PDA	CB-CA-N-C4A
2	J	1000	PDA	C3-C4-C4A-N
2	J	1000	PDA	C5-C4-C4A-N
2	J	1000	PDA	C5A-OP4-P-OP2
2	K	1000	PDA	C-CA-N-C4A
2	K	1000	PDA	C3-C4-C4A-N
2	K	1000	PDA	C5-C4-C4A-N
2	L	1000	PDA	C-CA-N-C4A
2	L	1000	PDA	C3-C4-C4A-N
2	L	1000	PDA	C5-C4-C4A-N
2	B	1000	PDA	C5-C4-C4A-N
2	E	1000	PDA	C5-C4-C4A-N
2	F	1000	PDA	C5-C4-C4A-N
2	G	1000	PDA	C5-C4-C4A-N
2	C	1000	PDA	C5-C4-C4A-N
2	F	1000	PDA	OXT-C-CA-CB
2	A	1000	PDA	C3-C4-C4A-N
2	C	1000	PDA	C3-C4-C4A-N
2	G	1000	PDA	C3-C4-C4A-N
2	I	1000	PDA	C3-C4-C4A-N
2	E	1000	PDA	O-C-CA-CB
2	E	1000	PDA	OXT-C-CA-CB
2	F	1000	PDA	O-C-CA-CB
2	B	1000	PDA	C3-C4-C4A-N
2	E	1000	PDA	C3-C4-C4A-N
2	F	1000	PDA	C3-C4-C4A-N
2	G	1000	PDA	C4-C5-C5A-OP4
2	A	1000	PDA	C-CA-N-C4A
2	B	1000	PDA	O-C-CA-CB
2	G	1000	PDA	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	J	1000	PDA	C-CA-N-C4A
2	B	1000	PDA	OXT-C-CA-CB
2	H	1000	PDA	O-C-CA-CB
2	L	1000	PDA	O-C-CA-CB
2	D	1000	PDA	O-C-CA-CB
2	G	1000	PDA	OXT-C-CA-CB
2	H	1000	PDA	OXT-C-CA-CB
2	I	1000	PDA	O-C-CA-CB
2	I	1000	PDA	OXT-C-CA-CB
2	K	1000	PDA	O-C-CA-CB
2	L	1000	PDA	OXT-C-CA-CB
2	C	1000	PDA	C5A-OP4-P-OP2
2	E	1000	PDA	CB-CA-N-C4A
2	A	1000	PDA	OXT-C-CA-CB
2	D	1000	PDA	OXT-C-CA-CB
2	K	1000	PDA	OXT-C-CA-CB
2	A	1000	PDA	O-C-CA-CB
2	D	1000	PDA	C-CA-N-C4A

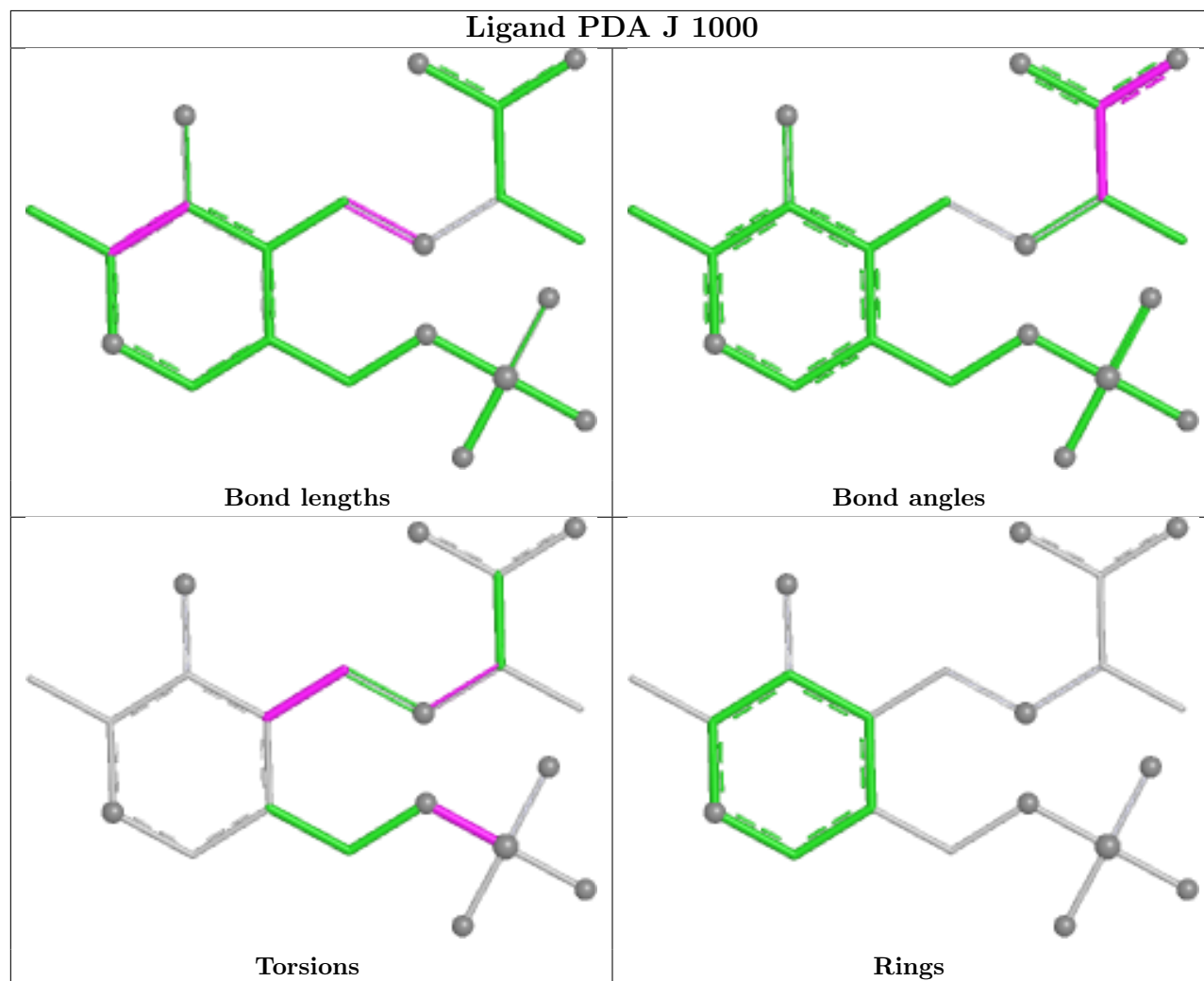
There are no ring outliers.

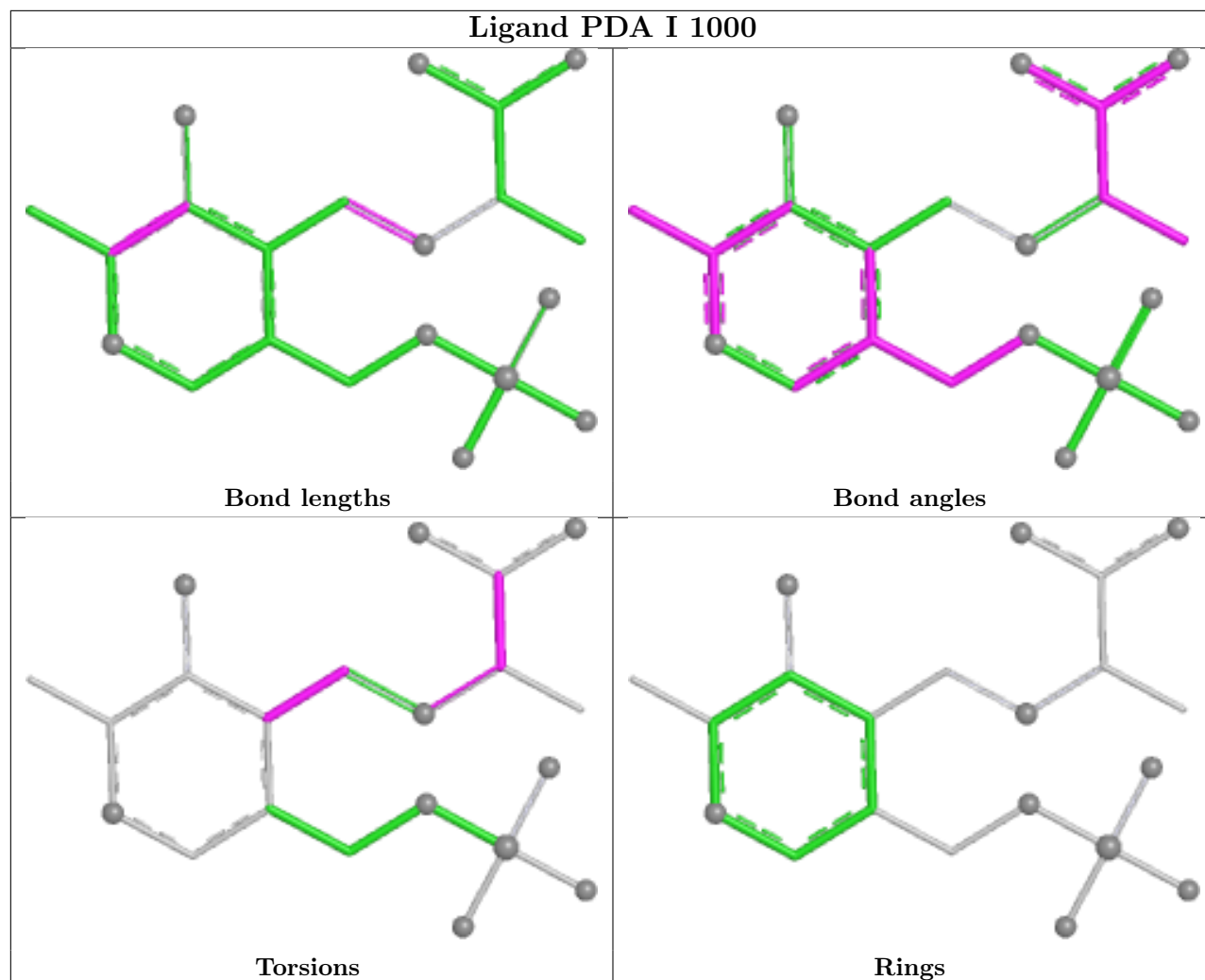
9 monomers are involved in 19 short contacts:

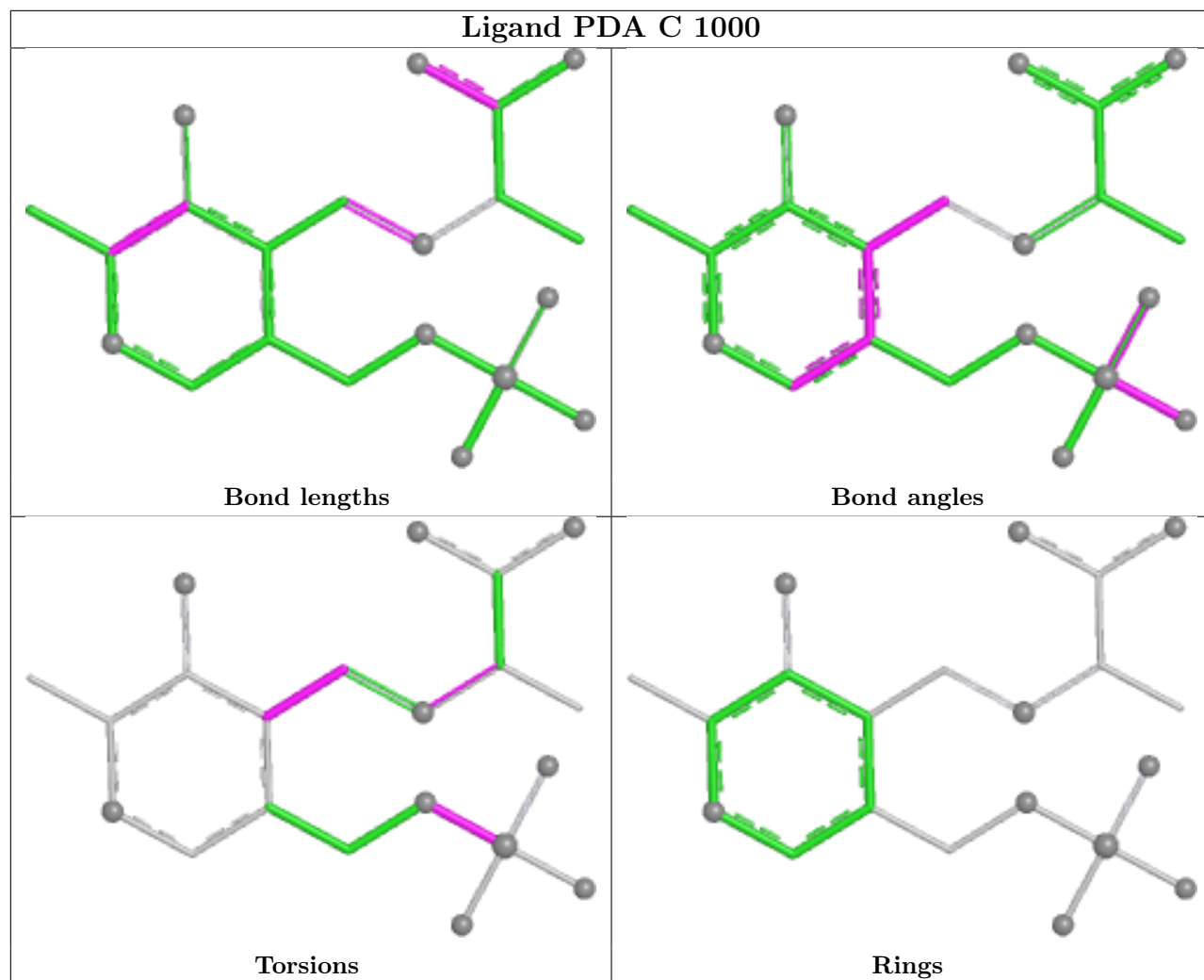
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1000	PDA	1	0
2	I	1000	PDA	2	0
2	C	1000	PDA	3	0
2	A	1000	PDA	2	0
2	L	1000	PDA	1	0
2	F	1000	PDA	4	0
2	D	1000	PDA	2	0
2	K	1000	PDA	1	0
2	B	1000	PDA	3	0

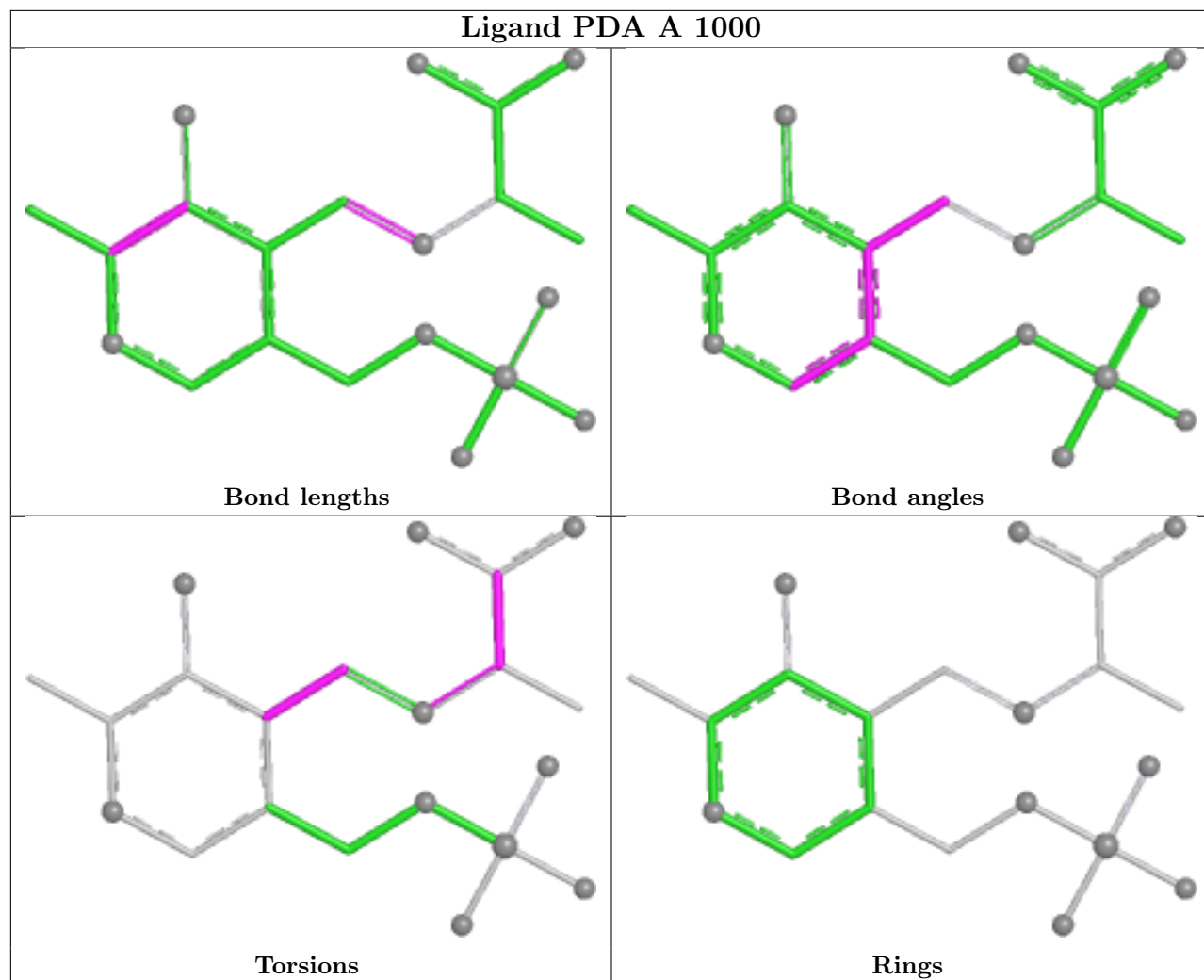
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

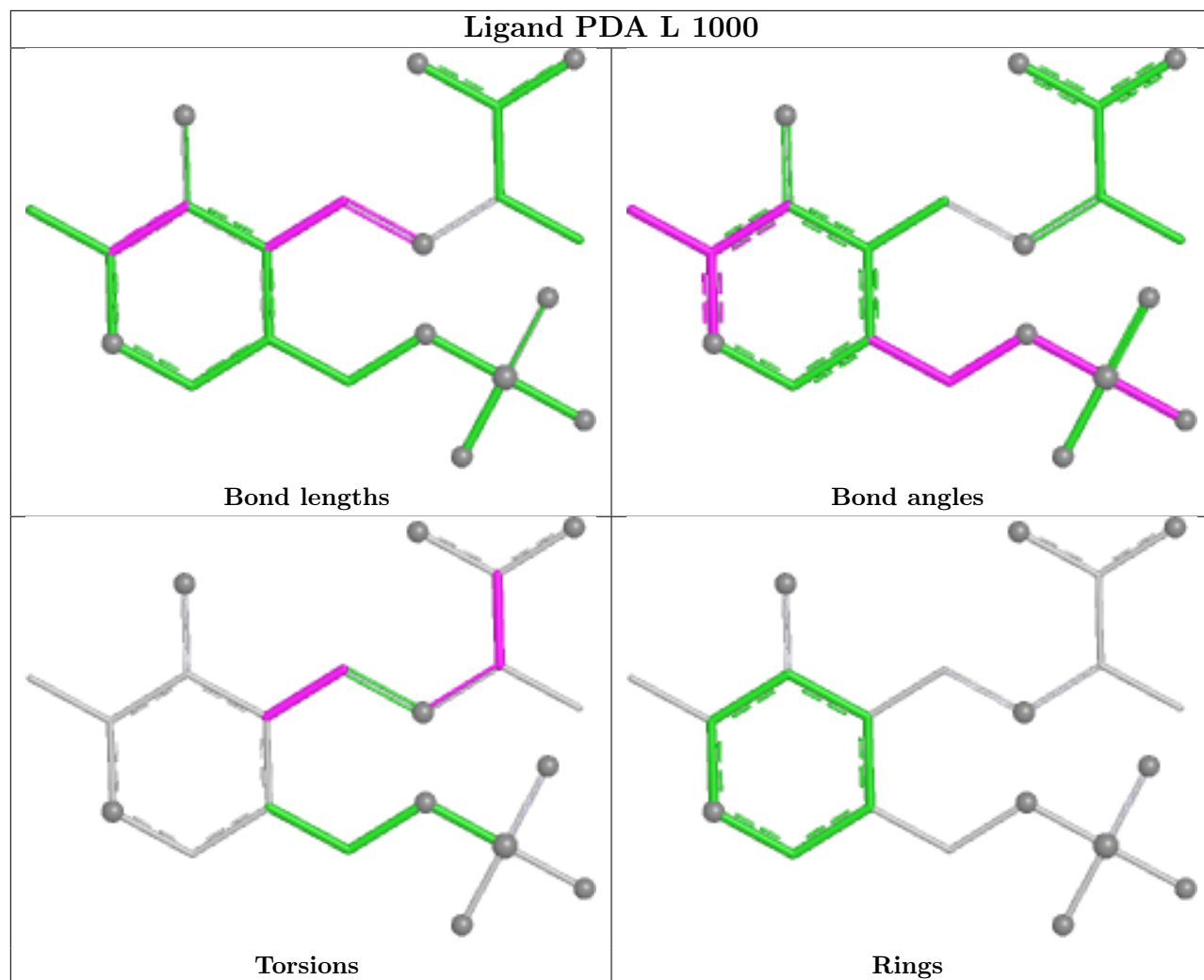
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

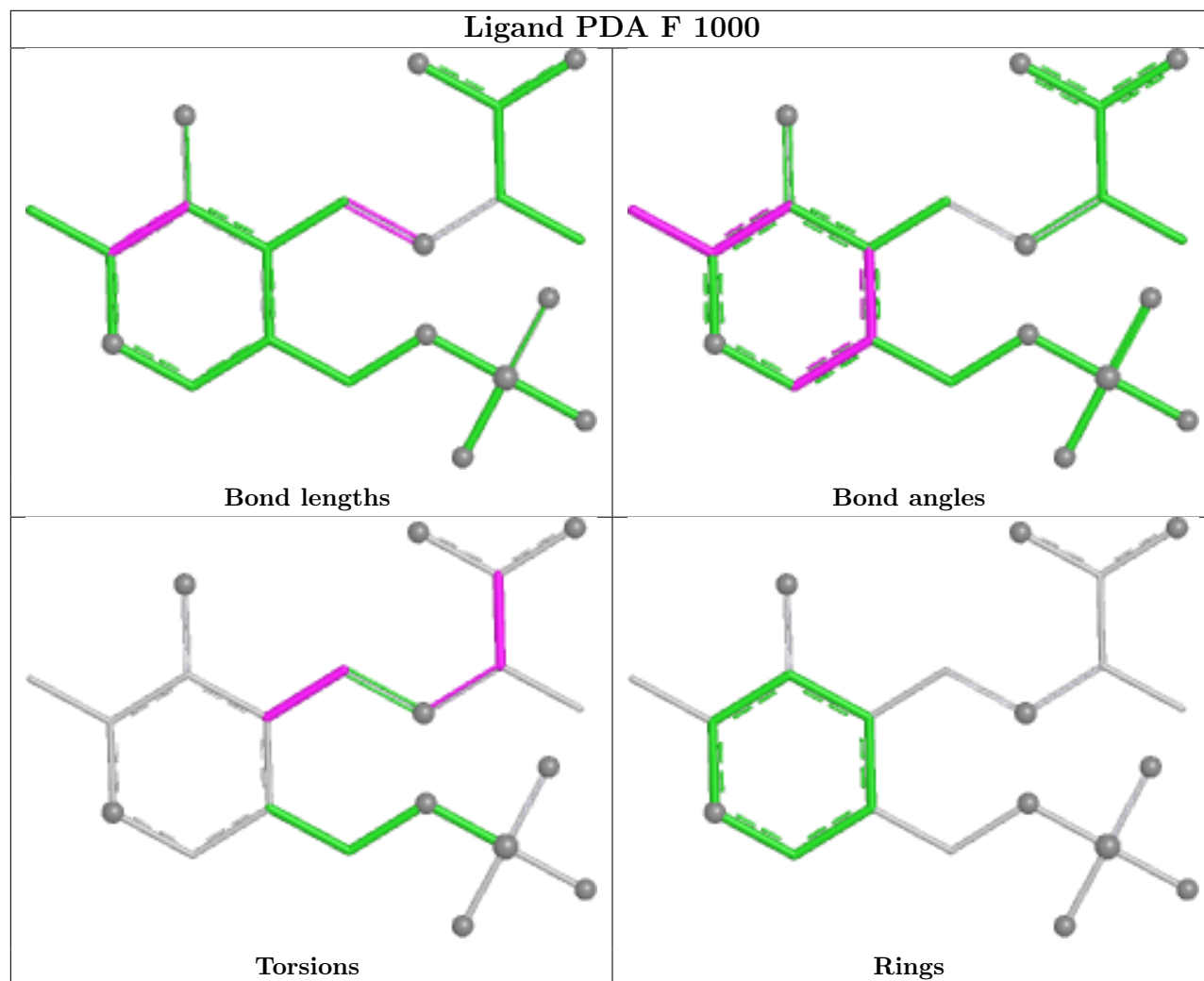


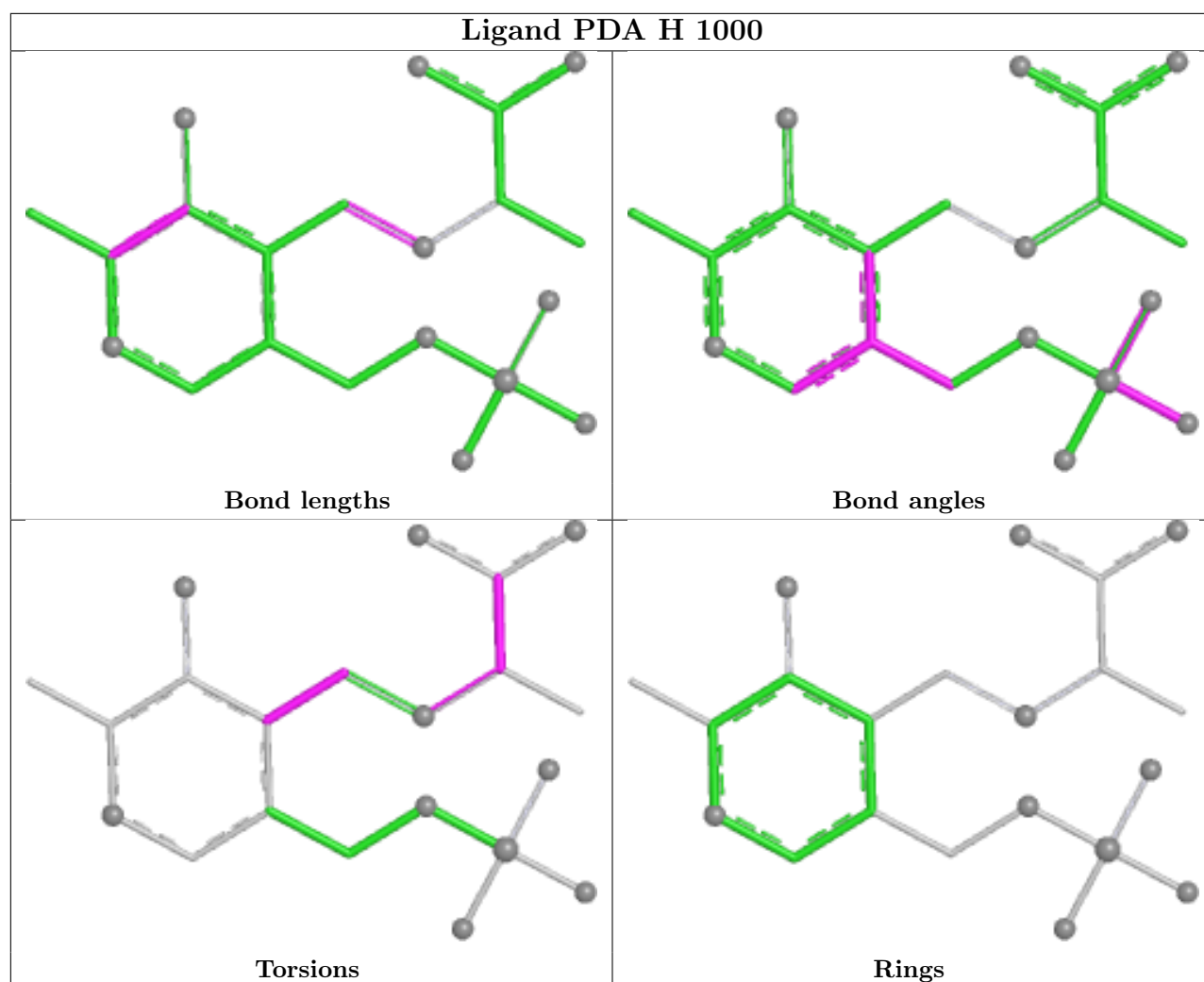


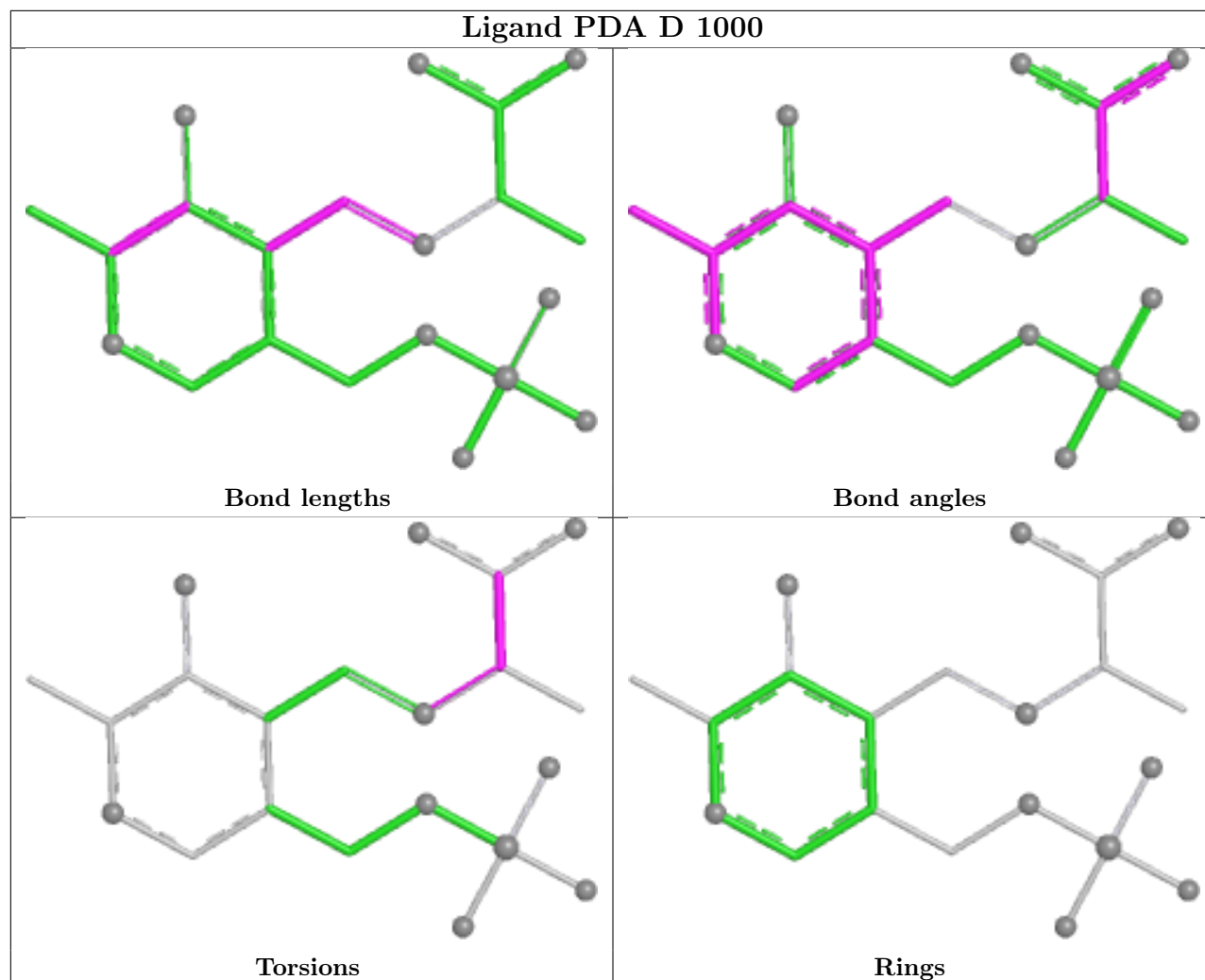


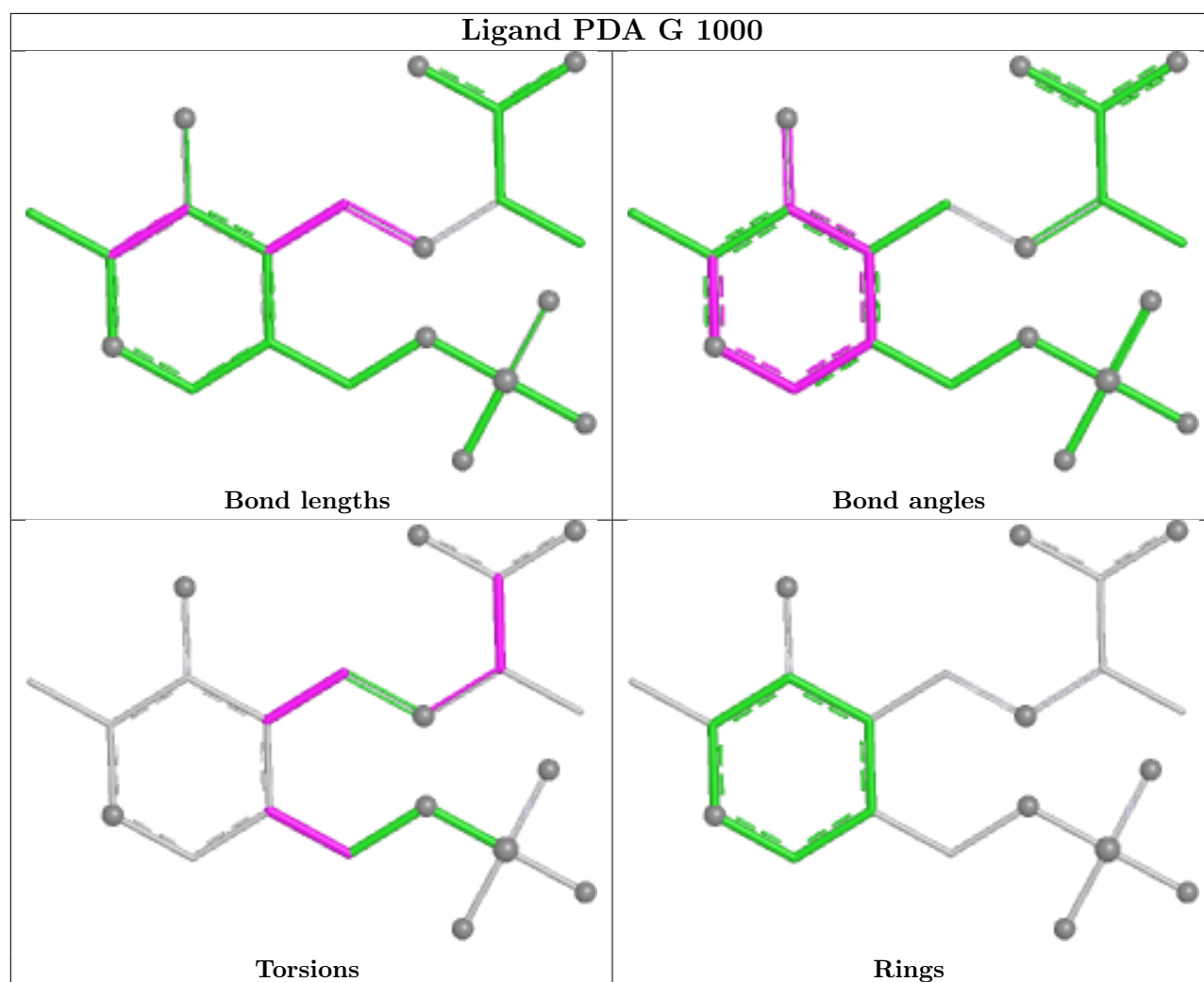


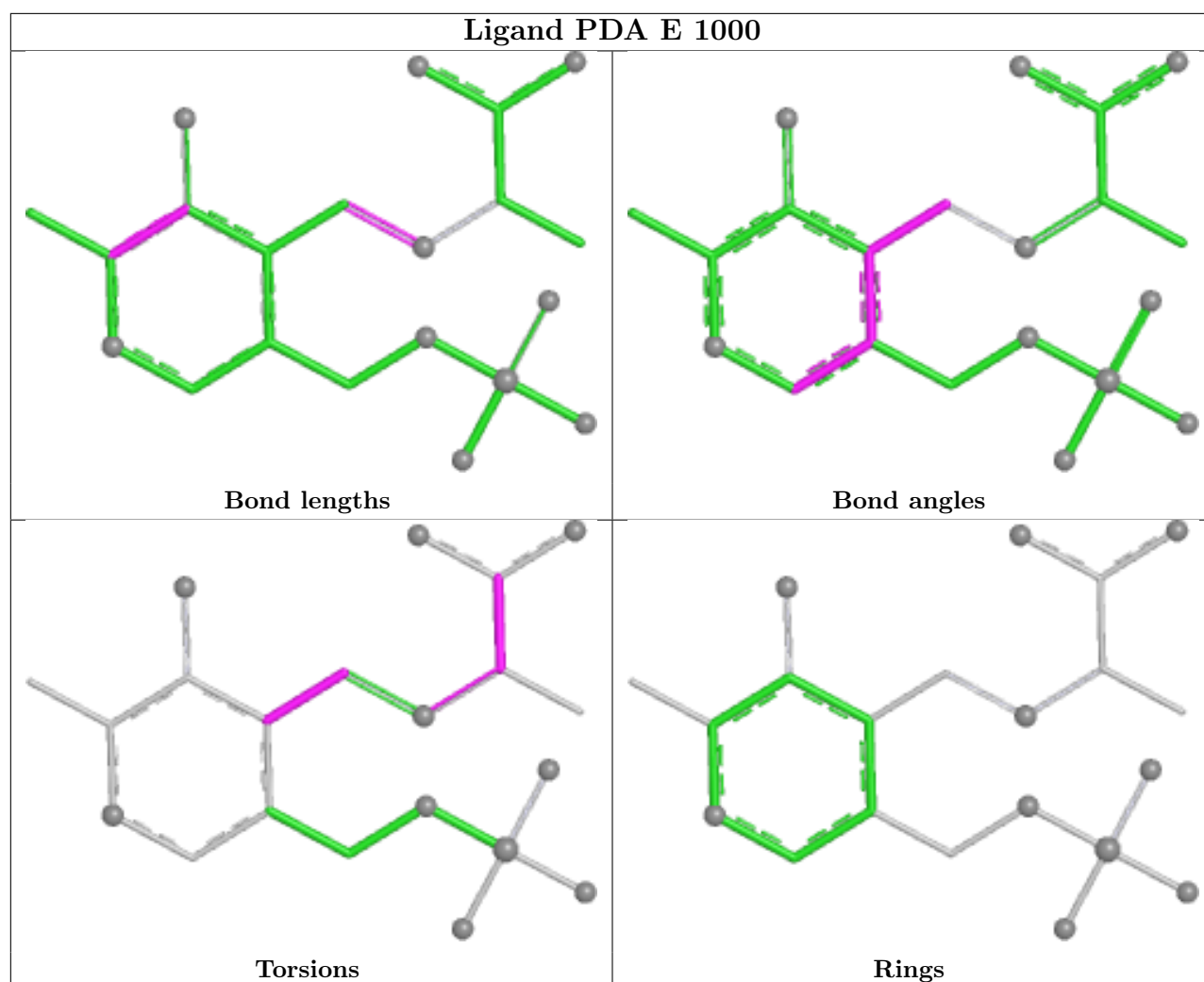


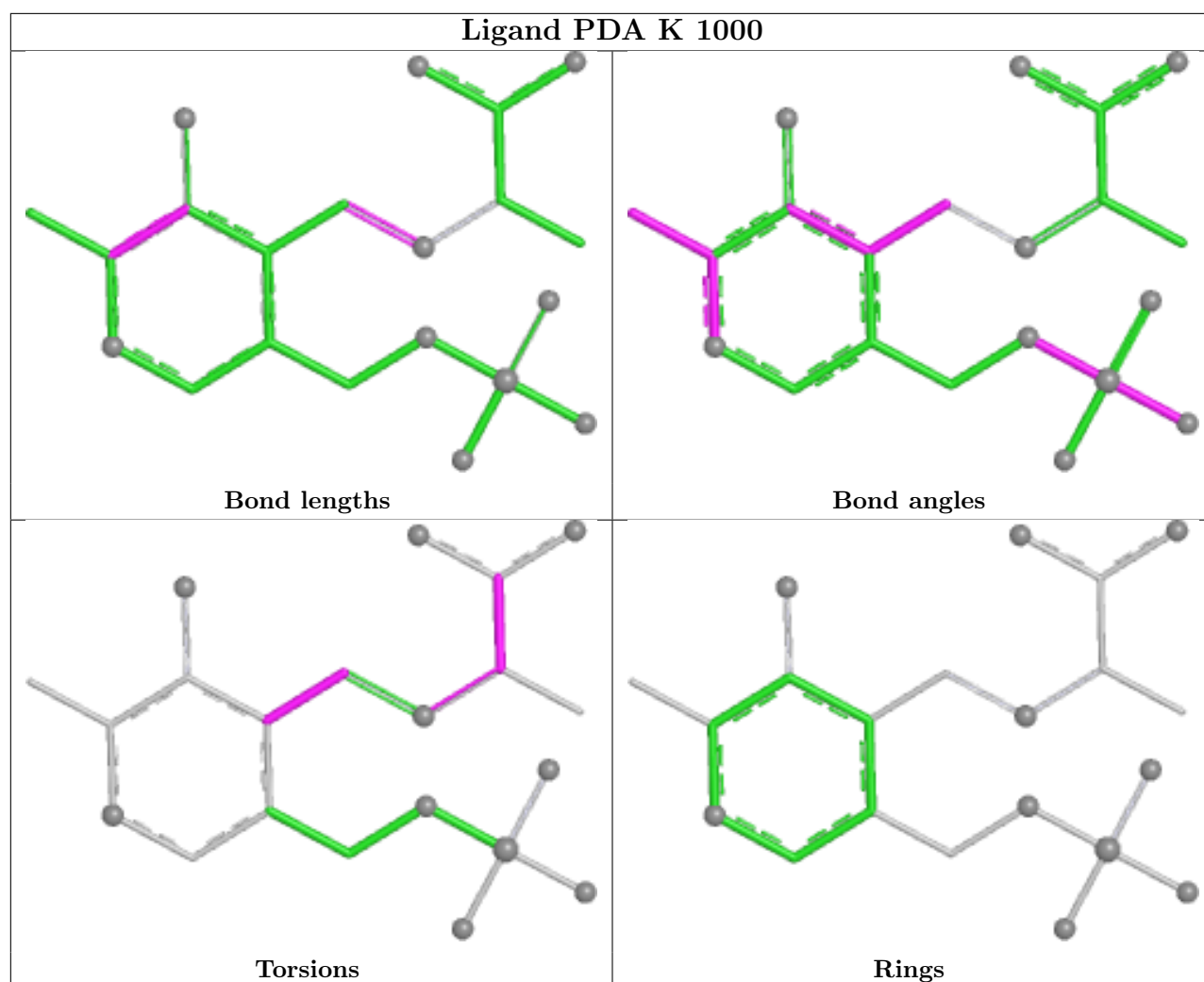


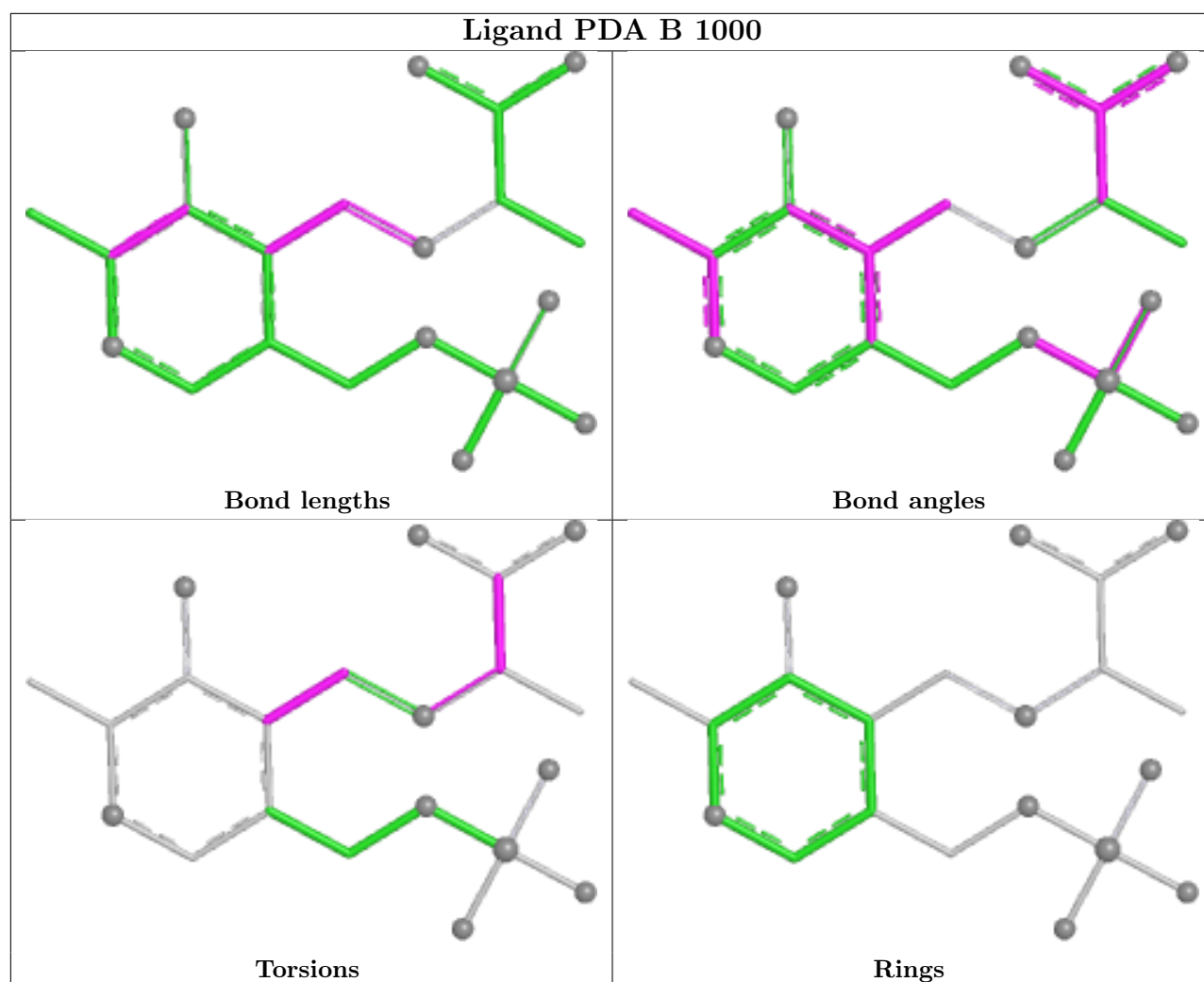












5.7 Other polymers [i](#)

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	461/485 (95%)	-0.19	2 (0%) 88 89	45, 55, 75, 94	0
1	B	461/485 (95%)	-0.25	0 100 100	43, 56, 74, 97	0
1	C	461/485 (95%)	-0.01	1 (0%) 91 91	49, 63, 81, 96	0
1	D	465/485 (95%)	0.03	1 (0%) 91 91	48, 63, 84, 116	0
1	E	461/485 (95%)	0.18	0 100 100	53, 72, 91, 107	0
1	F	465/485 (95%)	0.14	1 (0%) 91 91	51, 68, 88, 114	0
1	G	459/485 (94%)	-0.01	1 (0%) 91 91	49, 64, 87, 118	0
1	H	462/485 (95%)	-0.05	1 (0%) 91 91	47, 61, 81, 98	0
1	I	461/485 (95%)	0.40	6 (1%) 75 76	52, 77, 101, 127	0
1	J	461/485 (95%)	0.78	22 (4%) 35 37	59, 86, 114, 133	0
1	K	461/485 (95%)	0.73	16 (3%) 47 49	57, 96, 136, 163	0
1	L	460/485 (94%)	0.91	30 (6%) 25 27	63, 110, 164, 185	0
All	All	5538/5820 (95%)	0.22	81 (1%) 72 73	43, 69, 119, 185	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	461	LEU	3.7
1	K	82	TYR	3.6
1	H	200	ASP	3.6
1	L	370	LEU	3.5
1	J	467	TYR	3.4
1	K	276	GLY	3.2
1	L	431	VAL	3.2
1	L	214	LEU	3.2
1	J	370	LEU	3.0
1	J	34	VAL	2.9
1	K	93	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	38	SER	2.8
1	J	48	GLY	2.8
1	J	353	LEU	2.7
1	J	464	ALA	2.7
1	I	83	GLY	2.7
1	L	473	TRP	2.7
1	I	90	ALA	2.7
1	J	460	ALA	2.7
1	K	198	PHE	2.7
1	K	8	ILE	2.7
1	C	187	SER	2.6
1	L	83	GLY	2.6
1	J	371	LEU	2.5
1	K	381	PHE	2.5
1	I	85	VAL	2.5
1	L	354	VAL	2.5
1	J	368	LEU	2.5
1	L	427	LEU	2.5
1	L	445	ALA	2.5
1	J	211	GLY	2.5
1	L	198	PHE	2.4
1	K	243	GLY	2.4
1	L	436	ALA	2.4
1	L	379	GLY	2.3
1	J	422	ILE	2.3
1	J	272	LEU	2.3
1	L	368	LEU	2.3
1	L	249	TYR	2.3
1	J	36	ILE	2.3
1	L	8	ILE	2.3
1	L	36	ILE	2.3
1	L	175	SER	2.3
1	J	389	ILE	2.3
1	K	390	VAL	2.3
1	L	13	VAL	2.3
1	J	205	TYR	2.3
1	F	176	PHE	2.2
1	J	72	ASN	2.2
1	K	343	ALA	2.2
1	L	10	TRP	2.2
1	L	336	VAL	2.2
1	J	176	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	59	LEU	2.2
1	J	71	VAL	2.2
1	L	238	VAL	2.2
1	L	430	GLY	2.2
1	A	249	TYR	2.1
1	J	364	ILE	2.1
1	J	433	ILE	2.1
1	L	25	PHE	2.1
1	L	55	PHE	2.1
1	L	381	PHE	2.1
1	D	395	ALA	2.1
1	I	357	ALA	2.1
1	I	131	ILE	2.1
1	K	44	LEU	2.1
1	K	79	LEU	2.1
1	L	371	LEU	2.1
1	K	363	TYR	2.1
1	L	71	VAL	2.1
1	A	473	TRP	2.1
1	G	176	PHE	2.1
1	I	370	LEU	2.1
1	K	176	PHE	2.1
1	K	78	ALA	2.0
1	J	465	LEU	2.0
1	J	468	LEU	2.0
1	K	401	TYR	2.0
1	K	370	LEU	2.0
1	L	447	LEU	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,

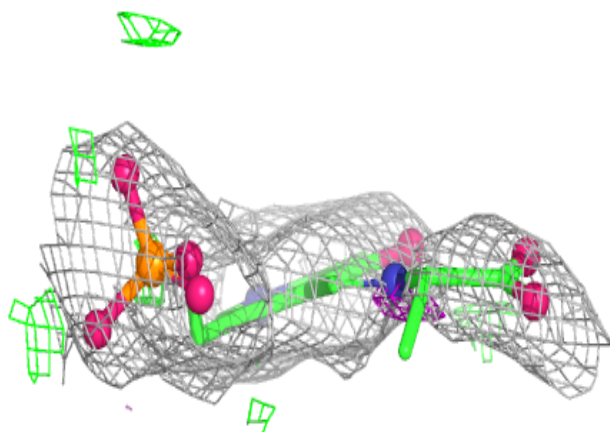
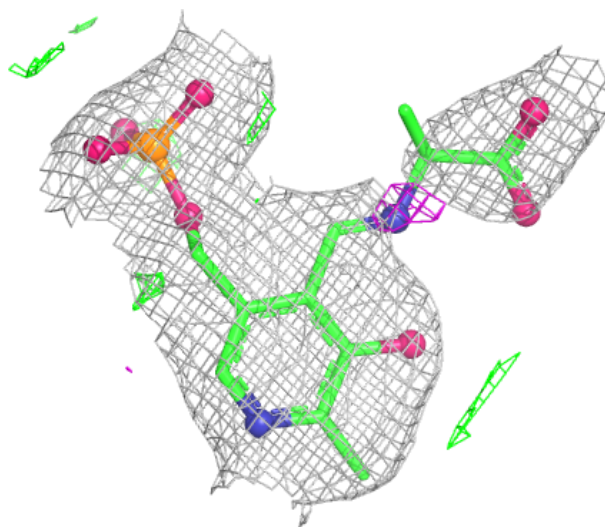
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PDA	J	1000	21/21	0.92	0.12	68,74,89,92	0
2	PDA	K	1000	21/21	0.94	0.12	76,83,87,88	0
2	PDA	L	1000	21/21	0.94	0.11	90,94,117,121	0
2	PDA	E	1000	21/21	0.96	0.09	65,69,81,84	0
2	PDA	F	1000	21/21	0.96	0.10	60,63,89,92	0
2	PDA	I	1000	21/21	0.96	0.10	60,62,85,91	0
2	PDA	H	1000	21/21	0.97	0.08	48,55,72,76	0
2	PDA	D	1000	21/21	0.97	0.09	55,60,71,75	0
2	PDA	B	1000	21/21	0.97	0.08	47,55,65,69	0
2	PDA	C	1000	21/21	0.97	0.09	49,57,74,76	0
2	PDA	G	1000	21/21	0.97	0.07	53,60,77,79	0
2	PDA	A	1000	21/21	0.98	0.07	48,52,66,69	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.

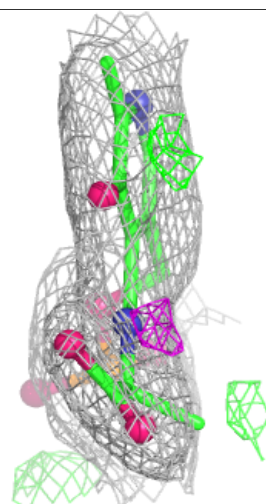
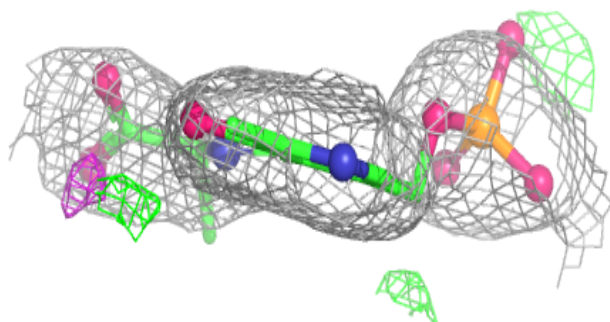
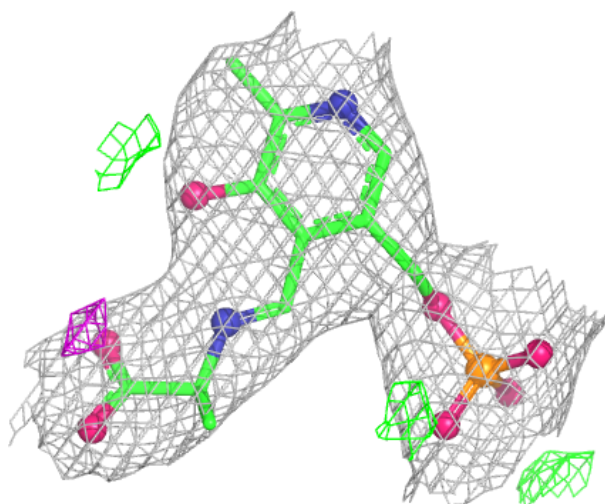
Electron density around PDA J 1000:

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



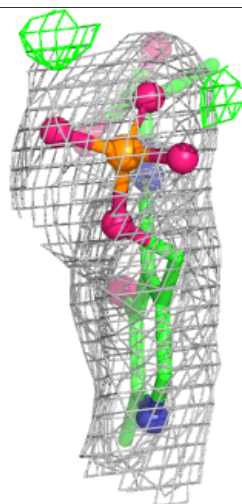
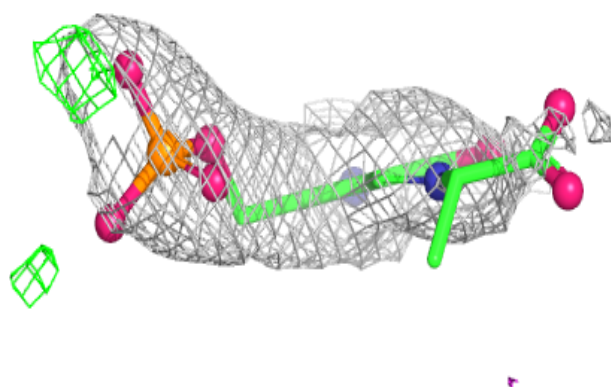
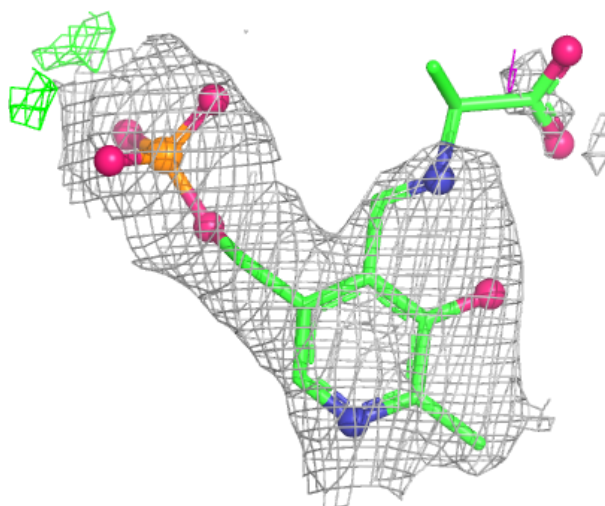
Electron density around PDA K 1000:

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



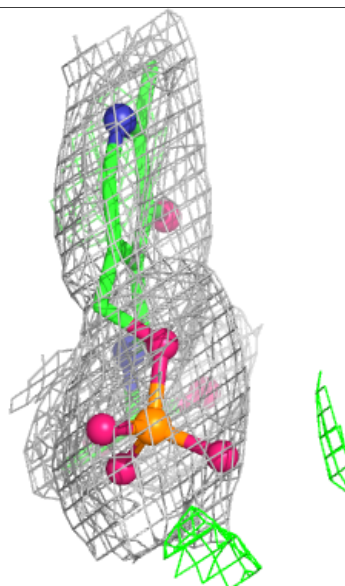
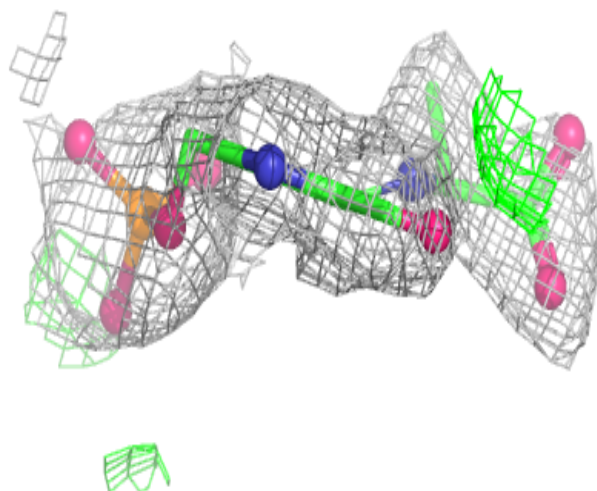
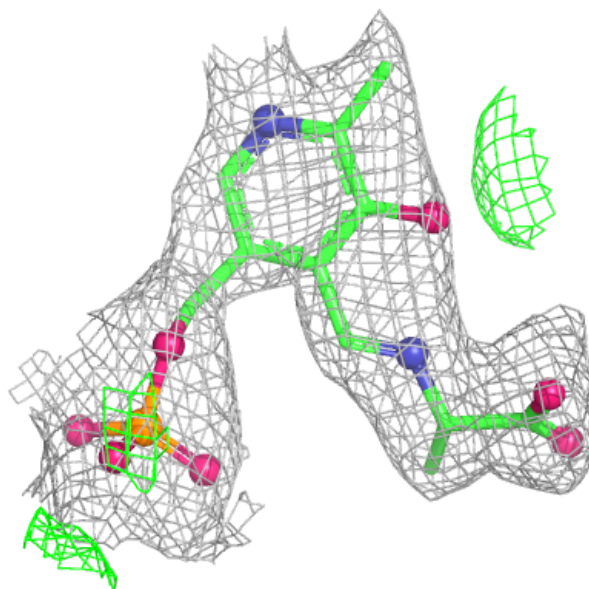
Electron density around PDA L 1000:

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



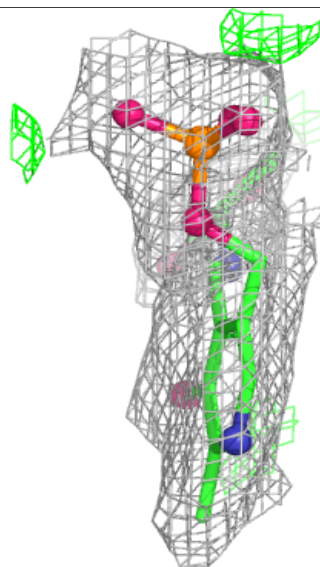
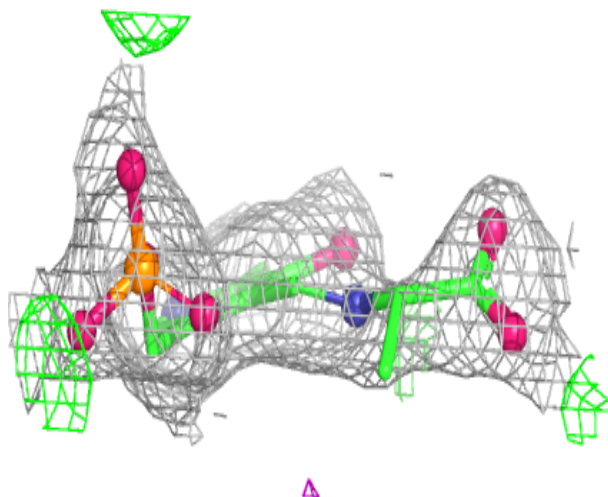
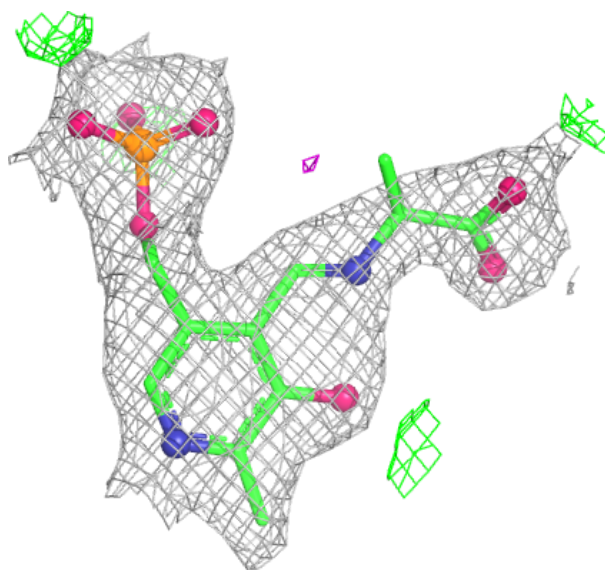
Electron density around PDA E 1000:

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



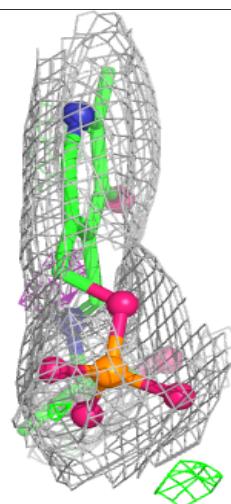
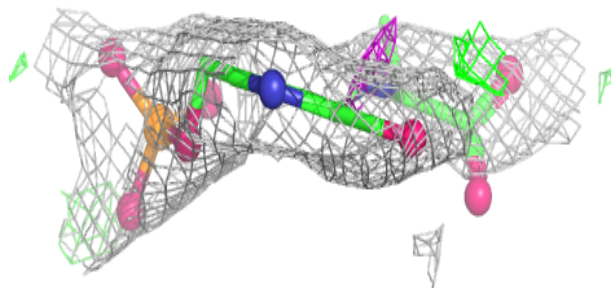
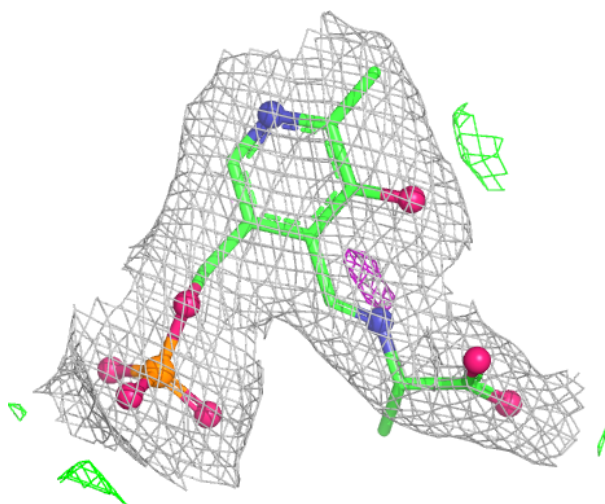
Electron density around PDA F 1000:

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



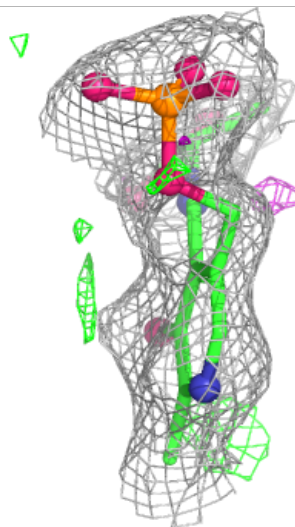
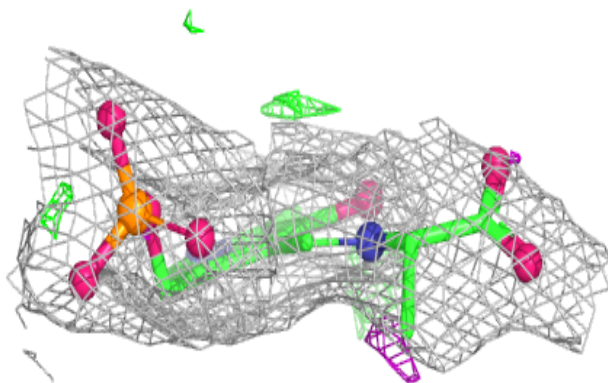
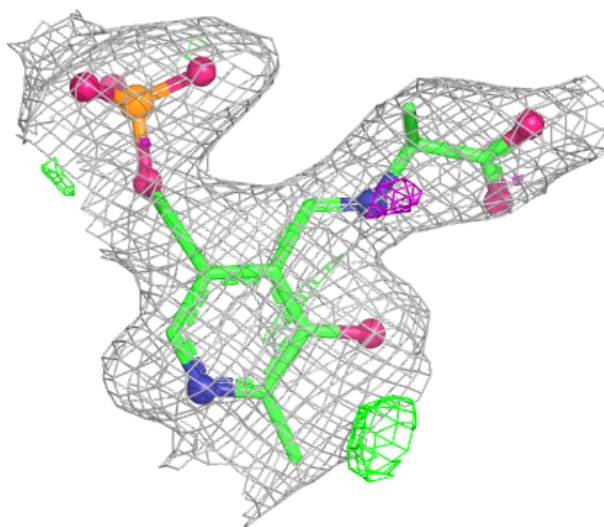
Electron density around PDA I 1000:

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



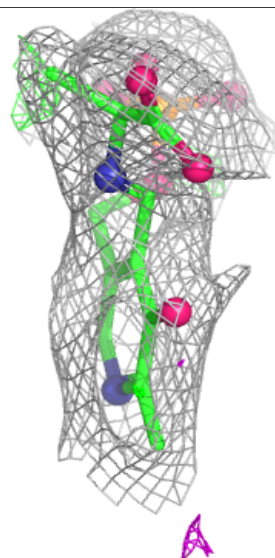
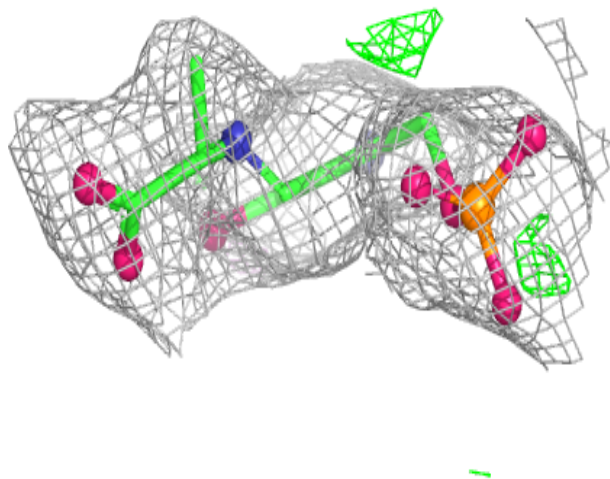
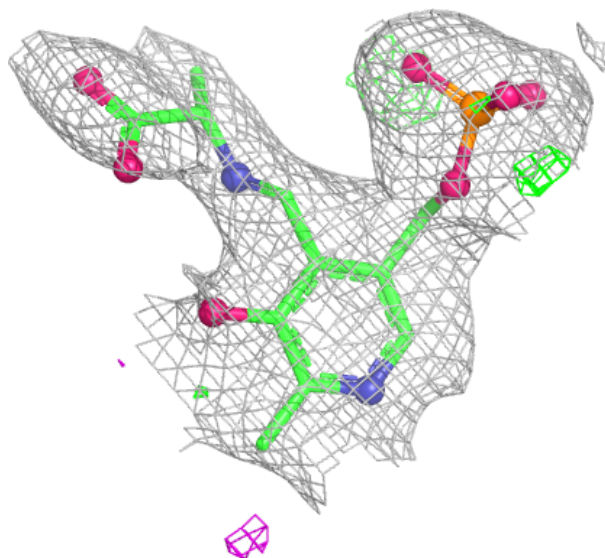
Electron density around PDA H 1000:

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



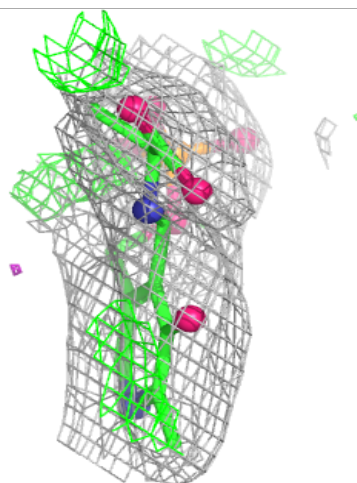
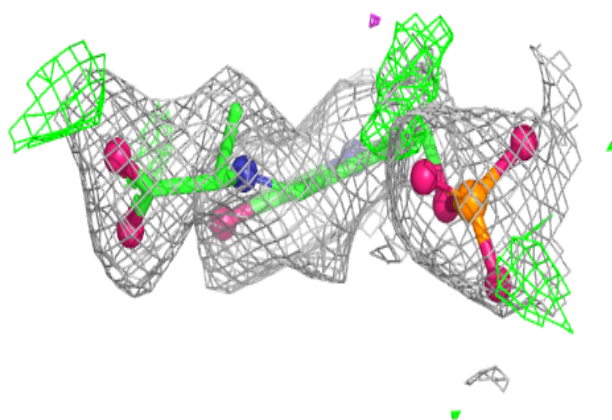
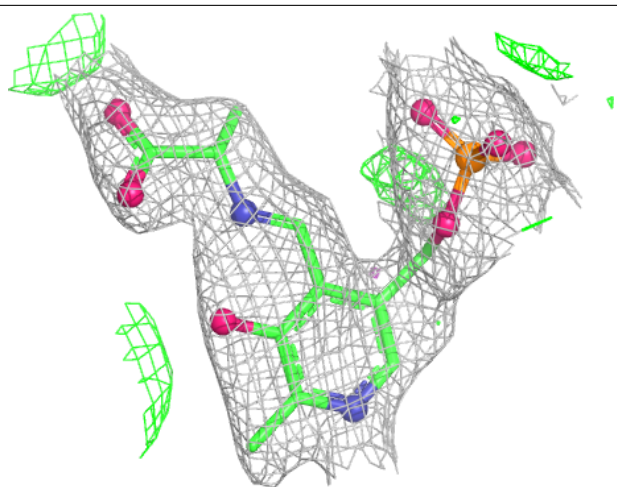
Electron density around PDA D 1000:

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



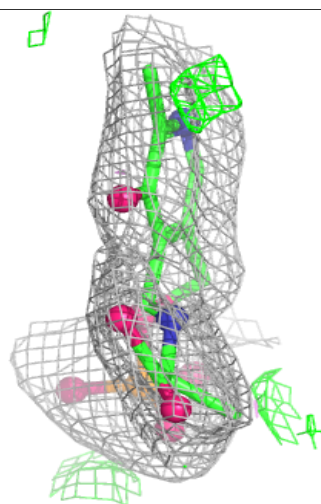
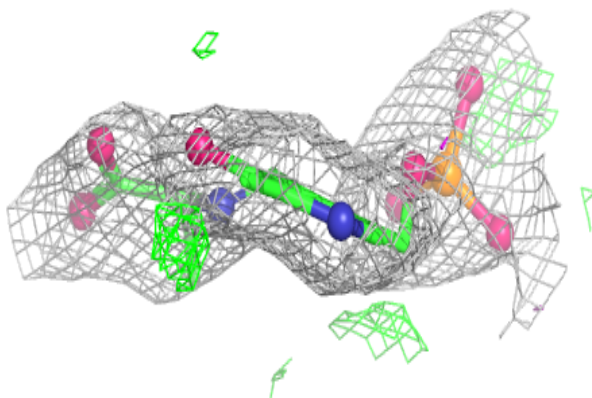
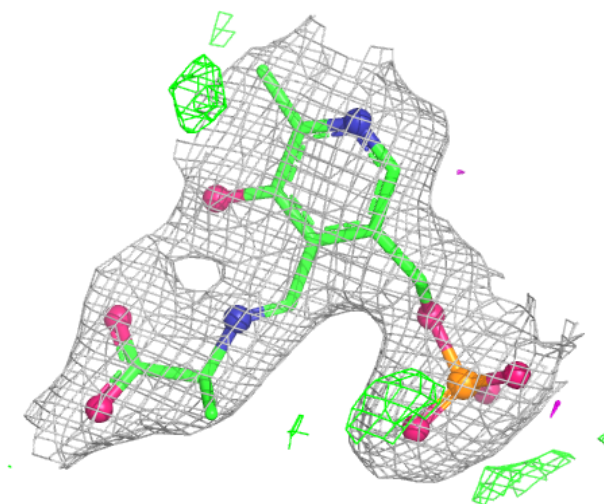
Electron density around PDA B 1000:

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



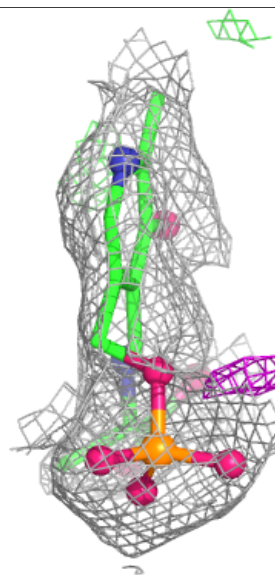
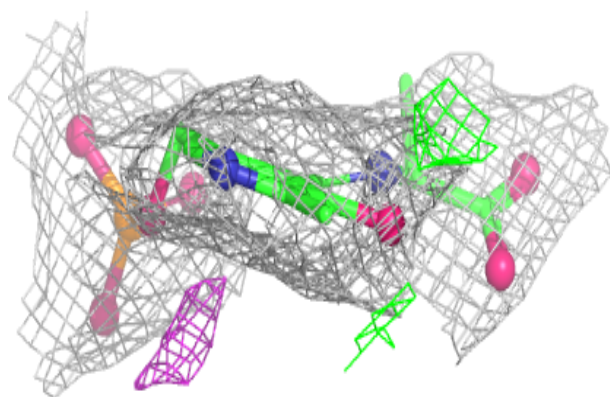
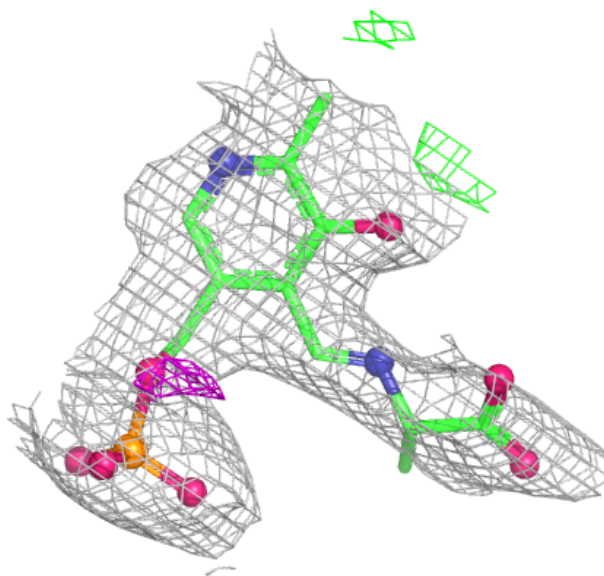
Electron density around PDA C 1000:

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



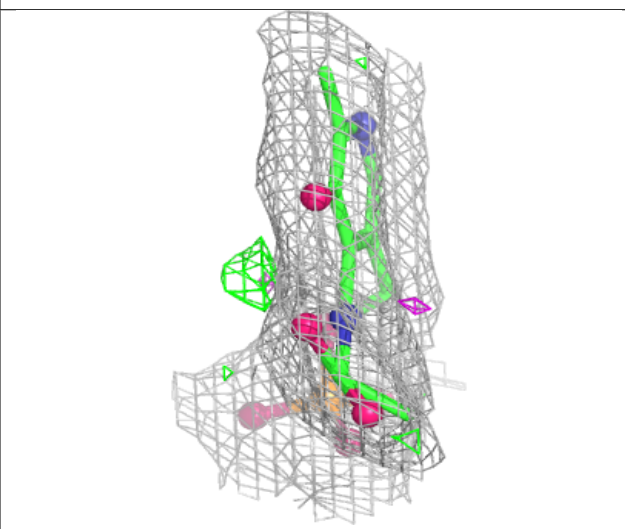
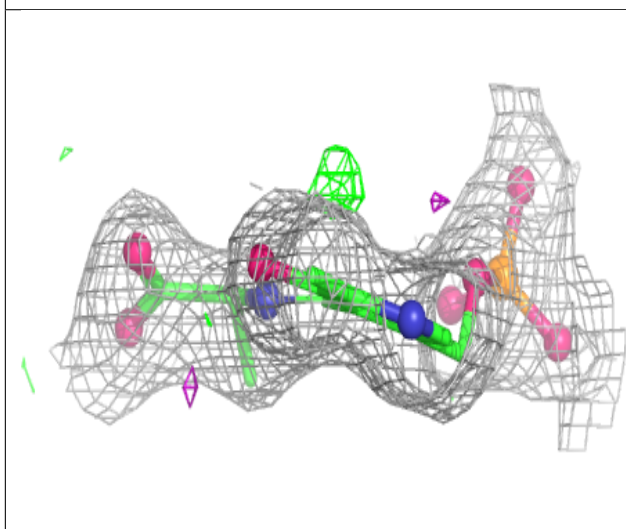
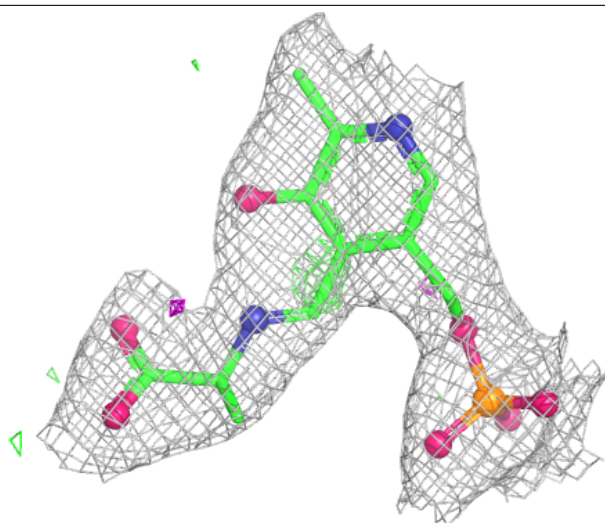
Electron density around PDA G 1000:

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



Electron density around PDA A 1000:

$2mF_o-DF_c$ (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.