



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:49 AM UTC

PDB ID : 8TBS / pdb_00008tbs
Title : Structure of human erythrocyte pyruvate kinase in complex with an allosteric activator AG-946
Authors : Jin, L.; Padyana, A.
Deposited on : 2023-06-29
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

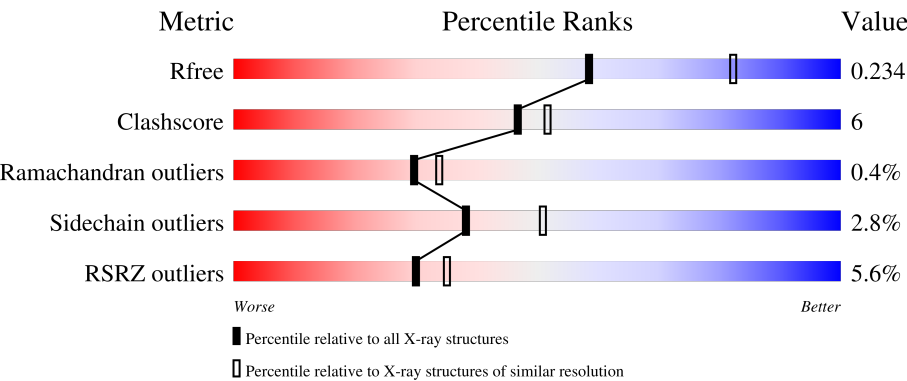
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	544	5% 78% 11% • 11%
1	B	544	6% 85% 10% • 5%
1	C	544	7% 82% 11% • 6%
1	D	544	6% 75% 14% 11%
1	E	544	7% 72% 21% • 5%

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Mol	Chain	Length	Quality of chain
1	F	544	
1	G	544	
1	H	544	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PYR	E	604	-	X	-	-
5	PYR	H	604	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31741 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 Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	1	0
			3693	2322	670	683	18			
1	B	517	Total	C	N	O	S	0	0	0
			3922	2468	708	728	18			
1	C	512	Total	C	N	O	S	0	2	0
			3895	2450	705	722	18			
1	D	483	Total	C	N	O	S	0	0	0
			3661	2303	664	676	18			
1	E	515	Total	C	N	O	S	0	1	0
			3908	2459	709	722	18			
1	F	520	Total	C	N	O	S	0	0	0
			3941	2479	712	732	18			
1	G	509	Total	C	N	O	S	0	6	0
			3901	2449	709	725	18			
1	H	519	Total	C	N	O	S	0	1	0
			3943	2480	712	733	18			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP P30613
A	32	GLY	-	expression tag	UNP P30613
A	33	SER	-	expression tag	UNP P30613
A	34	SER	-	expression tag	UNP P30613
A	35	HIS	-	expression tag	UNP P30613
A	36	HIS	-	expression tag	UNP P30613
A	37	HIS	-	expression tag	UNP P30613
A	38	HIS	-	expression tag	UNP P30613
A	39	HIS	-	expression tag	UNP P30613
A	40	HIS	-	expression tag	UNP P30613
A	41	SER	-	expression tag	UNP P30613
A	42	SER	-	expression tag	UNP P30613
A	43	GLY	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LEU	-	expression tag	UNP P30613
A	45	VAL	-	expression tag	UNP P30613
A	46	PRO	-	expression tag	UNP P30613
A	47	ARG	-	expression tag	UNP P30613
A	48	GLY	-	expression tag	UNP P30613
A	49	SER	-	expression tag	UNP P30613
B	31	MET	-	initiating methionine	UNP P30613
B	32	GLY	-	expression tag	UNP P30613
B	33	SER	-	expression tag	UNP P30613
B	34	SER	-	expression tag	UNP P30613
B	35	HIS	-	expression tag	UNP P30613
B	36	HIS	-	expression tag	UNP P30613
B	37	HIS	-	expression tag	UNP P30613
B	38	HIS	-	expression tag	UNP P30613
B	39	HIS	-	expression tag	UNP P30613
B	40	HIS	-	expression tag	UNP P30613
B	41	SER	-	expression tag	UNP P30613
B	42	SER	-	expression tag	UNP P30613
B	43	GLY	-	expression tag	UNP P30613
B	44	LEU	-	expression tag	UNP P30613
B	45	VAL	-	expression tag	UNP P30613
B	46	PRO	-	expression tag	UNP P30613
B	47	ARG	-	expression tag	UNP P30613
B	48	GLY	-	expression tag	UNP P30613
B	49	SER	-	expression tag	UNP P30613
C	31	MET	-	initiating methionine	UNP P30613
C	32	GLY	-	expression tag	UNP P30613
C	33	SER	-	expression tag	UNP P30613
C	34	SER	-	expression tag	UNP P30613
C	35	HIS	-	expression tag	UNP P30613
C	36	HIS	-	expression tag	UNP P30613
C	37	HIS	-	expression tag	UNP P30613
C	38	HIS	-	expression tag	UNP P30613
C	39	HIS	-	expression tag	UNP P30613
C	40	HIS	-	expression tag	UNP P30613
C	41	SER	-	expression tag	UNP P30613
C	42	SER	-	expression tag	UNP P30613
C	43	GLY	-	expression tag	UNP P30613
C	44	LEU	-	expression tag	UNP P30613
C	45	VAL	-	expression tag	UNP P30613
C	46	PRO	-	expression tag	UNP P30613
C	47	ARG	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	48	GLY	-	expression tag	UNP P30613
C	49	SER	-	expression tag	UNP P30613
D	31	MET	-	initiating methionine	UNP P30613
D	32	GLY	-	expression tag	UNP P30613
D	33	SER	-	expression tag	UNP P30613
D	34	SER	-	expression tag	UNP P30613
D	35	HIS	-	expression tag	UNP P30613
D	36	HIS	-	expression tag	UNP P30613
D	37	HIS	-	expression tag	UNP P30613
D	38	HIS	-	expression tag	UNP P30613
D	39	HIS	-	expression tag	UNP P30613
D	40	HIS	-	expression tag	UNP P30613
D	41	SER	-	expression tag	UNP P30613
D	42	SER	-	expression tag	UNP P30613
D	43	GLY	-	expression tag	UNP P30613
D	44	LEU	-	expression tag	UNP P30613
D	45	VAL	-	expression tag	UNP P30613
D	46	PRO	-	expression tag	UNP P30613
D	47	ARG	-	expression tag	UNP P30613
D	48	GLY	-	expression tag	UNP P30613
D	49	SER	-	expression tag	UNP P30613
E	31	MET	-	initiating methionine	UNP P30613
E	32	GLY	-	expression tag	UNP P30613
E	33	SER	-	expression tag	UNP P30613
E	34	SER	-	expression tag	UNP P30613
E	35	HIS	-	expression tag	UNP P30613
E	36	HIS	-	expression tag	UNP P30613
E	37	HIS	-	expression tag	UNP P30613
E	38	HIS	-	expression tag	UNP P30613
E	39	HIS	-	expression tag	UNP P30613
E	40	HIS	-	expression tag	UNP P30613
E	41	SER	-	expression tag	UNP P30613
E	42	SER	-	expression tag	UNP P30613
E	43	GLY	-	expression tag	UNP P30613
E	44	LEU	-	expression tag	UNP P30613
E	45	VAL	-	expression tag	UNP P30613
E	46	PRO	-	expression tag	UNP P30613
E	47	ARG	-	expression tag	UNP P30613
E	48	GLY	-	expression tag	UNP P30613
E	49	SER	-	expression tag	UNP P30613
F	31	MET	-	initiating methionine	UNP P30613
F	32	GLY	-	expression tag	UNP P30613

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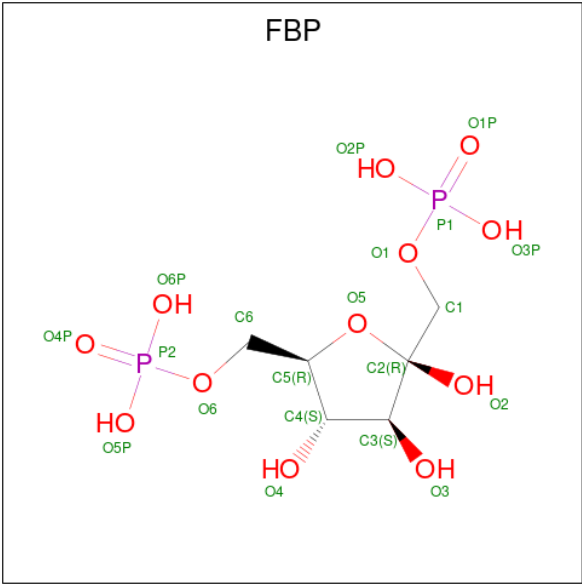
Chain	Residue	Modelled	Actual	Comment	Reference
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F	34	SER	-	expression tag	UNP P30613
F	35	HIS	-	expression tag	UNP P30613
F	36	HIS	-	expression tag	UNP P30613
F	37	HIS	-	expression tag	UNP P30613
F	38	HIS	-	expression tag	UNP P30613
F	39	HIS	-	expression tag	UNP P30613
F	40	HIS	-	expression tag	UNP P30613
F	41	SER	-	expression tag	UNP P30613
F	42	SER	-	expression tag	UNP P30613
F	43	GLY	-	expression tag	UNP P30613
F	44	LEU	-	expression tag	UNP P30613
F	45	VAL	-	expression tag	UNP P30613
F	46	PRO	-	expression tag	UNP P30613
F	47	ARG	-	expression tag	UNP P30613
F	48	GLY	-	expression tag	UNP P30613
F	49	SER	-	expression tag	UNP P30613
G	31	MET	-	initiating methionine	UNP P30613
G	32	GLY	-	expression tag	UNP P30613
G	33	SER	-	expression tag	UNP P30613
G	34	SER	-	expression tag	UNP P30613
G	35	HIS	-	expression tag	UNP P30613
G	36	HIS	-	expression tag	UNP P30613
G	37	HIS	-	expression tag	UNP P30613
G	38	HIS	-	expression tag	UNP P30613
G	39	HIS	-	expression tag	UNP P30613
G	40	HIS	-	expression tag	UNP P30613
G	41	SER	-	expression tag	UNP P30613
G	42	SER	-	expression tag	UNP P30613
G	43	GLY	-	expression tag	UNP P30613
G	44	LEU	-	expression tag	UNP P30613
G	45	VAL	-	expression tag	UNP P30613
G	46	PRO	-	expression tag	UNP P30613
G	47	ARG	-	expression tag	UNP P30613
G	48	GLY	-	expression tag	UNP P30613
G	49	SER	-	expression tag	UNP P30613
H	31	MET	-	initiating methionine	UNP P30613
H	32	GLY	-	expression tag	UNP P30613
H	33	SER	-	expression tag	UNP P30613
H	34	SER	-	expression tag	UNP P30613
H	35	HIS	-	expression tag	UNP P30613
H	36	HIS	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
H	37	HIS	-	expression tag	UNP P30613
H	38	HIS	-	expression tag	UNP P30613
H	39	HIS	-	expression tag	UNP P30613
H	40	HIS	-	expression tag	UNP P30613
H	41	SER	-	expression tag	UNP P30613
H	42	SER	-	expression tag	UNP P30613
H	43	GLY	-	expression tag	UNP P30613
H	44	LEU	-	expression tag	UNP P30613
H	45	VAL	-	expression tag	UNP P30613
H	46	PRO	-	expression tag	UNP P30613
H	47	ARG	-	expression tag	UNP P30613
H	48	GLY	-	expression tag	UNP P30613
H	49	SER	-	expression tag	UNP P30613

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C₆H₁₄O₁₂P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

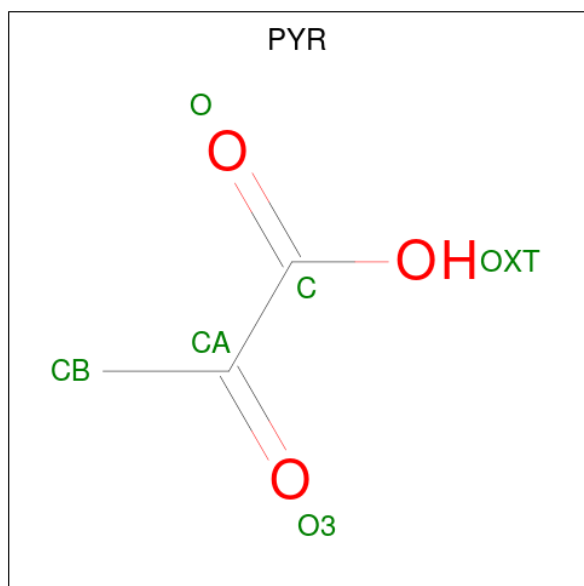
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

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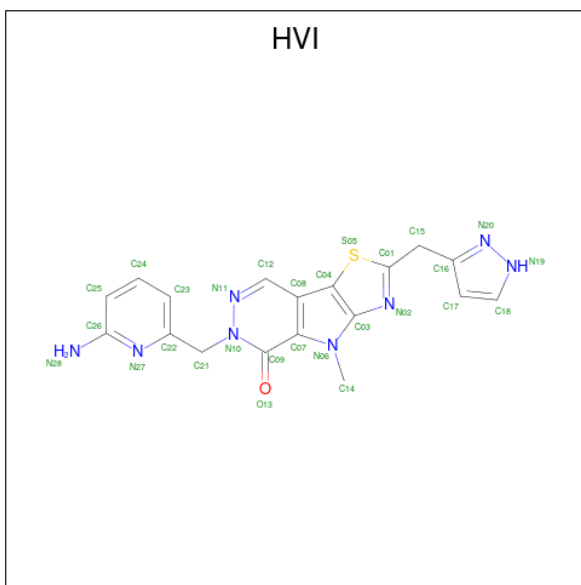
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total K 1 1	0	0

- Molecule 5 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 6 is 6-[(6-aminopyridin-2-yl)methyl]-4-methyl-2-[(1H-pyrazol-3-yl)methyl]-4,6-dihydro-5H-[1,3]thiazolo[5',4':4,5]pyrrolo[2,3-d]pyridazin-5-one (CCD ID: HVI) (formula: $C_{18}H_{16}N_8OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			28	18	8	1	1		
6	D	1	Total	C	N	O	S	0	0
			28	18	8	1	1		
6	F	1	Total	C	N	O	S	0	0
			28	18	8	1	1		
6	H	1	Total	C	N	O	S	0	0
			28	18	8	1	1		

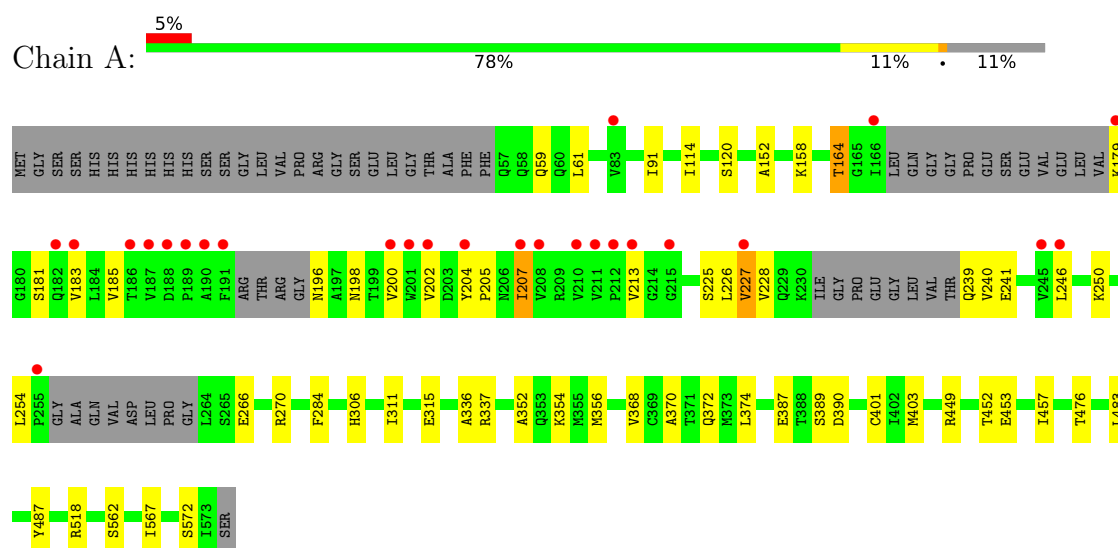
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	73	Total	O	0	0
			73	73		
7	B	64	Total	O	0	0
			64	64		
7	C	62	Total	O	0	0
			62	62		
7	D	55	Total	O	0	0
			55	55		
7	E	41	Total	O	0	0
			41	41		
7	F	91	Total	O	0	0
			91	91		
7	G	48	Total	O	0	0
			48	48		
7	H	109	Total	O	0	0
			109	109		

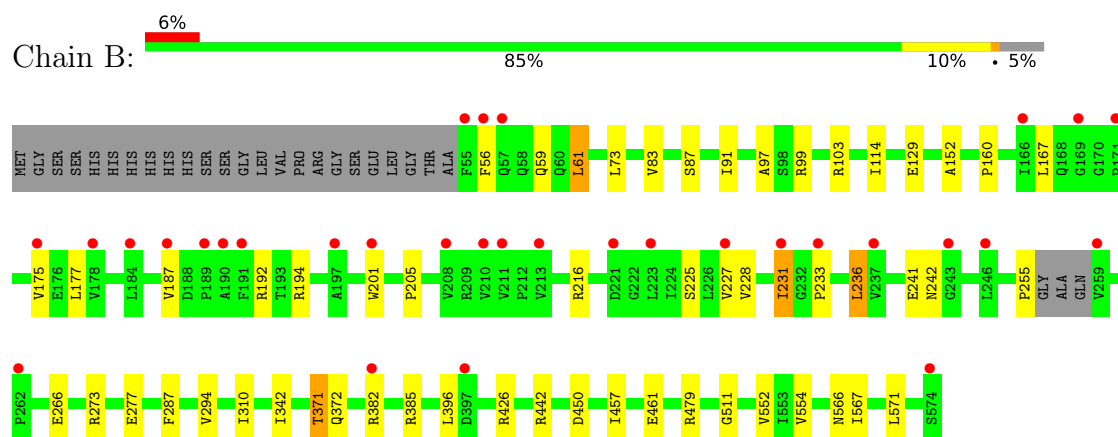
3 Residue-property plots [i](#)

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.

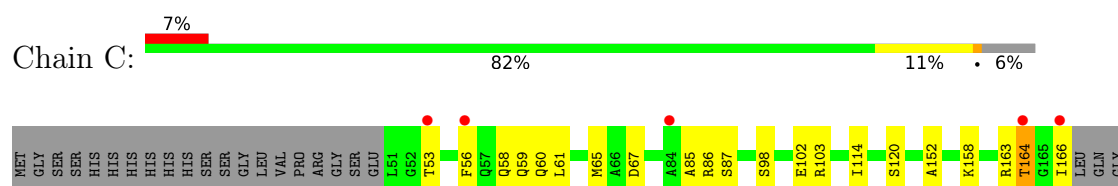
• Molecule 1: Pyruvate kinase PKLR

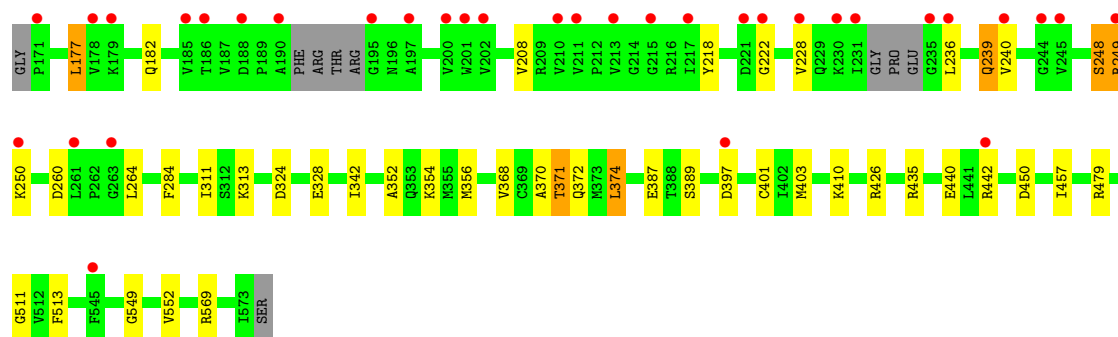


• Molecule 1: Pyruvate kinase PKLR

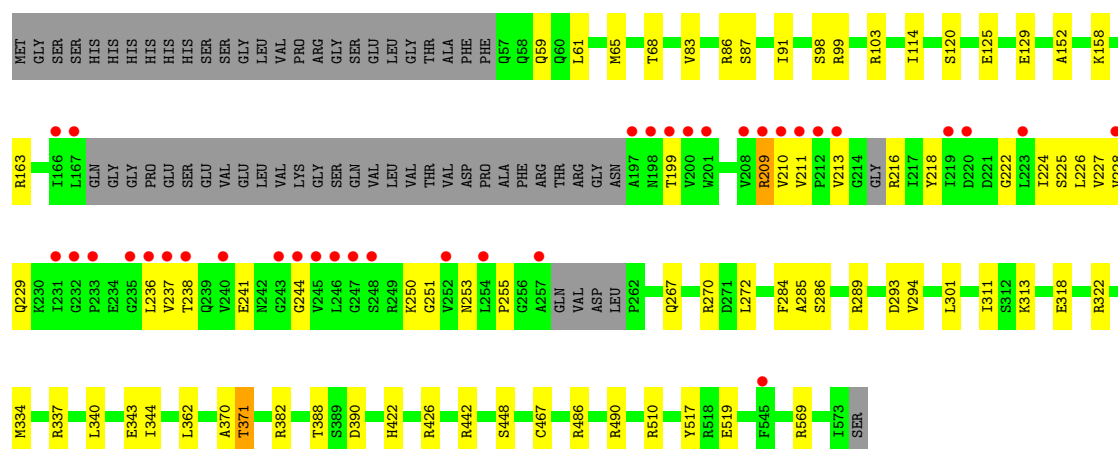
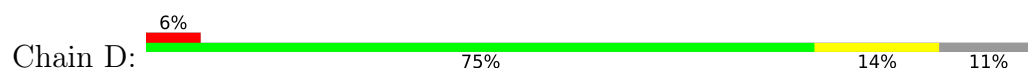


• Molecule 1: Pyruvate kinase PKLR

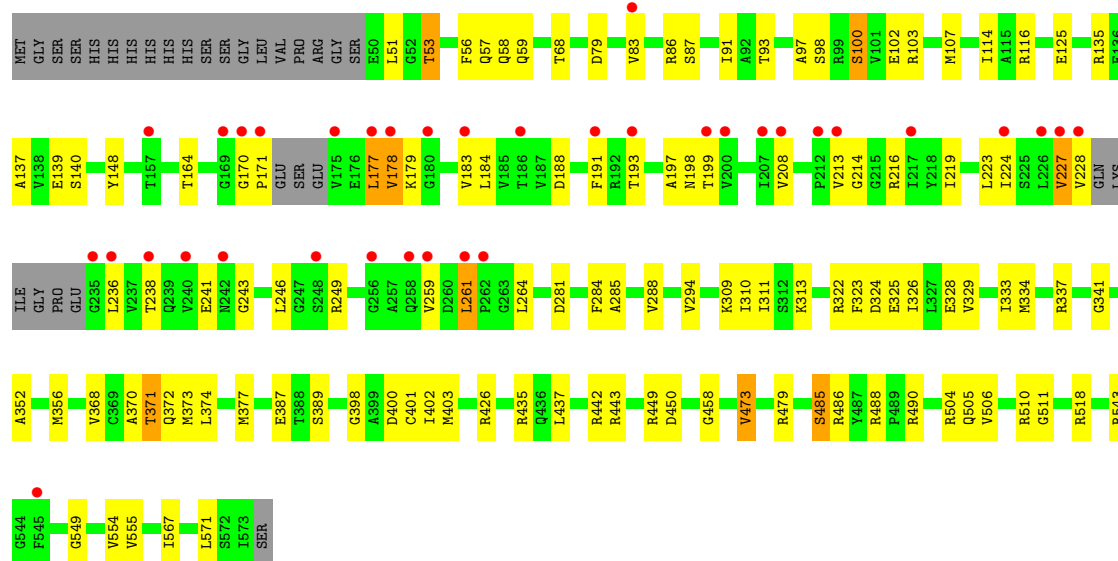




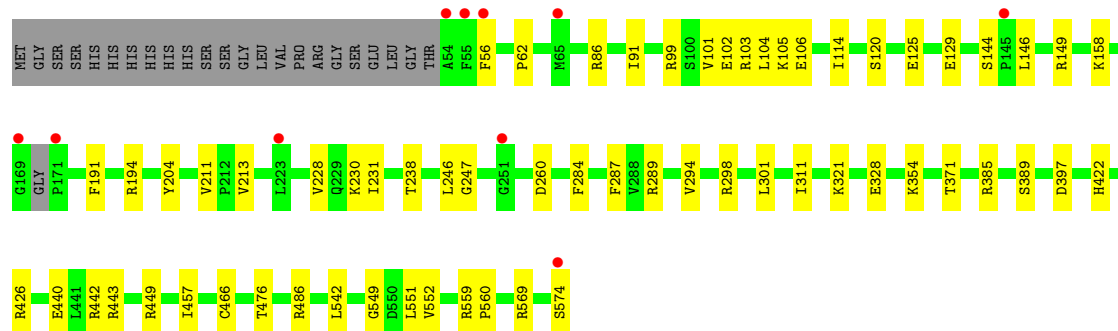
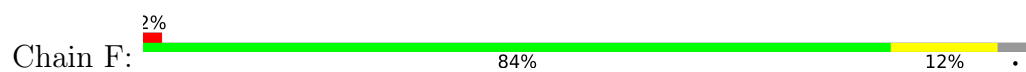
• Molecule 1: Pyruvate kinase PKLR



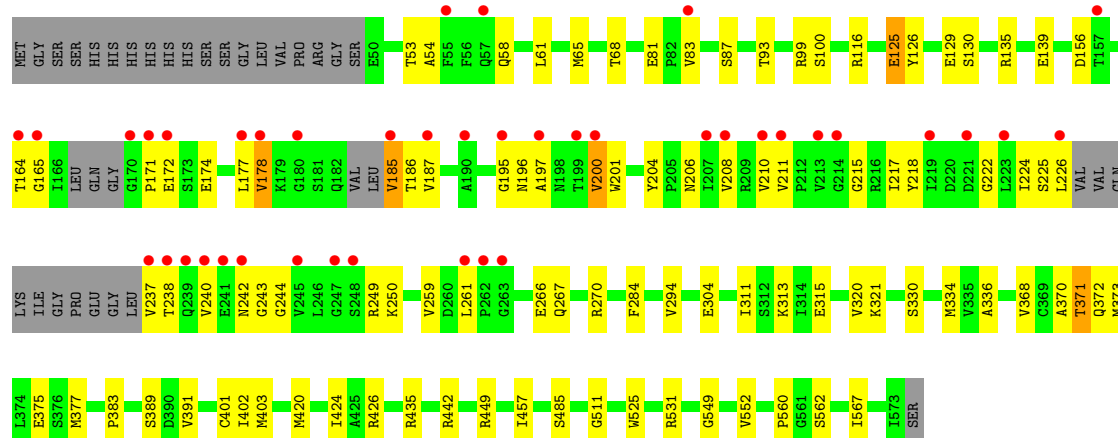
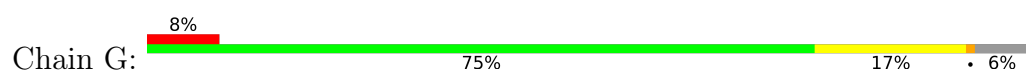
• Molecule 1: Pyruvate kinase PKLR



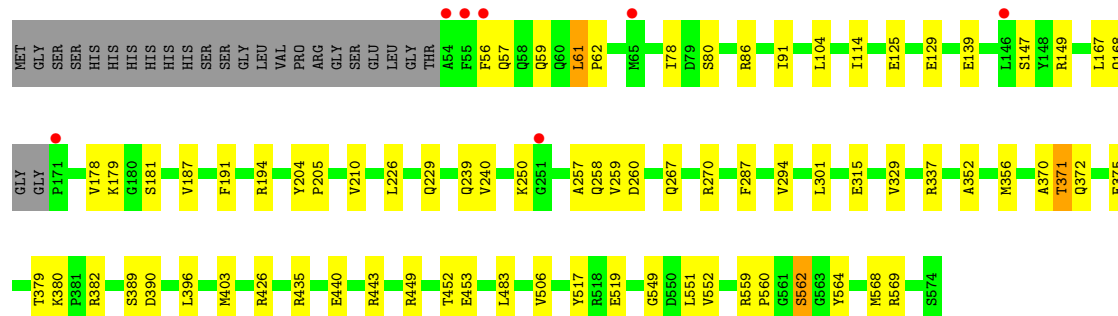
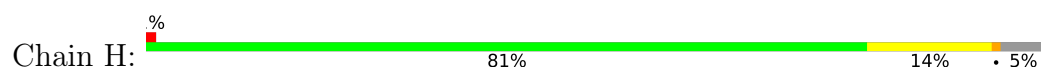
• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.32Å 122.60Å 378.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.35 29.44 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.44-2.35) 99.5 (29.44-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.02 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.193 , 0.234 0.193 , 0.234	Depositor DCC
R_{free} test set	10643 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31741	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 66.22 % 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 6.2563e-06. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, PYR, FBP, HVI, MN

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	0.16	0/3750	0.33	0/5076
1	B	0.17	0/3987	0.34	1/5403 (0.0%)
1	C	0.18	0/3956	0.36	0/5357
1	D	0.16	0/3719	0.33	0/5035
1	E	0.17	0/3971	0.34	0/5380
1	F	0.18	0/4006	0.34	0/5428
1	G	0.16	0/3975	0.37	0/5381
1	H	0.17	0/4008	0.36	0/5431
All	All	0.17	0/31372	0.35	1/42491 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	ILE	N-CA-C	-5.25	107.71	112.96

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	3693	0	3766	33	0
1	B	3922	0	3998	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3895	0	3974	43	0
1	D	3661	0	3741	50	0
1	E	3908	0	3987	78	0
1	F	3941	0	4016	39	0
1	G	3901	0	3971	58	1
1	H	3943	0	4018	47	0
2	A	20	0	9	0	0
2	B	20	0	9	0	0
2	C	20	0	9	0	0
2	D	20	0	9	0	0
2	E	20	0	9	0	0
2	F	20	0	9	0	0
2	G	20	0	9	0	0
2	H	20	0	9	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	6	0	0	2	0
5	H	6	0	0	0	0
6	B	28	0	0	0	0
6	D	28	0	0	0	0
6	F	28	0	0	0	0
6	H	28	0	0	0	0
7	A	73	0	0	1	0
7	B	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	62	0	0	2	0
7	D	55	0	0	0	0
7	E	41	0	0	3	0
7	F	91	0	0	6	0
7	G	48	0	0	1	0
7	H	109	0	0	0	0
All	All	31741	0	31543	356	1

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 6.

All (356) 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:E:179:LYS:HB2	1:E:243:GLY:HA3	1.55	0.87
1:G:99:ARG:NH2	1:G:126:TYR:O	2.12	0.82
1:E:59:GLN:O	1:E:490[A]:ARG:NH2	2.10	0.82
1:F:486:ARG:NH1	7:F:701:HOH:O	2.11	0.79
1:G:185:VAL:N	1:G:200:VAL:O	2.18	0.77
1:F:549:GLY:O	1:G:449:ARG:NH2	2.18	0.77
1:B:228:VAL:HG22	1:B:236:LEU:HD11	1.66	0.75
1:E:449:ARG:NH2	1:H:549:GLY:O	2.20	0.74
1:C:120:SER:HA	1:C:158:LYS:HG3	1.69	0.74
1:F:559:ARG:HD2	1:F:560:PRO:O	1.88	0.74
1:E:213:VAL:HA	1:E:228:VAL:HG21	1.70	0.73
1:E:373:MET:HE1	1:E:402:ILE:HB	1.68	0.73
1:G:267:GLN:OE1	1:G:270:ARG:NH2	2.22	0.72
1:F:191:PHE:HA	1:F:194:ARG:HG3	1.73	0.71
1:E:86:ARG:HB2	1:E:426:ARG:HG2	1.72	0.71
1:F:146:LEU:HD23	1:F:542:LEU:HG	1.72	0.71
1:E:426:ARG:NH1	7:E:702:HOH:O	2.23	0.70
1:C:450:ASP:OD2	1:C:479[A]:ARG:NH2	2.25	0.69
1:E:288:VAL:HG12	1:E:326:ILE:HD13	1.75	0.68
1:A:449:ARG:NH2	1:C:549:GLY:O	2.26	0.68
1:D:229:GLN:H	1:D:237:VAL:HG21	1.60	0.67
1:B:225:SER:HB3	1:B:242:ASN:HB2	1.77	0.66
1:D:86:ARG:HB3	1:D:426:ARG:HG3	1.75	0.66
1:G:315:GLU:HG2	1:G:336:ALA:HB3	1.76	0.66
1:H:371:THR:HG22	1:H:372:GLN:HG3	1.76	0.66
1:F:449:ARG:NH2	1:G:549:GLY:O	2.26	0.66
1:C:328:GLU:OE1	7:C:701:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ARG:NH2	7:E:701:HOH:O	2.18	0.66
1:F:328:GLU:OE1	7:F:702:HOH:O	2.14	0.65
1:E:450:ASP:OD2	1:E:479:ARG:NH2	2.29	0.65
1:B:382:ARG:NH2	1:B:385:ARG:HH12	1.94	0.65
1:F:204:TYR:OH	1:F:260:ASP:OD1	2.10	0.64
1:H:86:ARG:HB2	1:H:426:ARG:HG2	1.80	0.64
1:E:435:ARG:HH11	1:H:443:ARG:HE	1.45	0.63
1:H:178:VAL:O	1:H:181:SER:OG	2.16	0.63
1:B:187:VAL:HG21	1:B:205:PRO:HA	1.79	0.63
1:D:229:GLN:HG2	1:D:237:VAL:HG21	1.79	0.63
1:G:371:THR:HG22	1:G:372:GLN:HG3	1.79	0.63
1:A:306:HIS:CD2	1:A:306:HIS:H	2.18	0.62
1:D:199:THR:HG23	1:D:238:THR:HG21	1.82	0.62
1:H:379:THR:HG23	1:H:380:LYS:HG2	1.82	0.62
1:B:382:ARG:HH21	1:B:385:ARG:HH12	1.46	0.62
1:C:87:SER:HB2	1:C:511:GLY:HA2	1.80	0.62
1:F:149:ARG:NH2	7:F:703:HOH:O	2.33	0.62
1:C:67:ASP:OD2	7:C:702:HOH:O	2.16	0.61
1:E:371:THR:HG22	1:E:372:GLN:HG3	1.83	0.61
1:C:58:GLN:O	1:C:60:GLN:N	2.33	0.61
1:A:315:GLU:HG2	1:A:336:ALA:HB3	1.83	0.61
1:E:443:ARG:NH2	7:E:703:HOH:O	2.24	0.61
1:E:53:THR:O	1:E:57:GLN:NE2	2.34	0.60
1:E:435:ARG:NH1	1:H:443:ARG:HE	1.99	0.60
1:B:450:ASP:OD2	1:B:479:ARG:NH2	2.35	0.60
1:E:177:LEU:HD12	1:E:197:ALA:HA	1.85	0.59
1:D:86:ARG:HD3	1:D:422:HIS:ND1	2.18	0.59
1:D:337:ARG:NH2	1:D:390:ASP:OD1	2.34	0.59
1:G:313:LYS:HD2	1:G:334:MET:SD	2.42	0.59
1:B:273:ARG:O	1:B:277:GLU:HG3	2.03	0.58
1:C:218:TYR:HB3	1:C:222:GLY:HA2	1.85	0.58
1:E:178:VAL:HG12	1:E:179:LYS:H	1.67	0.58
1:G:99:ARG:NH2	1:G:130:SER:OG	2.36	0.58
1:C:368:VAL:HG22	1:C:401:CYS:HB2	1.86	0.58
1:A:185:VAL:HG12	1:A:200:VAL:HG23	1.85	0.58
1:E:91:ILE:HB	1:E:403:MET:HG3	1.84	0.58
1:E:437:LEU:HD21	1:E:488:ARG:HG2	1.86	0.58
1:G:373:MET:HE3	1:G:391:VAL:HG22	1.86	0.58
1:E:313:LYS:HD2	1:E:334:MET:SD	2.43	0.57
1:A:207:ILE:HD11	1:A:254:LEU:HD13	1.85	0.57
1:E:51:LEU:HD12	1:H:449:ARG:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLN:NE2	7:A:701:HOH:O	2.30	0.57
1:H:229:GLN:HE21	1:H:239:GLN:HB2	1.70	0.56
1:A:59:GLN:HG3	1:A:61:LEU:HD23	1.87	0.56
1:B:59:GLN:HG3	1:B:61:LEU:HD22	1.87	0.56
1:A:179:LYS:N	1:A:239:GLN:OE1	2.38	0.56
1:D:267:GLN:OE1	1:D:270:ARG:NH2	2.38	0.56
1:F:442:ARG:HG2	1:F:457:ILE:HD11	1.88	0.56
1:A:337:ARG:NH2	1:A:390:ASP:OD1	2.31	0.56
1:E:284:PHE:HD1	1:E:311:ILE:HB	1.71	0.56
1:H:226:LEU:HD22	1:H:240:VAL:HG12	1.88	0.55
1:A:164:THR:HG1	1:A:250:LYS:H	1.54	0.55
1:C:182:GLN:HG2	1:C:239:GLN:HG3	1.86	0.55
1:H:57:GLN:O	1:H:80:SER:OG	2.17	0.55
1:H:337:ARG:NH2	1:H:390:ASP:OD1	2.36	0.55
1:H:372:GLN:HA	1:H:375:GLU:HG2	1.87	0.55
1:E:208:VAL:HA	1:E:236:LEU:HD21	1.87	0.55
1:G:54:ALA:O	1:G:58:GLN:NE2	2.39	0.55
1:G:93:THR:OG1	1:G:116:ARG:NH1	2.37	0.55
1:G:224:ILE:HB	1:G:243:GLY:HA3	1.89	0.55
1:E:337:ARG:NH2	1:E:373:MET:HG2	2.21	0.55
1:E:97:ALA:O	1:E:103:ARG:NH2	2.36	0.55
1:G:304:GLU:OE2	1:G:304:GLU:N	2.26	0.54
1:A:453:GLU:HG2	1:A:483:LEU:HD13	1.88	0.54
1:D:218:TYR:HB3	1:D:222:GLY:HA2	1.88	0.54
1:F:443:ARG:CZ	1:G:435:ARG:HD3	2.38	0.54
1:D:224:ILE:HG12	1:D:244:GLY:HA3	1.88	0.54
1:E:473:VAL:HG13	1:E:555:VAL:HB	1.88	0.54
1:B:382:ARG:HH21	1:B:385:ARG:NH1	2.06	0.54
1:C:371:THR:HG22	1:C:372:GLN:HG3	1.89	0.54
1:H:167:LEU:O	1:H:168:GLN:HB2	2.06	0.54
1:A:352:ALA:O	1:A:356:MET:HG3	2.08	0.54
1:D:218:TYR:CE2	1:D:255:PRO:HG3	2.43	0.54
1:F:569:ARG:HG2	1:G:567:ILE:HG23	1.90	0.53
1:E:183:VAL:HG22	1:E:198:ASN:HA	1.91	0.53
1:G:185:VAL:N	1:G:200:VAL:H	2.06	0.53
1:H:59:GLN:HG3	1:H:61:LEU:HD22	1.90	0.53
1:B:442:ARG:HG2	1:B:457:ILE:HD11	1.91	0.53
1:F:120:SER:HA	1:F:158:LYS:HG3	1.91	0.53
1:D:61:LEU:HD12	1:D:65:MET:HE3	1.90	0.53
1:E:79:ASP:OD2	1:F:321:LYS:HE3	2.09	0.53
1:D:313:LYS:HD2	1:D:334:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:TYR:OH	1:H:260:ASP:OD1	2.20	0.52
1:E:53:THR:C	1:E:57:GLN:HE21	2.16	0.52
1:H:370:ALA:HB1	1:H:403:MET:HE2	1.91	0.52
1:G:266:GLU:HG3	1:G:270:ARG:HH12	1.75	0.52
1:D:125:GLU:O	1:D:129:GLU:HG3	2.09	0.52
1:D:209:ARG:HA	1:D:209:ARG:HH11	1.75	0.52
1:E:368:VAL:HG22	1:E:401:CYS:HB2	1.91	0.52
1:C:370:ALA:HB1	1:C:403:MET:HE2	1.91	0.52
1:E:135:ARG:O	1:E:139:GLU:HG2	2.10	0.52
1:F:86:ARG:HB2	1:F:426:ARG:HG2	1.92	0.52
1:E:177:LEU:HB3	1:E:246:LEU:HB3	1.92	0.51
1:H:229:GLN:HE21	1:H:239:GLN:CB	2.23	0.51
1:F:230:LYS:HG2	1:F:231:ILE:N	2.26	0.51
1:G:135:ARG:O	1:G:139:GLU:HG2	2.10	0.51
1:E:400:ASP:HA	1:E:510:ARG:HB2	1.92	0.51
1:F:486:ARG:HG2	7:F:701:HOH:O	2.11	0.51
1:B:167:LEU:HD21	1:B:175:VAL:HG23	1.91	0.51
1:F:101:VAL:HG12	1:F:105:LYS:HD2	1.92	0.51
1:B:227:VAL:HG23	1:B:241:GLU:HB2	1.93	0.51
1:G:259:VAL:HG22	1:G:261:LEU:H	1.76	0.51
1:A:204:TYR:HD1	1:A:205:PRO:HD2	1.76	0.51
1:G:211:VAL:HG13	1:G:215:GLY:HA3	1.93	0.51
1:G:217:ILE:HB	1:G:226:LEU:HD23	1.93	0.50
1:G:442:ARG:NH1	7:G:704:HOH:O	2.40	0.50
1:C:284:PHE:HB3	1:C:313:LYS:HD2	1.92	0.50
1:G:284:PHE:HD1	1:G:311:ILE:HB	1.76	0.50
1:H:125:GLU:O	1:H:129:GLU:HG3	2.12	0.50
1:C:102:GLU:CD	1:C:102:GLU:H	2.19	0.50
1:E:398:GLY:O	1:E:488:ARG:NH2	2.44	0.50
1:G:208:VAL:HG22	1:G:237:VAL:HG11	1.93	0.50
1:A:370:ALA:HB1	1:A:403:MET:HE2	1.94	0.50
1:C:166:ILE:HG13	1:C:249:ARG:HG3	1.93	0.50
1:G:224:ILE:HG22	1:G:244:GLY:H	1.76	0.50
1:A:196:ASN:HD21	1:A:198:ASN:HB2	1.77	0.50
1:C:442[A]:ARG:HB2	1:C:457:ILE:HD11	1.94	0.50
1:G:81[B]:GLU:H	1:G:81[B]:GLU:CD	2.16	0.50
1:G:372:GLN:HG2	1:G:375:GLU:OE1	2.11	0.50
1:A:567:ILE:HG12	1:C:569:ARG:HG2	1.94	0.50
1:G:195:GLY:O	1:G:197:ALA:N	2.45	0.50
1:E:341:GLY:HA3	1:F:385:ARG:HE	1.76	0.49
1:H:147[A]:SER:O	1:H:149:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:GLU:CD	1:F:125:GLU:H	2.20	0.49
1:G:336:ALA:HB1	5:G:604:PYR:C	2.42	0.49
1:H:559:ARG:HD2	1:H:560:PRO:O	2.13	0.49
1:G:266:GLU:HG3	1:G:270:ARG:NH1	2.27	0.49
1:D:225:SER:OG	1:D:241:GLU:OE1	2.29	0.49
1:E:214:GLY:H	1:E:228:VAL:CG2	2.24	0.49
1:H:187:VAL:HG11	1:H:205:PRO:HA	1.94	0.49
1:C:164:THR:HG23	1:C:250:LYS:O	2.13	0.49
1:B:114:ILE:HG12	1:B:152:ALA:HB3	1.95	0.49
1:C:352:ALA:O	1:C:356:MET:HG3	2.13	0.49
1:E:93:THR:OG1	1:E:116:ARG:NH1	2.40	0.49
1:E:125:GLU:OE2	1:E:125:GLU:N	2.43	0.49
1:C:177:LEU:CD2	1:C:240:VAL:HG21	2.43	0.48
1:E:219:ILE:HB	1:E:224:ILE:HD11	1.95	0.48
1:B:91:ILE:HG12	1:B:114:ILE:HB	1.95	0.48
1:B:567:ILE:HG12	1:D:569:ARG:HG2	1.95	0.48
1:C:61:LEU:O	1:C:65:MET:HG2	2.13	0.48
1:D:286:SER:HA	1:D:313:LYS:HE2	1.94	0.48
1:B:461:GLU:OE2	1:D:442:ARG:HD2	2.13	0.48
1:C:260:ASP:OD1	1:C:260:ASP:N	2.37	0.48
1:E:228:VAL:HA	1:E:238:THR:HA	1.95	0.48
1:E:294:VAL:HG23	1:E:310:ILE:HG21	1.96	0.48
1:F:125:GLU:O	1:F:129:GLU:HG3	2.13	0.48
1:G:373:MET:HE1	1:G:402:ILE:HB	1.95	0.48
1:A:179:LYS:C	1:A:239:GLN:HE22	2.20	0.48
1:E:370:ALA:HB1	1:E:403:MET:HE2	1.94	0.48
1:C:166:ILE:HG23	1:C:248:SER:HB3	1.96	0.48
1:A:368:VAL:HG22	1:A:401:CYS:HB2	1.96	0.48
1:E:281:ASP:CG	1:E:504:ARG:HE	2.22	0.48
1:A:284:PHE:HD1	1:A:311:ILE:HB	1.79	0.48
1:D:362:LEU:O	1:D:486:ARG:NH2	2.47	0.47
1:G:87:SER:HB2	1:G:511:GLY:HA2	1.95	0.47
1:E:148:TYR:O	1:E:543:ARG:NH2	2.47	0.47
1:E:177:LEU:HD13	1:E:246:LEU:HD23	1.96	0.47
1:E:554:VAL:HG21	1:E:571:LEU:HD12	1.96	0.47
1:A:354:LYS:HB3	1:B:73:LEU:HD22	1.96	0.47
1:A:204:TYR:CE2	1:A:207:ILE:HG12	2.49	0.47
1:G:156:ASP:HA	1:G:284:PHE:HB2	1.96	0.47
1:D:229:GLN:H	1:D:237:VAL:CG2	2.27	0.47
1:D:213:VAL:HG23	1:D:229:GLN:HA	1.97	0.47
1:E:216:ARG:NH1	1:E:241:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:VAL:HA	1:F:238:THR:HG22	1.96	0.47
1:F:246:LEU:HD13	1:F:247:GLY:O	2.14	0.47
1:F:476:THR:HG23	7:F:756:HOH:O	2.14	0.47
1:G:321:LYS:HA	1:G:321:LYS:HD3	1.63	0.47
1:G:68:THR:HB	1:H:440:GLU:CD	2.40	0.47
1:E:322:ARG:NH1	1:E:325:GLU:OE1	2.48	0.47
1:G:177:LEU:O	1:G:178:VAL:HB	2.15	0.47
1:G:370:ALA:HB1	1:G:403:MET:HE2	1.97	0.46
1:D:59:GLN:HG2	1:D:83:VAL:HB	1.98	0.46
1:E:68:THR:HB	1:F:440:GLU:CD	2.40	0.46
1:B:97:ALA:O	1:B:103:ARG:NH1	2.46	0.46
1:C:208:VAL:HA	1:C:236:LEU:HD21	1.96	0.46
1:D:284:PHE:HD1	1:D:311:ILE:HB	1.79	0.46
1:E:188:ASP:HB3	1:E:191:PHE:HD2	1.81	0.46
1:B:216:ARG:NH2	1:B:255:PRO:HB2	2.30	0.46
1:C:56:PHE:HZ	1:C:65:MET:HG3	1.80	0.46
1:B:371:THR:HG22	1:B:372:GLN:HG3	1.98	0.46
1:E:91:ILE:HG12	1:E:114:ILE:HB	1.97	0.46
1:G:225:SER:OG	1:G:242:ASN:OD1	2.30	0.46
1:A:452:THR:HG22	1:A:483:LEU:HD12	1.97	0.46
1:E:100:SER:OG	1:E:102:GLU:HG2	2.16	0.46
1:F:298:ARG:HD2	7:F:771:HOH:O	2.16	0.46
1:G:61:LEU:O	1:G:65:MET:HG2	2.16	0.46
1:G:171:PRO:O	1:G:174:GLU:HG2	2.16	0.46
1:F:354:LYS:NZ	1:F:397:ASP:OD2	2.41	0.45
1:A:120:SER:HA	1:A:158:LYS:HG3	1.97	0.45
1:D:114:ILE:HG12	1:D:152:ALA:HB3	1.97	0.45
1:D:490:ARG:HE	1:D:490:ARG:HB2	1.57	0.45
1:F:102:GLU:O	1:F:106:GLU:HG3	2.16	0.45
1:F:103:ARG:HD3	1:F:103:ARG:HA	1.71	0.45
1:C:102:GLU:OE1	1:C:102:GLU:N	2.40	0.45
1:C:324:ASP:O	1:C:328:GLU:HG2	2.16	0.45
1:D:120:SER:HA	1:D:158:LYS:HG3	1.98	0.45
1:E:137:ALA:O	1:E:140:SER:OG	2.35	0.45
1:H:210:VAL:CG1	1:H:257:ALA:HB1	2.46	0.45
1:D:99:ARG:NH2	1:D:129:GLU:OE1	2.49	0.45
1:H:559:ARG:NH2	1:H:564:TYR:OH	2.49	0.45
1:A:181:SER:HA	1:A:239:GLN:HB3	1.97	0.45
1:E:324:ASP:O	1:E:328:GLU:HG3	2.17	0.45
1:A:91:ILE:HG12	1:A:114:ILE:HB	1.98	0.45
1:A:374:LEU:HD23	1:A:387:GLU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:SER:HB2	1:C:511:GLY:CA	2.43	0.45
1:C:163:ARG:HG2	1:C:249:ARG:NE	2.32	0.45
1:E:323:PHE:HE1	1:E:333:ILE:HG21	1.82	0.44
1:B:294:VAL:HG13	1:B:310:ILE:HG21	2.00	0.44
1:D:250:LYS:HD2	1:D:250:LYS:HA	1.79	0.44
1:G:320:VAL:HG11	1:H:78:ILE:HD13	1.98	0.44
1:B:231:ILE:HA	1:B:236:LEU:HD22	1.99	0.44
1:C:86:ARG:HB2	1:C:426:ARG:HG2	1.99	0.44
1:C:374:LEU:HD12	1:C:387:GLU:HB3	1.99	0.44
1:D:253:ASN:ND2	1:D:343:GLU:OE1	2.45	0.44
1:E:337:ARG:HH21	1:E:373:MET:HG2	1.83	0.44
1:F:287:PHE:CE2	1:F:289:ARG:HD3	2.52	0.44
1:D:163:ARG:HH11	1:D:251:GLY:N	2.15	0.44
1:D:255:PRO:HB3	1:D:343:GLU:O	2.18	0.44
1:E:87:SER:HB2	1:E:511:GLY:HA2	2.00	0.44
1:E:170:GLY:HA3	1:E:171:PRO:HD3	1.83	0.44
1:E:374:LEU:HD23	1:E:387:GLU:HB3	2.00	0.44
1:D:272:LEU:HD22	1:D:301:LEU:HD21	1.99	0.44
1:D:284:PHE:HB3	1:D:313:LYS:HD3	1.98	0.44
1:D:289:ARG:HG2	1:D:293:ASP:OD1	2.18	0.44
1:F:56:PHE:O	1:F:62:PRO:HD3	2.18	0.44
1:E:567:ILE:HG23	1:H:569:ARG:HG2	1.99	0.44
1:D:517:TYR:CE2	1:D:519:GLU:HB2	2.53	0.44
1:E:58:GLN:NE2	1:E:83:VAL:HG21	2.32	0.44
1:E:285:ALA:O	1:E:313:LYS:HG3	2.17	0.44
1:H:147[B]:SER:O	1:H:149:ARG:NH1	2.50	0.44
1:H:191:PHE:HA	1:H:194:ARG:HG3	2.00	0.44
1:A:225:SER:OG	1:A:240:VAL:HG13	2.18	0.44
1:C:264:LEU:HD12	1:C:264:LEU:HA	1.83	0.44
1:D:213:VAL:HA	1:D:228:VAL:HG23	2.00	0.44
1:C:85:ALA:HB1	1:C:513:PHE:CZ	2.52	0.44
1:F:146:LEU:HB2	1:F:542:LEU:HD21	1.99	0.44
1:B:554:VAL:HG21	1:B:571:LEU:HD12	2.00	0.43
1:H:287:PHE:N	1:H:315:GLU:OE2	2.50	0.43
1:D:210:VAL:HG23	1:D:211:VAL:HG23	1.98	0.43
1:E:98:SER:HB2	1:E:107:MET:HE1	1.99	0.43
1:H:91:ILE:HG12	1:H:114:ILE:HB	2.00	0.43
1:E:435:ARG:HD3	1:H:443:ARG:NH2	2.33	0.43
1:C:98:SER:HA	1:C:103:ARG:HG2	2.00	0.43
1:F:144:SER:C	1:F:146:LEU:H	2.26	0.43
1:C:410:LYS:HE2	1:C:410:LYS:HB2	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:CYS:HB2	1:F:551:LEU:HD12	2.01	0.43
1:B:192:ARG:HG3	1:B:201:TRP:CZ2	2.54	0.43
1:D:99:ARG:HH22	1:D:129:GLU:HB2	1.83	0.43
1:G:371:THR:OG1	5:G:604:PYR:O	2.28	0.43
1:H:562:SER:OG	2:H:602:FBP:O6P	2.37	0.43
1:A:266:GLU:O	1:A:270:ARG:HG3	2.19	0.42
1:C:440:GLU:CD	1:D:68:THR:HB	2.44	0.42
1:C:435:ARG:HE	1:C:435:ARG:HB2	1.64	0.42
1:E:309:LYS:NZ	1:E:505:GLN:OE1	2.50	0.42
1:E:549:GLY:O	1:H:449:ARG:NH2	2.47	0.42
1:H:179:LYS:HA	1:H:240:VAL:HG23	2.01	0.42
1:C:114:ILE:HG12	1:C:152:ALA:HB3	2.01	0.42
1:G:250:LYS:HD2	1:G:250:LYS:HA	1.80	0.42
1:D:98:SER:HA	1:D:103:ARG:HG2	2.00	0.42
1:F:99:ARG:HH22	1:F:129:GLU:CD	2.28	0.42
1:G:218:TYR:HB3	1:G:222:GLY:HA2	2.01	0.42
1:G:377:MET:HE2	1:G:377:MET:HB3	1.93	0.42
1:D:250:LYS:HE3	1:D:251:GLY:H	1.83	0.42
1:E:322:ARG:O	1:E:326:ILE:HG13	2.20	0.42
1:H:250:LYS:HA	1:H:250:LYS:HD3	1.63	0.42
1:H:267:GLN:HE21	1:H:270:ARG:HH21	1.67	0.42
1:H:382:ARG:HA	1:H:382:ARG:HD2	1.79	0.42
1:A:225:SER:O	1:A:226:LEU:HD23	2.20	0.42
1:E:352:ALA:O	1:E:356:MET:HG3	2.20	0.42
1:G:368:VAL:HG22	1:G:401:CYS:HB2	2.01	0.42
1:D:209:ARG:HA	1:D:209:ARG:HD2	1.56	0.42
1:D:216:ARG:HA	1:D:226:LEU:O	2.20	0.42
1:E:56:PHE:HB2	1:E:57:GLN:NE2	2.35	0.42
1:H:517:TYR:CZ	1:H:519:GLU:HB2	2.55	0.42
1:A:476[B]:THR:OG1	1:A:562:SER:HB3	2.19	0.42
1:H:56:PHE:O	1:H:62:PRO:HD3	2.19	0.42
1:D:87:SER:HB2	1:D:510:ARG:HG2	2.02	0.42
1:E:458:GLY:HA3	1:H:568:MET:HE1	2.01	0.42
1:F:284:PHE:HD1	1:F:311:ILE:HB	1.84	0.42
1:G:164:THR:OG1	1:G:250:LYS:N	2.52	0.42
1:B:216:ARG:HH12	1:B:255:PRO:C	2.28	0.42
1:D:318:GLU:O	1:D:322:ARG:HG3	2.19	0.42
1:E:377:MET:HE2	1:E:377:MET:HB3	1.82	0.42
1:G:83:VAL:O	1:G:426:ARG:HD2	2.19	0.42
1:A:114:ILE:HG12	1:A:152:ALA:HB3	2.00	0.41
1:E:264:LEU:HD12	1:E:264:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:VAL:HG22	1:G:237:VAL:O	2.20	0.41
1:E:261:LEU:HD12	1:E:261:LEU:HA	1.85	0.41
1:G:165:GLY:N	1:G:201:TRP:O	2.54	0.41
1:G:383:PRO:HG3	1:G:420:MET:HG2	2.03	0.41
1:G:435:ARG:HE	1:G:435:ARG:HB2	1.68	0.41
1:H:352:ALA:O	1:H:356:MET:HG3	2.20	0.41
1:H:517:TYR:CE2	1:H:519:GLU:HB2	2.54	0.41
1:A:457:ILE:HD12	1:A:487:TYR:CE1	2.56	0.41
1:B:87:SER:HB3	1:B:511:GLY:HA2	2.02	0.41
1:B:160:PRO:HD2	1:B:287:PHE:HB2	2.02	0.41
1:F:551:LEU:HD23	1:F:551:LEU:HA	1.82	0.41
1:B:228:VAL:HG22	1:B:236:LEU:CD1	2.46	0.41
1:D:285:ALA:O	1:D:313:LYS:HG3	2.20	0.41
1:B:194:ARG:O	1:B:194:ARG:HG3	2.21	0.41
1:D:91:ILE:HG12	1:D:114:ILE:HB	2.02	0.41
1:C:342:ILE:HG12	1:D:382:ARG:HH22	1.86	0.41
1:C:354:LYS:NZ	1:C:397:ASP:OD1	2.54	0.41
1:D:340:LEU:O	1:D:344:ILE:HG12	2.21	0.41
1:G:525:TRP:CD1	1:G:560:PRO:HG3	2.56	0.41
1:H:452:THR:HG22	1:H:483:LEU:HD12	2.03	0.41
1:B:566:ASN:OD1	1:B:567:ILE:HG13	2.21	0.41
1:E:164:THR:O	1:E:249:ARG:HA	2.21	0.41
1:E:485:SER:HB2	1:E:510:ARG:O	2.20	0.41
1:B:87:SER:CB	1:B:511:GLY:HA2	2.51	0.40
1:C:177:LEU:HD22	1:C:240:VAL:HG21	2.03	0.40
1:C:284:PHE:HD1	1:C:311:ILE:HB	1.84	0.40
1:C:250:LYS:HD3	1:C:250:LYS:HA	1.85	0.40
1:E:285:ALA:C	1:E:313:LYS:HG3	2.46	0.40
1:G:442:ARG:HG2	1:G:457:ILE:HD11	2.03	0.40
1:D:370:ALA:O	1:D:371:THR:HB	2.22	0.40
1:E:449:ARG:CZ	1:H:551:LEU:HD23	2.50	0.40
1:H:267:GLN:NE2	1:H:270:ARG:HH21	2.19	0.40
1:H:435:ARG:HE	1:H:435:ARG:HB2	1.70	0.40
1:A:204:TYR:HE2	1:A:207:ILE:HG12	1.87	0.40
1:B:83:VAL:O	1:B:426:ARG:HD2	2.22	0.40
1:F:86:ARG:HD3	1:F:422:HIS:HA	2.03	0.40
1:F:91:ILE:HG12	1:F:114:ILE:HB	2.04	0.40
1:G:125:GLU:O	1:G:129:GLU:HG3	2.21	0.40
1:G:204:TYR:CE1	1:G:206:ASN:HB2	2.57	0.40
1:G:420:MET:HE3	1:G:424:ILE:HD11	2.03	0.40
1:B:99:ARG:NH2	1:B:129:GLU:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:HG	1:E:178:VAL:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:THR:OG1	1:G:304:GLU:OE1[4_544]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/544 (88%)	458 (96%)	16 (3%)	2 (0%)	30	34
1	B	513/544 (94%)	498 (97%)	13 (2%)	2 (0%)	30	34
1	C	506/544 (93%)	489 (97%)	12 (2%)	5 (1%)	12	12
1	D	475/544 (87%)	460 (97%)	14 (3%)	1 (0%)	43	52
1	E	510/544 (94%)	491 (96%)	17 (3%)	2 (0%)	30	34
1	F	516/544 (95%)	505 (98%)	10 (2%)	1 (0%)	43	52
1	G	507/544 (93%)	485 (96%)	18 (4%)	4 (1%)	16	17
1	H	516/544 (95%)	507 (98%)	8 (2%)	1 (0%)	43	52
All	All	4019/4352 (92%)	3893 (97%)	108 (3%)	18 (0%)	30	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	GLN
1	G	178	VAL
1	E	227	VAL
1	G	196	ASN

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Mol	Chain	Res	Type
1	C	164	THR
1	D	371	THR
1	E	371	THR
1	B	371	THR
1	C	249	ARG
1	C	371	THR
1	F	371	THR
1	G	371	THR
1	B	233	PRO
1	G	249	ARG
1	H	371	THR
1	A	228	VAL
1	C	228	VAL
1	A	227	VAL

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	391/436 (90%)	380 (97%)	11 (3%)	38	51
1	B	416/436 (95%)	408 (98%)	8 (2%)	50	65
1	C	412/436 (94%)	405 (98%)	7 (2%)	53	68
1	D	386/436 (88%)	379 (98%)	7 (2%)	51	66
1	E	412/436 (94%)	394 (96%)	18 (4%)	25	33
1	F	417/436 (96%)	409 (98%)	8 (2%)	50	65
1	G	413/436 (95%)	394 (95%)	19 (5%)	24	31
1	H	418/436 (96%)	404 (97%)	14 (3%)	33	44
All	All	3265/3488 (94%)	3173 (97%)	92 (3%)	38	51

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	THR

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Mol	Chain	Res	Type
1	A	183	VAL
1	A	202	VAL
1	A	207	ILE
1	A	213	VAL
1	A	227	VAL
1	A	241	GLU
1	A	246	LEU
1	A	389	SER
1	A	518	ARG
1	A	572	SER
1	B	56	PHE
1	B	61	LEU
1	B	177	LEU
1	B	231	ILE
1	B	236	LEU
1	B	266	GLU
1	B	396	LEU
1	B	552	VAL
1	C	53	THR
1	C	177	LEU
1	C	239	GLN
1	C	248	SER
1	C	374	LEU
1	C	389	SER
1	C	552	VAL
1	D	209	ARG
1	D	227	VAL
1	D	236	LEU
1	D	294	VAL
1	D	388	THR
1	D	448	SER
1	D	467	CYS
1	E	53	THR
1	E	100	SER
1	E	177	LEU
1	E	178	VAL
1	E	184	LEU
1	E	193	THR
1	E	199	THR
1	E	223	LEU
1	E	227	VAL
1	E	259	VAL

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Mol	Chain	Res	Type
1	E	261	LEU
1	E	329	VAL
1	E	389	SER
1	E	473	VAL
1	E	485	SER
1	E	486	ARG
1	E	506	VAL
1	E	518	ARG
1	F	104	LEU
1	F	211	VAL
1	F	213	VAL
1	F	294	VAL
1	F	301	LEU
1	F	389	SER
1	F	552	VAL
1	F	574	SER
1	G	100	SER
1	G	125	GLU
1	G	172	GLU
1	G	185	VAL
1	G	186	THR
1	G	187	VAL
1	G	200	VAL
1	G	210	VAL
1	G	238	THR
1	G	240	VAL
1	G	294	VAL
1	G	330	SER
1	G	389	SER
1	G	485	SER
1	G	531[A]	ARG
1	G	531[B]	ARG
1	G	552	VAL
1	G	562[A]	SER
1	G	562[B]	SER
1	H	61	LEU
1	H	104	LEU
1	H	139	GLU
1	H	258	GLN
1	H	259	VAL
1	H	294	VAL
1	H	301	LEU

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Mol	Chain	Res	Type
1	H	329	VAL
1	H	389	SER
1	H	396	LEU
1	H	453	GLU
1	H	506	VAL
1	H	552	VAL
1	H	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	306	HIS
1	A	501	GLN
1	B	229	GLN
1	B	482	GLN
1	C	229	GLN
1	E	57	GLN
1	E	58	GLN
1	E	239	GLN
1	E	482	GLN
1	F	57	GLN
1	F	229	GLN
1	F	278	HIS
1	G	421	GLN
1	G	501	GLN
1	H	229	GLN
1	H	239	GLN
1	H	258	GLN
1	H	267	GLN
1	H	501	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PYR	B	605	3	5,5,5	3.16	3 (60%)	3,6,6	1.41	0
5	PYR	C	604	3	5,5,5	3.15	3 (60%)	3,6,6	1.50	1 (33%)
6	HVI	B	601	-	31,32,32	1.74	6 (19%)	27,47,47	2.51	11 (40%)
2	FBP	H	602	-	18,20,20	3.42	6 (33%)	21,32,32	0.71	0
5	PYR	D	604	3	5,5,5	3.01	3 (60%)	3,6,6	1.92	1 (33%)
5	PYR	F	605	-	5,5,5	3.07	3 (60%)	3,6,6	1.64	1 (33%)
2	FBP	D	602	-	18,20,20	3.42	5 (27%)	21,32,32	0.73	0
2	FBP	C	601	-	18,20,20	3.58	6 (33%)	21,32,32	1.52	5 (23%)
6	HVI	H	601	-	31,32,32	1.66	8 (25%)	27,47,47	2.52	11 (40%)
5	PYR	A	604	3	5,5,5	3.02	3 (60%)	3,6,6	1.82	2 (66%)
5	PYR	H	604	-	5,5,5	3.05	3 (60%)	3,6,6	1.56	1 (33%)
2	FBP	E	601	-	18,20,20	3.39	6 (33%)	21,32,32	0.79	0
5	PYR	G	604	3	5,5,5	3.02	3 (60%)	3,6,6	1.82	1 (33%)
2	FBP	F	602	-	18,20,20	3.37	5 (27%)	21,32,32	0.69	0
2	FBP	A	601	-	18,20,20	3.41	5 (27%)	21,32,32	0.75	0
6	HVI	D	601	-	31,32,32	1.68	7 (22%)	27,47,47	2.46	11 (40%)
5	PYR	E	604	3	5,5,5	3.02	3 (60%)	3,6,6	1.87	2 (66%)
6	HVI	F	601	-	31,32,32	1.64	6 (19%)	27,47,47	2.46	11 (40%)
2	FBP	B	602	-	18,20,20	3.41	5 (27%)	21,32,32	0.77	0
2	FBP	G	601	-	18,20,20	3.40	5 (27%)	21,32,32	0.83	0

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
5	PYR	B	605	3	-	0/4/4/4	-
5	PYR	C	604	3	-	0/4/4/4	-
6	HVI	B	601	-	-	4/8/8/8	0/5/5/5
2	FBP	H	602	-	-	2/13/32/32	0/1/1/1
5	PYR	D	604	3	-	0/4/4/4	-
5	PYR	F	605	-	-	0/4/4/4	-
2	FBP	D	602	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
6	HVI	H	601	-	-	4/8/8/8	0/5/5/5
5	PYR	A	604	3	-	0/4/4/4	-
5	PYR	H	604	-	-	4/4/4/4	-
2	FBP	E	601	-	-	4/13/32/32	0/1/1/1
5	PYR	G	604	3	-	0/4/4/4	-
2	FBP	F	602	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
6	HVI	D	601	-	-	3/8/8/8	0/5/5/5
5	PYR	E	604	3	-	4/4/4/4	-
6	HVI	F	601	-	-	4/8/8/8	0/5/5/5
2	FBP	B	602	-	-	2/13/32/32	0/1/1/1
2	FBP	G	601	-	-	4/13/32/32	0/1/1/1

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	FBP	O5-C2	-8.74	1.29	1.43
2	C	601	FBP	O5-C5	8.66	1.62	1.43
2	C	601	FBP	O5-C2	-8.38	1.30	1.43
2	A	601	FBP	O5-C5	8.35	1.62	1.43
2	G	601	FBP	O5-C5	8.16	1.61	1.43
2	B	602	FBP	O5-C2	-8.15	1.30	1.43
2	H	602	FBP	O5-C5	8.14	1.61	1.43
2	F	602	FBP	O5-C2	-8.08	1.30	1.43
2	G	601	FBP	O5-C2	-8.06	1.30	1.43
2	E	601	FBP	O5-C2	-8.05	1.30	1.43
2	B	602	FBP	O5-C5	8.04	1.61	1.43
2	H	602	FBP	O5-C2	-8.03	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	FBP	O5-C5	7.95	1.61	1.43
2	F	602	FBP	O5-C5	7.91	1.61	1.43
2	A	601	FBP	O5-C2	-7.77	1.31	1.43
2	D	602	FBP	O5-C5	7.64	1.60	1.43
2	C	601	FBP	C4-C5	-7.35	1.34	1.53
2	F	602	FBP	C4-C5	-7.08	1.35	1.53
2	H	602	FBP	C4-C5	-7.05	1.35	1.53
2	D	602	FBP	C4-C5	-7.02	1.35	1.53
2	E	601	FBP	C4-C5	-6.94	1.35	1.53
2	G	601	FBP	C4-C5	-6.92	1.35	1.53
2	A	601	FBP	C4-C5	-6.91	1.35	1.53
2	B	602	FBP	C4-C5	-6.90	1.35	1.53
5	C	604	PYR	CA-C	-4.83	1.38	1.54
5	B	605	PYR	CA-C	-4.78	1.38	1.54
5	H	604	PYR	CA-C	-4.52	1.39	1.54
5	F	605	PYR	CA-C	-4.43	1.39	1.54
5	G	604	PYR	CA-C	-4.34	1.40	1.54
5	D	604	PYR	CA-C	-4.33	1.40	1.54
5	A	604	PYR	CA-C	-4.31	1.40	1.54
5	E	604	PYR	CA-C	-4.27	1.40	1.54
6	B	601	HVI	C12-N11	4.04	1.34	1.29
6	B	601	HVI	C01-N02	4.01	1.36	1.31
6	D	601	HVI	C12-N11	3.97	1.34	1.29
6	D	601	HVI	C01-N02	3.93	1.35	1.31
5	F	605	PYR	O3-CA	3.76	1.31	1.23
5	E	604	PYR	O3-CA	3.73	1.31	1.23
5	D	604	PYR	O3-CA	3.69	1.31	1.23
5	A	604	PYR	O3-CA	3.68	1.31	1.23
5	B	605	PYR	O3-CA	3.67	1.31	1.23
6	F	601	HVI	C12-N11	3.66	1.34	1.29
5	B	605	PYR	O-C	3.66	1.31	1.22
5	H	604	PYR	O-C	3.66	1.31	1.22
5	A	604	PYR	O-C	3.66	1.31	1.22
5	G	604	PYR	O3-CA	3.65	1.31	1.23
5	F	605	PYR	O-C	3.64	1.31	1.22
5	C	604	PYR	O3-CA	3.63	1.31	1.23
5	G	604	PYR	O-C	3.63	1.31	1.22
5	E	604	PYR	O-C	3.62	1.31	1.22
5	C	604	PYR	O-C	3.62	1.31	1.22
6	H	601	HVI	C12-N11	3.61	1.34	1.29
5	D	604	PYR	O-C	3.59	1.31	1.22
5	H	604	PYR	O3-CA	3.55	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	602	FBP	O3-C3	-3.55	1.35	1.42
6	H	601	HVI	C01-N02	3.54	1.35	1.31
2	A	601	FBP	O3-C3	-3.48	1.35	1.42
6	F	601	HVI	C01-N02	3.47	1.35	1.31
2	B	602	FBP	O3-C3	-3.47	1.35	1.42
2	E	601	FBP	O3-C3	-3.43	1.36	1.42
2	G	601	FBP	O3-C3	-3.35	1.36	1.42
2	D	602	FBP	O3-C3	-3.29	1.36	1.42
2	F	602	FBP	O3-C3	-3.17	1.36	1.42
2	C	601	FBP	O3-C3	-3.08	1.36	1.42
2	C	601	FBP	P1-O1	2.82	1.69	1.60
6	B	601	HVI	N10-N11	-2.69	1.31	1.36
6	F	601	HVI	N10-N11	-2.68	1.31	1.36
2	A	601	FBP	O4-C4	2.67	1.49	1.43
2	B	602	FBP	O4-C4	2.66	1.49	1.43
6	H	601	HVI	N10-N11	-2.62	1.31	1.36
6	B	601	HVI	C26-N28	2.61	1.42	1.35
6	H	601	HVI	C26-N28	2.60	1.42	1.35
2	E	601	FBP	O4-C4	2.58	1.49	1.43
6	D	601	HVI	C26-N28	2.54	1.42	1.35
6	F	601	HVI	C26-N28	2.53	1.42	1.35
2	G	601	FBP	O4-C4	2.52	1.49	1.43
2	F	602	FBP	O4-C4	2.47	1.49	1.43
6	B	601	HVI	C03-N02	2.47	1.41	1.36
6	D	601	HVI	C03-N02	2.47	1.41	1.36
6	D	601	HVI	N10-N11	-2.46	1.32	1.36
2	H	602	FBP	O4-C4	2.44	1.49	1.43
6	B	601	HVI	C18-C17	2.38	1.43	1.37
2	D	602	FBP	O4-C4	2.38	1.48	1.43
2	C	601	FBP	O4-C4	2.30	1.48	1.43
6	F	601	HVI	C18-C17	2.28	1.42	1.37
6	H	601	HVI	C18-C17	2.23	1.42	1.37
6	D	601	HVI	N19-N20	-2.22	1.31	1.36
6	F	601	HVI	C03-N02	2.18	1.40	1.36
2	E	601	FBP	P1-O1	2.18	1.67	1.60
6	H	601	HVI	C03-N02	2.18	1.40	1.36
6	D	601	HVI	C18-C17	2.10	1.42	1.37
2	H	602	FBP	P1-O1	2.06	1.66	1.60
6	H	601	HVI	C21-C22	2.05	1.54	1.51
6	H	601	HVI	N19-N20	-2.04	1.32	1.36

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	HVI	C07-N06-C03	7.10	110.17	106.27
6	D	601	HVI	C07-N06-C03	7.04	110.14	106.27
6	H	601	HVI	C07-N06-C03	6.88	110.05	106.27
6	F	601	HVI	C07-N06-C03	6.57	109.88	106.27
6	B	601	HVI	S05-C01-N02	-5.38	108.89	116.18
6	D	601	HVI	S05-C01-N02	-5.18	109.15	116.18
6	F	601	HVI	S05-C01-N02	-5.06	109.33	116.18
6	H	601	HVI	S05-C01-N02	-4.94	109.49	116.18
6	B	601	HVI	C26-N27-C22	4.79	121.65	118.07
6	H	601	HVI	C26-N27-C22	4.48	121.42	118.07
6	D	601	HVI	C26-N27-C22	4.06	121.11	118.07
6	F	601	HVI	C08-C04-C03	-3.83	105.66	108.28
6	H	601	HVI	C21-N10-N11	3.79	118.90	114.38
2	C	601	FBP	O2-C2-O5	3.68	116.38	109.33
6	H	601	HVI	C08-C04-C03	-3.57	105.84	108.28
6	F	601	HVI	C26-N27-C22	3.54	120.72	118.07
6	F	601	HVI	C21-N10-N11	3.54	118.60	114.38
6	B	601	HVI	O13-C09-C07	-3.06	120.12	126.38
6	F	601	HVI	C25-C24-C23	-3.05	116.33	120.24
6	D	601	HVI	O13-C09-C07	-3.04	120.14	126.38
6	D	601	HVI	C08-C04-C03	-2.96	106.26	108.28
6	B	601	HVI	C08-C04-C03	-2.90	106.30	108.28
6	D	601	HVI	C21-N10-N11	2.85	117.78	114.38
6	B	601	HVI	C21-N10-N11	2.82	117.74	114.38
6	B	601	HVI	C16-N20-N19	2.78	111.68	105.38
6	H	601	HVI	C25-C24-C23	-2.77	116.68	120.24
6	B	601	HVI	C01-N02-C03	2.75	114.84	108.01
6	F	601	HVI	C01-N02-C03	2.70	114.73	108.01
5	D	604	PYR	OXT-C-CA	2.67	121.00	113.59
6	D	601	HVI	C01-N02-C03	2.67	114.65	108.01
6	H	601	HVI	C09-C07-N06	2.67	134.38	131.26
2	C	601	FBP	O1-P1-O1P	2.65	113.61	106.44
6	H	601	HVI	C01-N02-C03	2.61	114.50	108.01
6	F	601	HVI	O13-C09-C07	-2.55	121.16	126.38
6	D	601	HVI	C25-C24-C23	-2.55	116.97	120.24
6	F	601	HVI	C16-N20-N19	2.51	111.07	105.38
6	H	601	HVI	C16-N20-N19	2.51	111.06	105.38
6	D	601	HVI	C09-C07-N06	2.50	134.18	131.26
6	B	601	HVI	C09-C07-N06	2.49	134.17	131.26
5	G	604	PYR	OXT-C-CA	2.46	120.42	113.59
2	C	601	FBP	C6-C5-C4	-2.45	106.40	115.21
5	E	604	PYR	OXT-C-CA	2.45	120.37	113.59
6	D	601	HVI	C16-N20-N19	2.44	110.91	105.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	601	HVI	O13-C09-C07	-2.44	121.39	126.38
2	C	601	FBP	O3-C3-C4	-2.36	104.91	113.25
5	A	604	PYR	OXT-C-CA	2.33	120.06	113.59
5	F	605	PYR	OXT-C-CA	2.29	119.94	113.59
6	B	601	HVI	C25-C24-C23	-2.26	117.34	120.24
6	F	601	HVI	C09-C07-N06	2.24	133.88	131.26
5	C	604	PYR	OXT-C-CA	2.23	119.76	113.59
6	F	601	HVI	C03-C04-S05	-2.22	105.65	109.62
6	D	601	HVI	C03-C04-S05	-2.21	105.67	109.62
5	H	604	PYR	OXT-C-CA	2.18	119.64	113.59
6	H	601	HVI	C03-C04-S05	-2.17	105.75	109.62
6	B	601	HVI	C03-C04-S05	-2.14	105.79	109.62
5	E	604	PYR	OXT-C-O	-2.11	118.87	123.90
2	C	601	FBP	O3P-P1-O1	2.11	112.17	106.67
5	A	604	PYR	OXT-C-O	-2.10	118.90	123.90

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O1-C1-C2-O2
2	E	601	FBP	O1-C1-C2-O5
2	G	601	FBP	O1-C1-C2-O2
5	E	604	PYR	O-C-CA-CB
5	E	604	PYR	OXT-C-CA-CB
5	H	604	PYR	O-C-CA-O3
5	H	604	PYR	OXT-C-CA-O3
6	D	601	HVI	N02-C01-C15-C16
2	A	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C4-C5-C6-O6
2	G	601	FBP	C4-C5-C6-O6
2	H	602	FBP	C4-C5-C6-O6
2	B	602	FBP	C4-C5-C6-O6
2	F	602	FBP	C4-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	B	602	FBP	O5-C5-C6-O6
2	D	602	FBP	C4-C5-C6-O6
2	D	602	FBP	O5-C5-C6-O6

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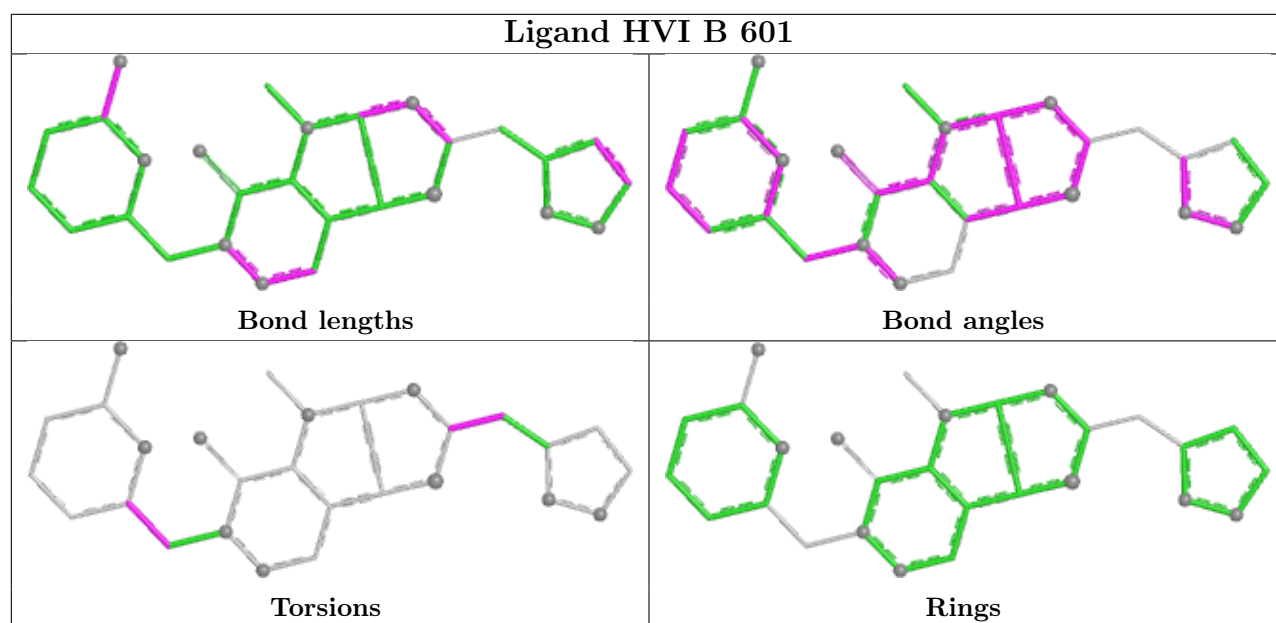
Mol	Chain	Res	Type	Atoms
2	F	602	FBP	O5-C5-C6-O6
2	H	602	FBP	O5-C5-C6-O6
5	H	604	PYR	O-C-CA-CB
6	B	601	HVI	N02-C01-C15-C16
6	F	601	HVI	N02-C01-C15-C16
6	H	601	HVI	N02-C01-C15-C16
5	E	604	PYR	OXT-C-CA-O3
5	H	604	PYR	OXT-C-CA-CB
6	B	601	HVI	N10-C21-C22-N27
6	D	601	HVI	N10-C21-C22-N27
6	F	601	HVI	N10-C21-C22-N27
6	H	601	HVI	N10-C21-C22-N27
6	B	601	HVI	N10-C21-C22-C23
6	D	601	HVI	N10-C21-C22-C23
6	F	601	HVI	N10-C21-C22-C23
6	H	601	HVI	N10-C21-C22-C23
6	B	601	HVI	S05-C01-C15-C16
6	F	601	HVI	S05-C01-C15-C16
6	H	601	HVI	S05-C01-C15-C16
2	G	601	FBP	O1-C1-C2-O5
5	E	604	PYR	O-C-CA-O3

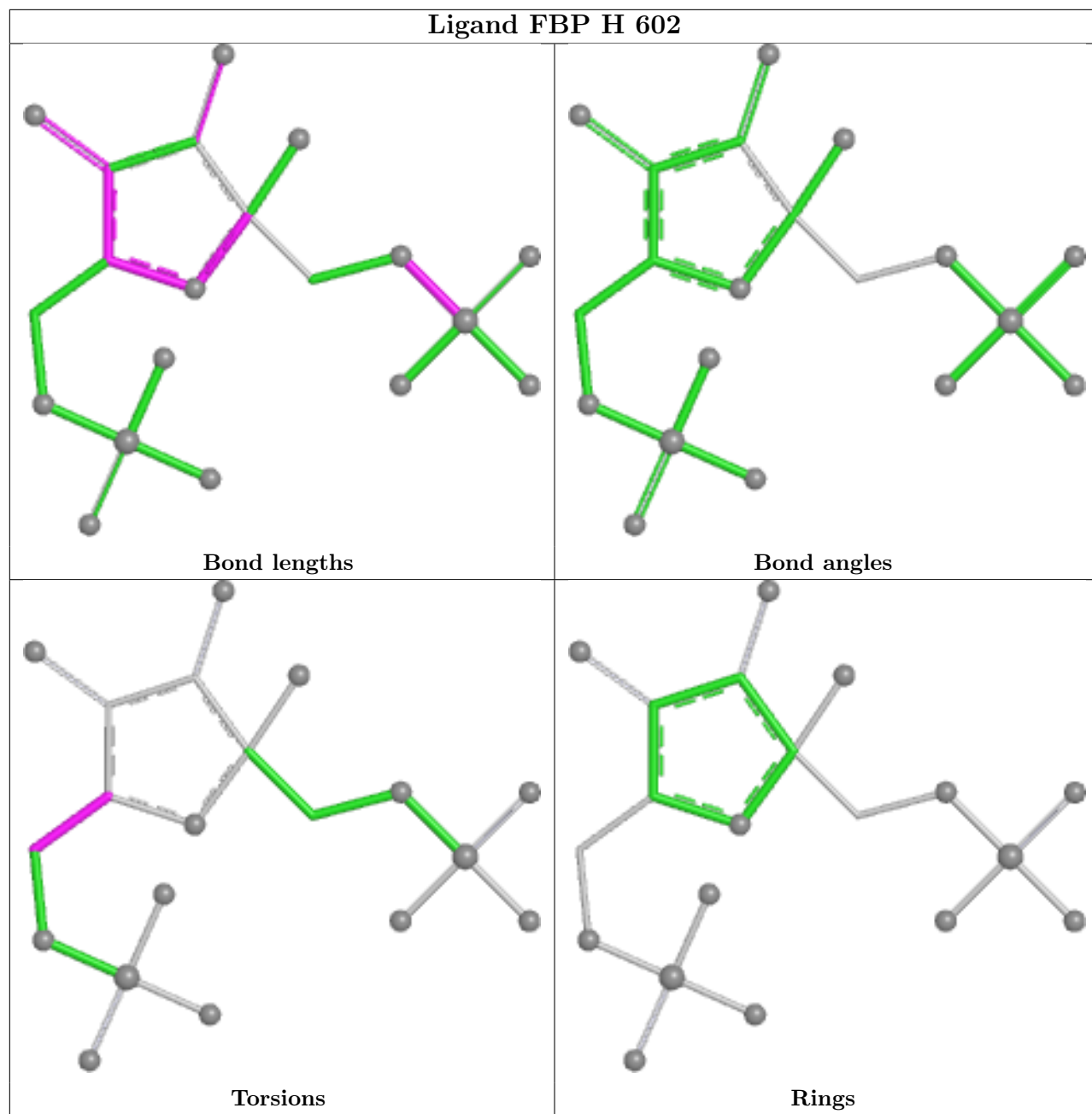
There are no ring outliers.

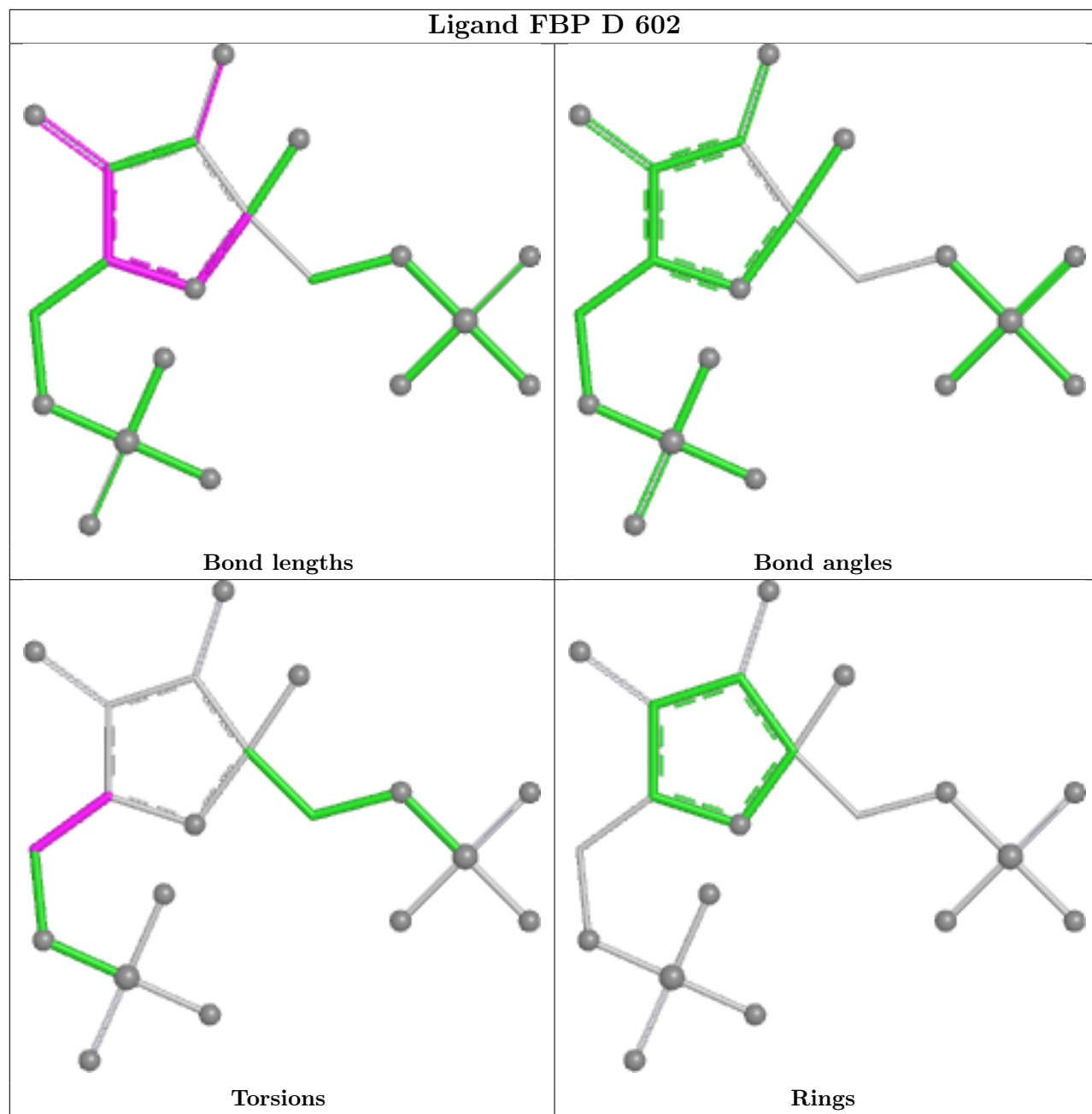
2 monomers are involved in 3 short contacts:

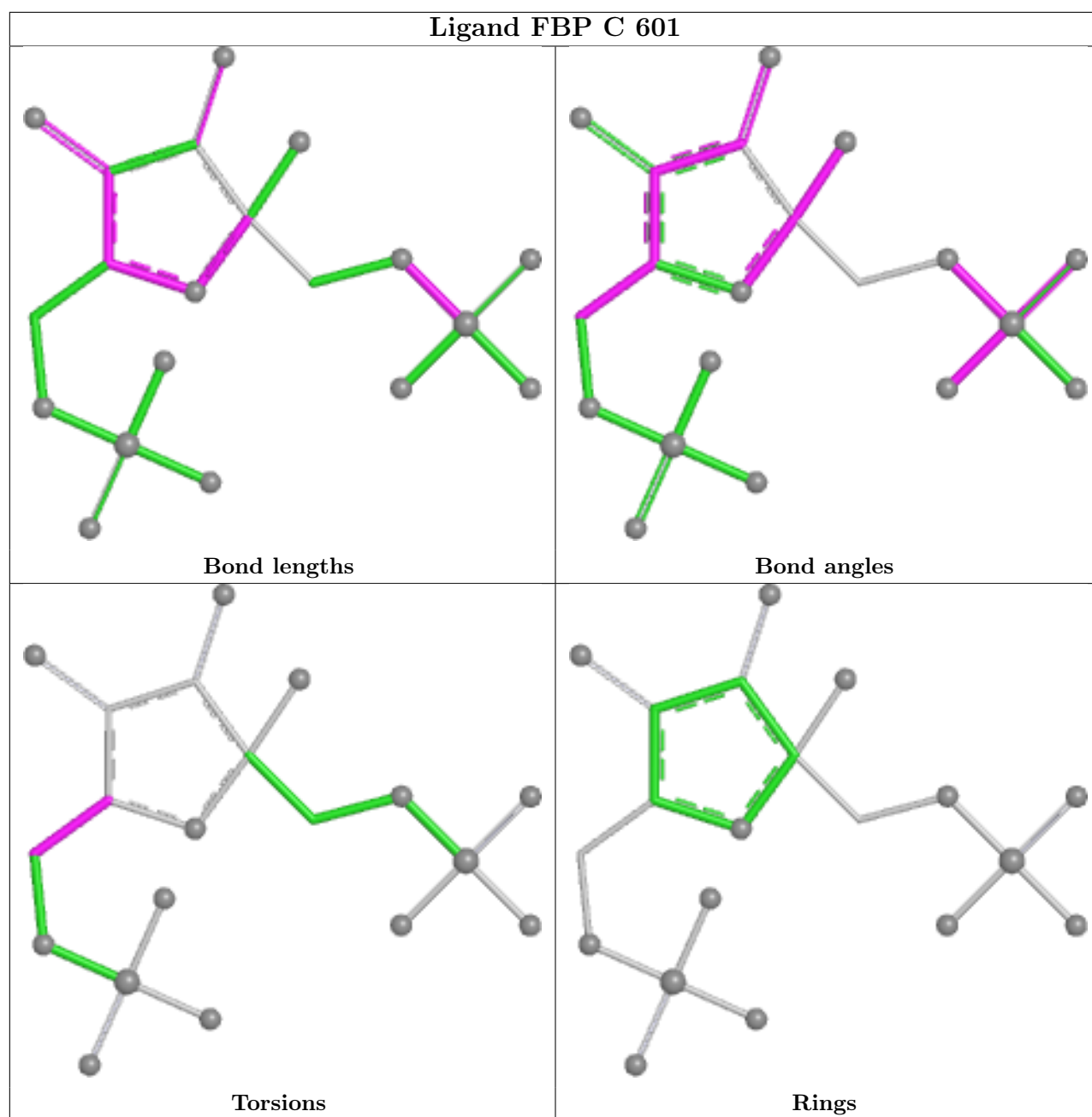
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	602	FBP	1	0
5	G	604	PYR	2	0

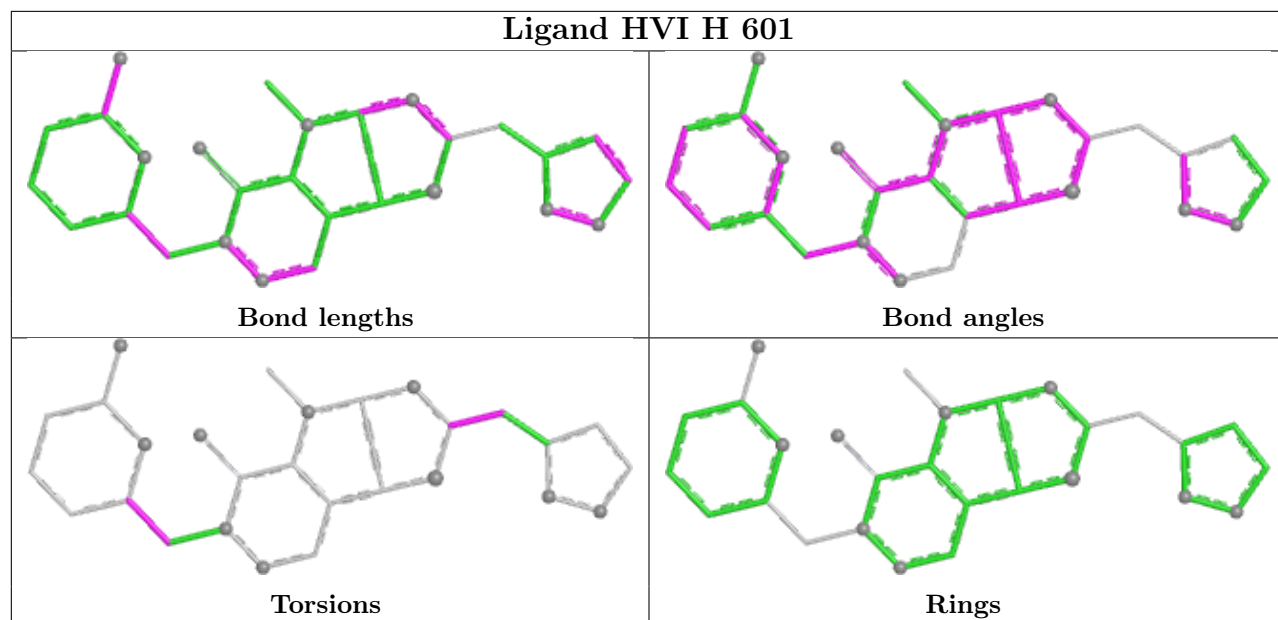
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



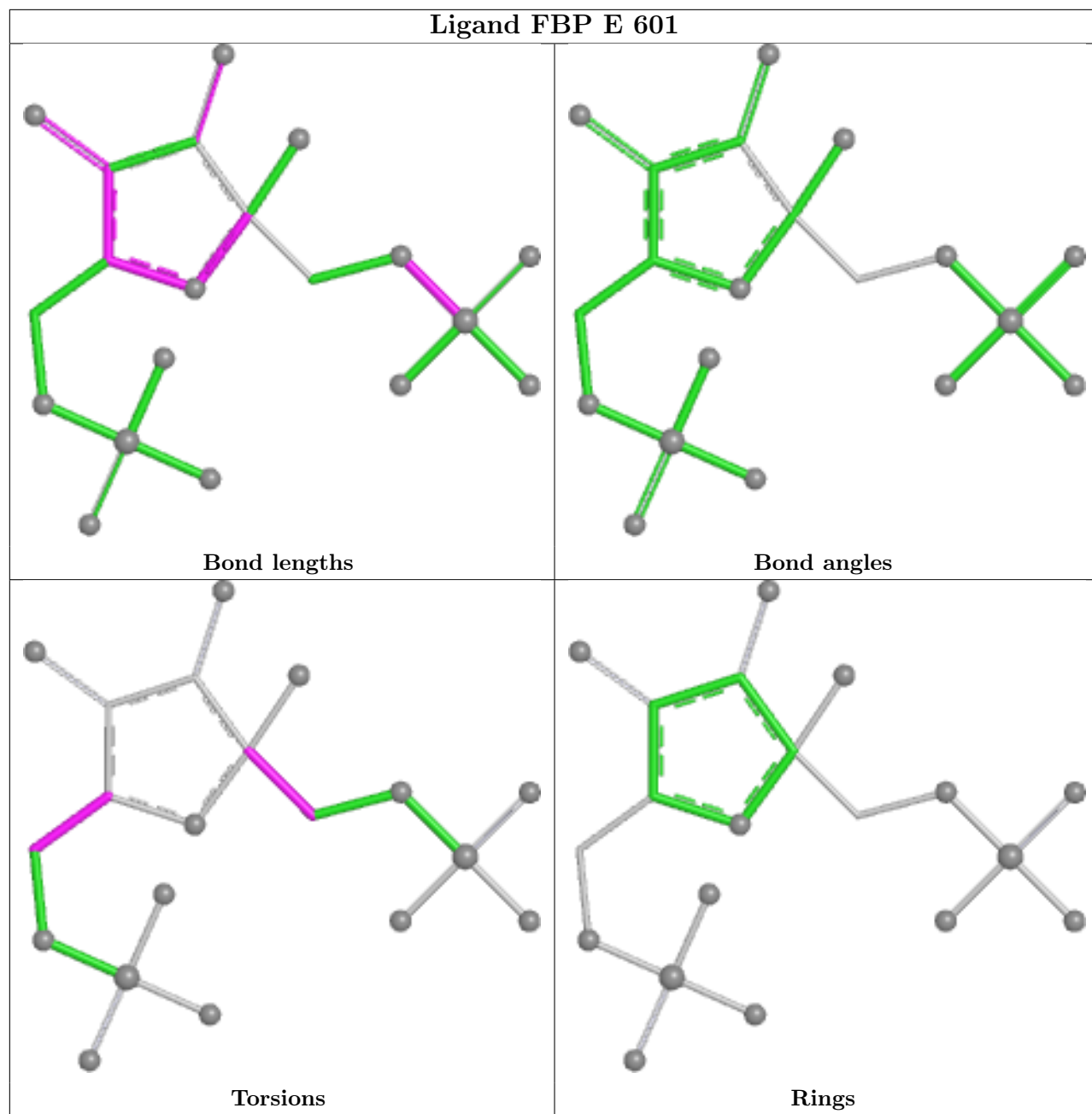




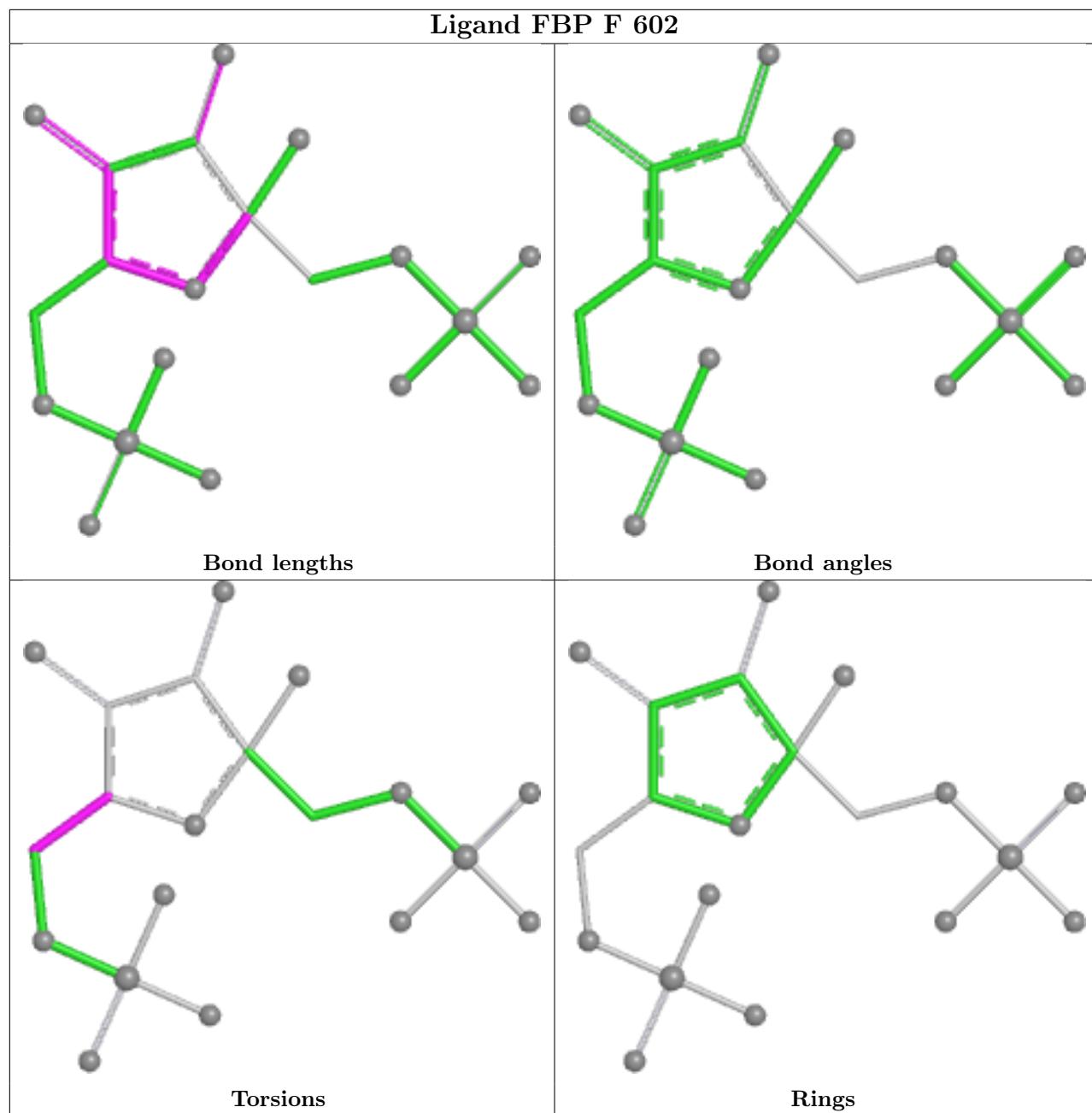


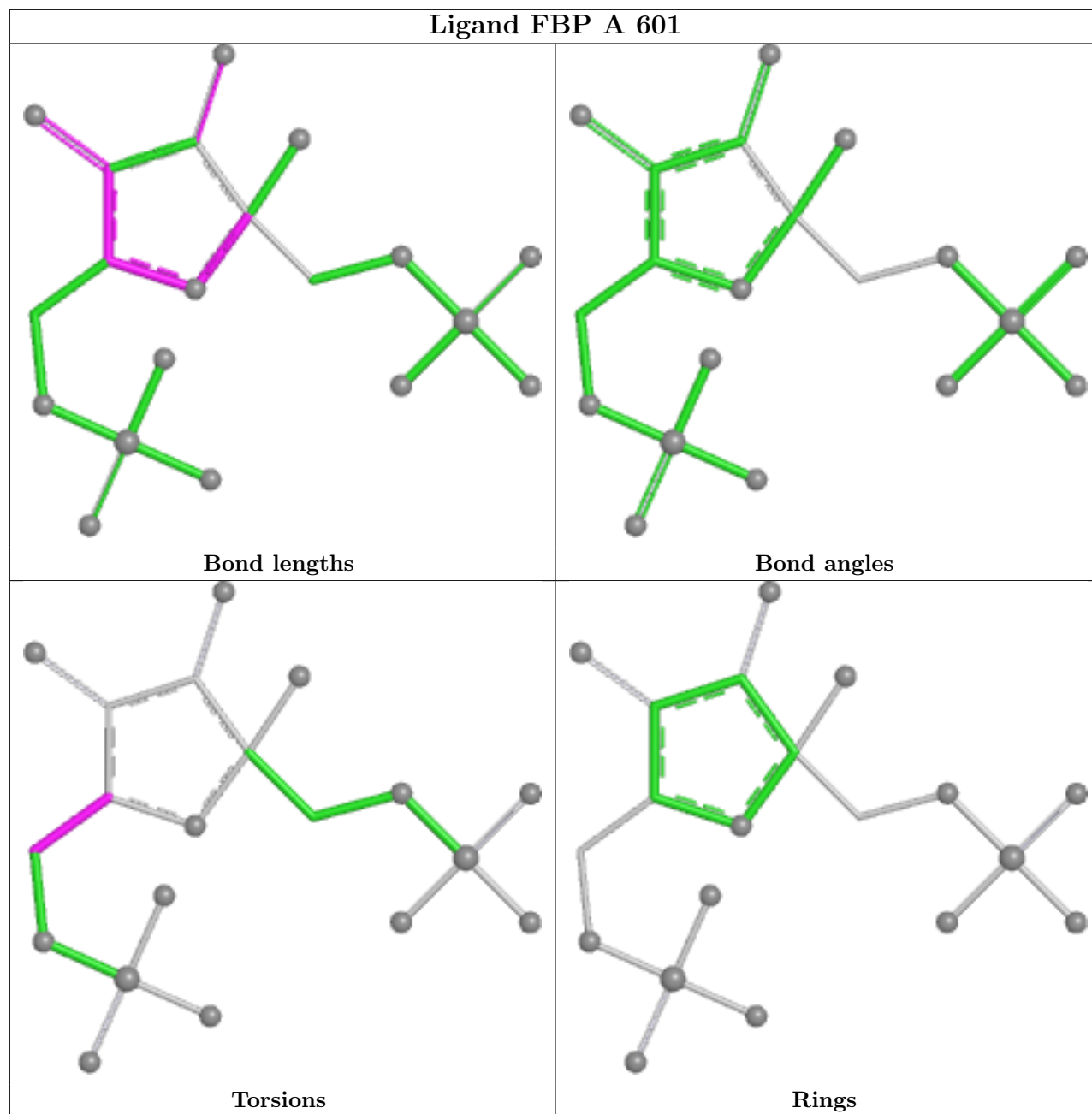


Ligand FBP E 601

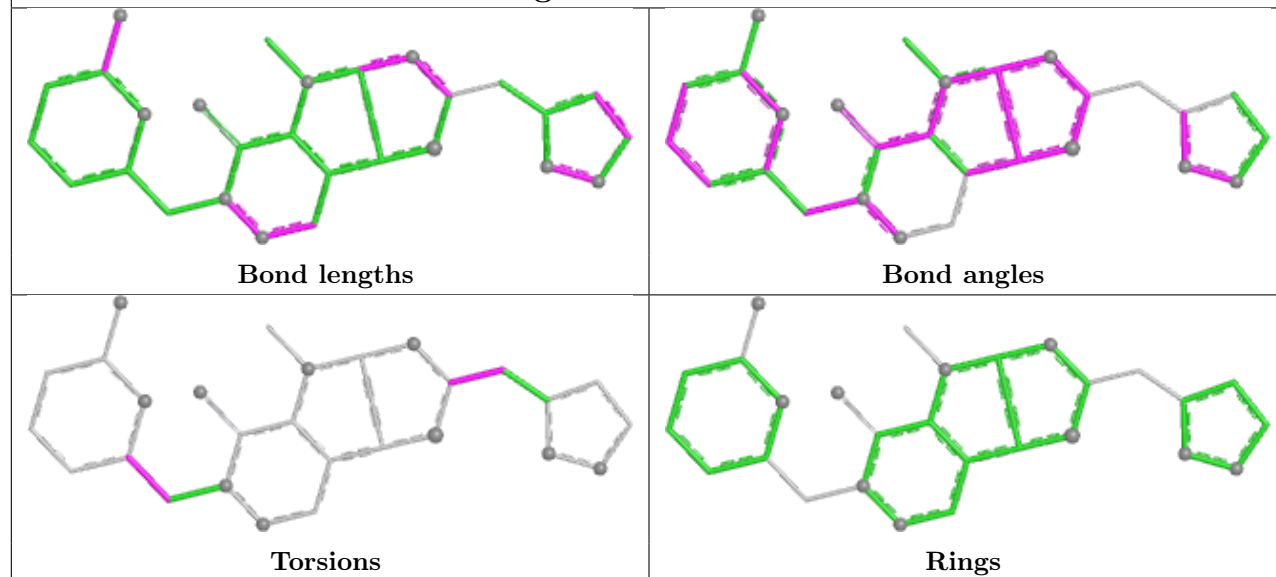


Ligand FBP F 602

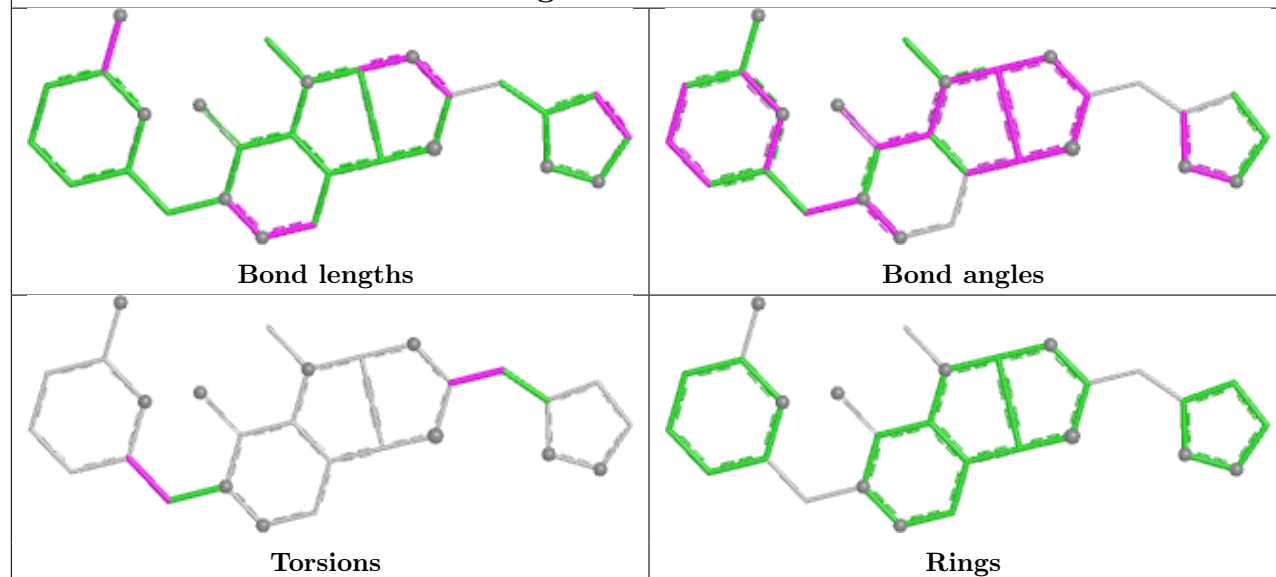


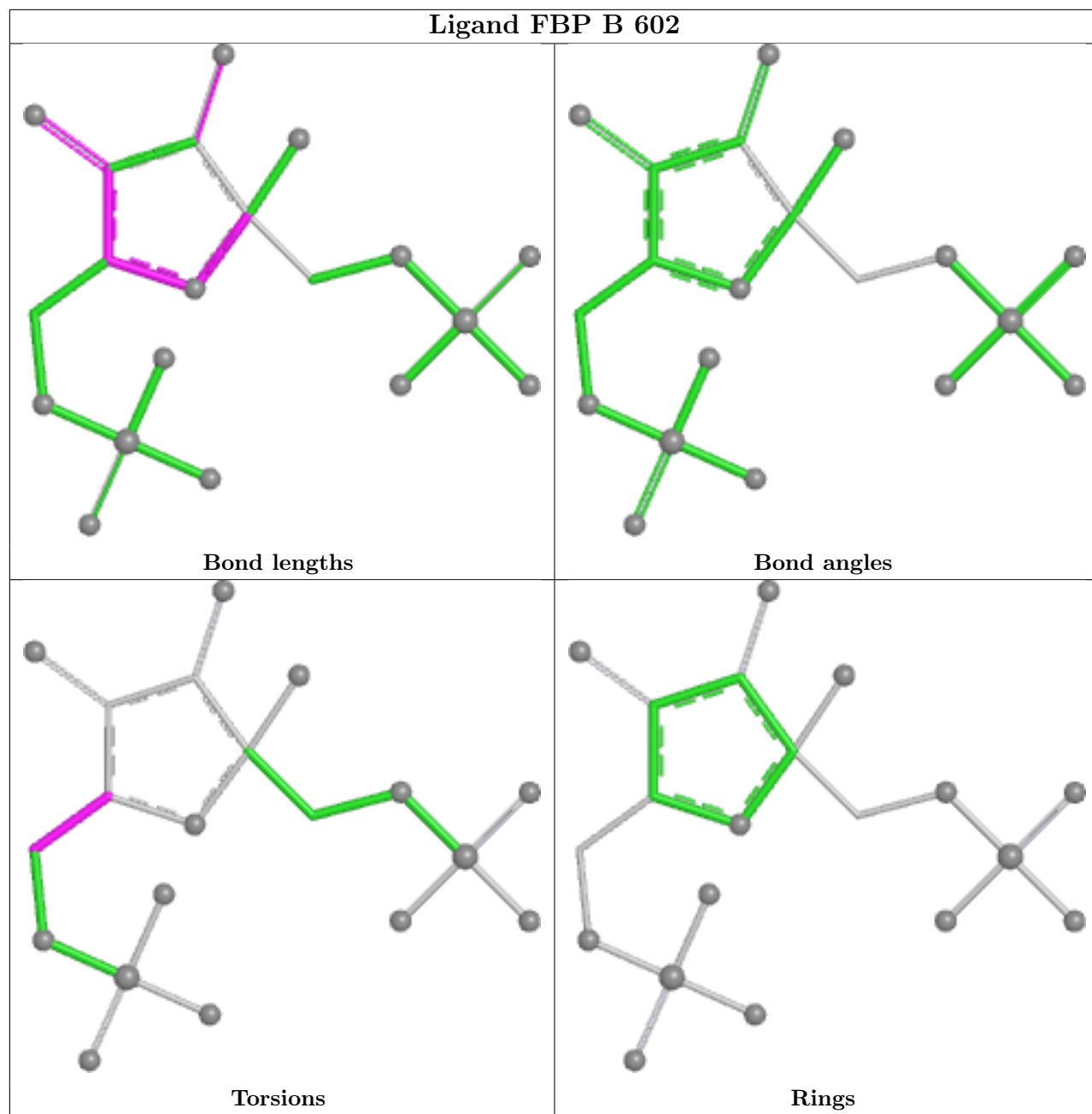


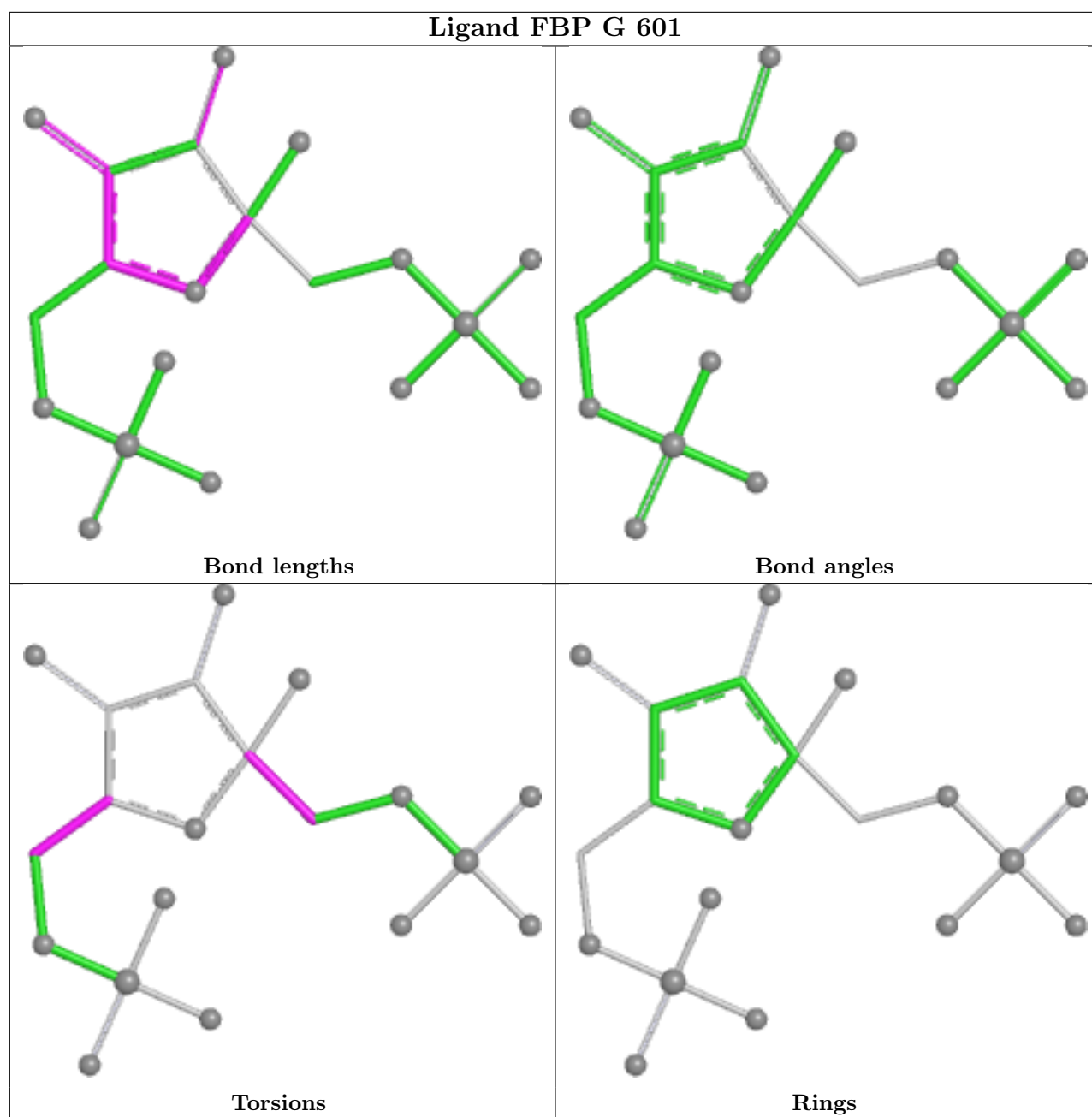
Ligand HVI D 601



Ligand HVI F 601







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	485/544 (89%)	0.16	26 (5%)	31	37	26, 51, 124, 158	1 (0%)
1	B	517/544 (95%)	0.18	32 (6%)	26	30	35, 51, 132, 162	0
1	C	512/544 (94%)	0.19	39 (7%)	20	22	24, 50, 135, 181	2 (0%)
1	D	483/544 (88%)	0.20	35 (7%)	21	24	36, 50, 110, 153	0
1	E	515/544 (94%)	0.39	36 (6%)	22	25	23, 62, 102, 155	1 (0%)
1	F	520/544 (95%)	-0.11	10 (1%)	66	71	31, 46, 75, 138	0
1	G	509/544 (93%)	0.38	41 (8%)	18	20	26, 61, 109, 155	6 (1%)
1	H	519/544 (95%)	-0.11	7 (1%)	75	79	29, 45, 73, 124	1 (0%)
All	All	4060/4352 (93%)	0.16	226 (5%)	30	35	23, 51, 116, 181	11 (0%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	LEU	6.7
1	D	245	VAL	6.2
1	A	245	VAL	5.8
1	G	185	VAL	5.8
1	D	208	VAL	5.4
1	H	171	PRO	5.1
1	E	208	VAL	5.0
1	E	178	VAL	4.9
1	G	170	GLY	4.9
1	G	208	VAL	4.8
1	G	240	VAL	4.8
1	D	167	LEU	4.7
1	A	166	ILE	4.6
1	B	231	ILE	4.5
1	D	247	GLY	4.5
1	C	231	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	207	ILE	4.4
1	D	197	ALA	4.3
1	D	233	PRO	4.3
1	E	171	PRO	4.2
1	C	235	GLY	4.2
1	C	213	VAL	4.2
1	D	236	LEU	4.2
1	C	186	THR	4.2
1	A	200	VAL	4.2
1	C	171	PRO	4.1
1	E	177	LEU	4.1
1	E	83	VAL	4.1
1	E	175	VAL	4.1
1	A	191	PHE	4.1
1	D	238	THR	4.1
1	C	201	TRP	4.0
1	D	220	ASP	4.0
1	B	171	PRO	3.9
1	G	241	GLU	3.9
1	A	187	VAL	3.8
1	A	210	VAL	3.8
1	G	237	VAL	3.8
1	G	226	LEU	3.8
1	D	201	TRP	3.8
1	B	55	PHE	3.8
1	C	245	VAL	3.8
1	G	248	SER	3.7
1	F	171	PRO	3.7
1	A	201	TRP	3.7
1	F	145	PRO	3.6
1	D	235	GLY	3.5
1	A	186	THR	3.5
1	B	211	VAL	3.4
1	C	84	ALA	3.4
1	H	56	PHE	3.4
1	A	211	VAL	3.3
1	B	166	ILE	3.3
1	H	251	GLY	3.3
1	C	545	PHE	3.3
1	F	56	PHE	3.2
1	E	180	GLY	3.2
1	A	246	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	233	PRO	3.2
1	A	83	VAL	3.1
1	A	213	VAL	3.1
1	C	178	VAL	3.1
1	G	171	PRO	3.1
1	F	169	GLY	3.1
1	A	212	PRO	3.1
1	B	259	VAL	3.1
1	G	213	VAL	3.1
1	E	224	ILE	3.0
1	E	186	THR	3.0
1	E	213	VAL	3.0
1	G	210	VAL	3.0
1	C	166	ILE	3.0
1	A	227	VAL	3.0
1	D	240	VAL	3.0
1	C	215	GLY	3.0
1	G	245	VAL	2.9
1	F	251	GLY	2.9
1	G	262	PRO	2.9
1	G	211	VAL	2.9
1	E	248	SER	2.9
1	B	397	ASP	2.9
1	C	195	GLY	2.8
1	G	263	GLY	2.8
1	B	175	VAL	2.8
1	D	232	GLY	2.8
1	E	169	GLY	2.8
1	E	261	LEU	2.8
1	C	397	ASP	2.8
1	A	190	ALA	2.8
1	C	190	ALA	2.8
1	G	190	ALA	2.8
1	B	382	ARG	2.8
1	G	178	VAL	2.8
1	G	177	LEU	2.7
1	G	207	ILE	2.7
1	G	219	ILE	2.7
1	A	189	PRO	2.7
1	C	197	ALA	2.7
1	C	240	VAL	2.7
1	C	164	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	242	ASN	2.7
1	F	65	MET	2.7
1	H	65	MET	2.7
1	C	236	LEU	2.7
1	D	198	ASN	2.6
1	D	243	GLY	2.6
1	E	170	GLY	2.6
1	E	207	ILE	2.6
1	B	201	TRP	2.6
1	B	56	PHE	2.6
1	D	210	VAL	2.6
1	C	250	LYS	2.6
1	B	178	VAL	2.6
1	B	208	VAL	2.6
1	C	185	VAL	2.6
1	C	211	VAL	2.6
1	E	183	VAL	2.6
1	D	223	LEU	2.5
1	G	172	GLU	2.5
1	A	188	ASP	2.5
1	G	214	GLY	2.5
1	A	202	VAL	2.5
1	E	228	VAL	2.5
1	A	204	TYR	2.5
1	H	55	PHE	2.5
1	A	208	VAL	2.5
1	C	202	VAL	2.5
1	E	227	VAL	2.5
1	E	258	GLN	2.5
1	D	254	LEU	2.5
1	E	226	LEU	2.5
1	D	257	ALA	2.5
1	G	164	THR	2.5
1	D	545	PHE	2.5
1	C	210	VAL	2.5
1	G	187	VAL	2.5
1	C	222	GLY	2.5
1	B	237	VAL	2.4
1	F	55	PHE	2.4
1	D	231	ILE	2.4
1	F	223	LEU	2.4
1	G	197	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	199	THR	2.4
1	B	187	VAL	2.4
1	G	261	LEU	2.4
1	B	221	ASP	2.4
1	C	221	ASP	2.4
1	D	212	PRO	2.4
1	E	262	PRO	2.4
1	G	195	GLY	2.4
1	A	182	GLN	2.4
1	E	235	GLY	2.3
1	E	256	GLY	2.3
1	D	219	ILE	2.3
1	D	200	VAL	2.3
1	D	237	VAL	2.3
1	E	259	VAL	2.3
1	A	215	GLY	2.3
1	B	190	ALA	2.3
1	F	574	SER	2.3
1	D	166	ILE	2.3
1	C	56	PHE	2.3
1	D	213	VAL	2.3
1	E	200	VAL	2.3
1	G	180	GLY	2.3
1	E	157	THR	2.3
1	G	238	THR	2.3
1	B	191	PHE	2.2
1	C	228	VAL	2.3
1	E	236	LEU	2.2
1	E	240	VAL	2.3
1	G	200	VAL	2.3
1	C	263	GLY	2.2
1	E	193	THR	2.2
1	E	238	THR	2.2
1	G	57	GLN	2.2
1	B	213	VAL	2.2
1	B	223	LEU	2.2
1	D	252	VAL	2.2
1	E	242	ASN	2.2
1	B	189	PRO	2.2
1	B	262	PRO	2.2
1	H	146	LEU	2.2
1	C	200	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	209	ARG	2.2
1	G	247	GLY	2.2
1	B	197	ALA	2.2
1	H	54	ALA	2.2
1	B	210	VAL	2.1
1	D	228	VAL	2.1
1	E	212	PRO	2.1
1	G	55	PHE	2.1
1	C	244	GLY	2.1
1	G	157	THR	2.1
1	A	183	VAL	2.1
1	A	255	PRO	2.1
1	G	83	VAL	2.1
1	B	57	GLN	2.1
1	E	217	ILE	2.1
1	B	243	GLY	2.1
1	C	53	THR	2.1
1	G	199	THR	2.1
1	C	230	LYS	2.1
1	F	54	ALA	2.1
1	G	223	LEU	2.1
1	C	188	ASP	2.1
1	G	221	ASP	2.1
1	B	169	GLY	2.1
1	D	244	GLY	2.1
1	E	545	PHE	2.1
1	G	165	GLY	2.1
1	C	249	ARG	2.1
1	A	179	LYS	2.0
1	D	248	SER	2.0
1	E	199	THR	2.0
1	B	184	LEU	2.0
1	B	227	VAL	2.0
1	C	442[A]	ARG	2.0
1	D	211	VAL	2.0
1	E	191	PHE	2.0
1	C	179	LYS	2.0
1	B	574	SER	2.0
1	G	239	GLN	2.0
1	B	246	LEU	2.0
1	C	261	LEU	2.0
1	C	217	ILE	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
3	MN	H	603	1/1	0.58	0.31	210,210,210,210	0
5	PYR	F	605	6/6	0.70	0.16	74,75,85,90	0
4	K	G	603	1/1	0.71	0.13	119,119,119,119	0
4	K	E	603	1/1	0.71	0.19	140,140,140,140	0
4	K	C	603	1/1	0.78	0.14	102,102,102,102	0
4	K	B	604	1/1	0.78	0.16	98,98,98,98	0
5	PYR	H	604	6/6	0.81	0.13	80,81,83,86	0
5	PYR	E	604	6/6	0.83	0.12	61,75,77,84	0
3	MN	F	603	1/1	0.84	0.24	160,160,160,160	0
4	K	F	604	1/1	0.85	0.21	107,107,107,107	0
5	PYR	D	604	6/6	0.86	0.12	58,68,78,84	0
4	K	A	603	1/1	0.89	0.12	90,90,90,90	0
5	PYR	B	605	6/6	0.89	0.14	51,72,77,78	0
5	PYR	C	604	6/6	0.91	0.11	52,60,68,72	0
5	PYR	G	604	6/6	0.92	0.10	63,70,75,78	0
6	HVI	B	601	28/28	0.93	0.08	31,46,52,58	0
3	MN	G	602	1/1	0.94	0.12	133,133,133,133	0
2	FBP	C	601	20/20	0.94	0.09	37,42,56,57	0
3	MN	D	603	1/1	0.95	0.07	99,99,99,99	0
2	FBP	E	601	20/20	0.95	0.07	41,48,56,61	0
2	FBP	G	601	20/20	0.95	0.08	38,47,58,61	0
6	HVI	H	601	28/28	0.95	0.08	31,38,45,48	0
6	HVI	D	601	28/28	0.96	0.07	33,45,55,59	0
6	HVI	F	601	28/28	0.96	0.07	31,38,46,50	0
2	FBP	D	602	20/20	0.96	0.07	40,49,55,62	0
5	PYR	A	604	6/6	0.97	0.14	50,59,65,65	0
2	FBP	A	601	20/20	0.97	0.05	39,46,56,61	0

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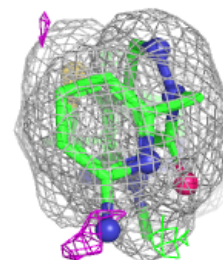
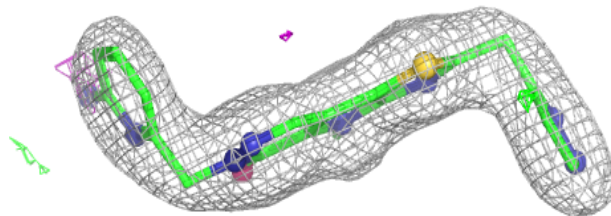
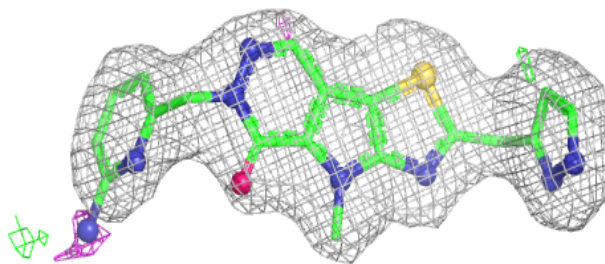
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	F	602	20/20	0.97	0.06	31,41,47,48	0
3	MN	E	602	1/1	0.97	0.08	93,93,93,93	0
3	MN	B	603	1/1	0.98	0.06	87,87,87,87	0
2	FBP	B	602	20/20	0.98	0.04	32,39,44,47	0
2	FBP	H	602	20/20	0.98	0.06	35,41,51,51	0
3	MN	C	602	1/1	0.99	0.05	67,67,67,67	0
3	MN	A	602	1/1	0.99	0.04	61,61,61,61	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.

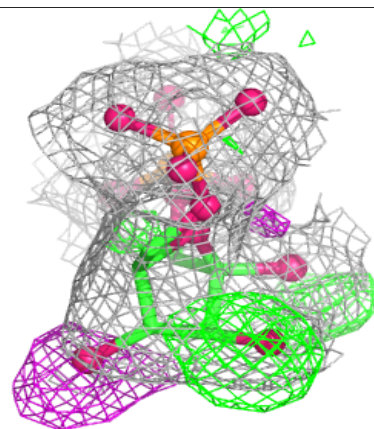
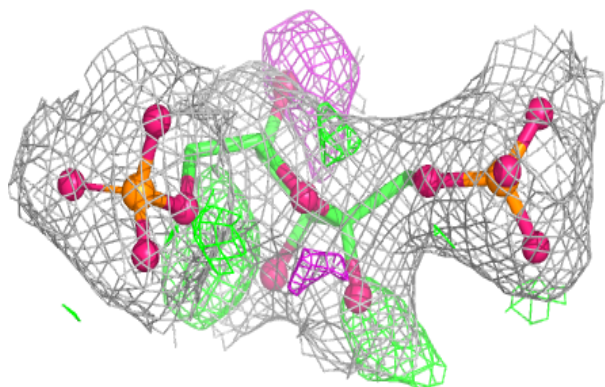
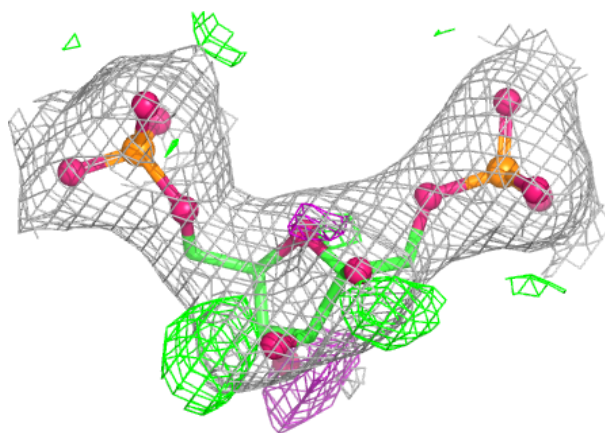
Electron density around HVI B 601:

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

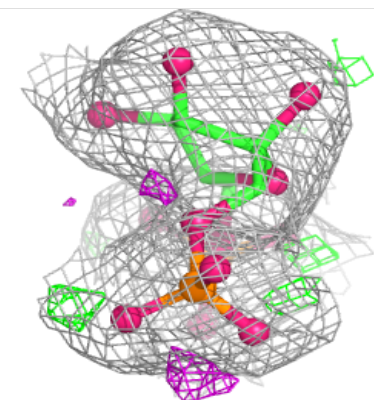
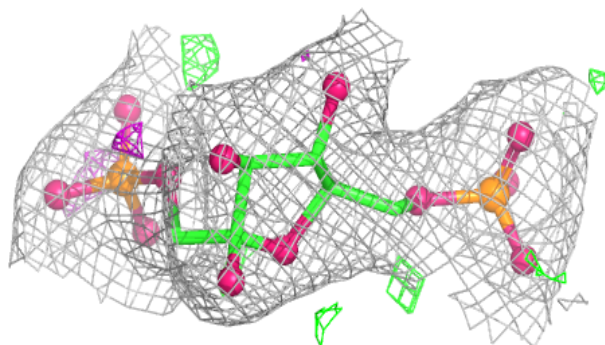
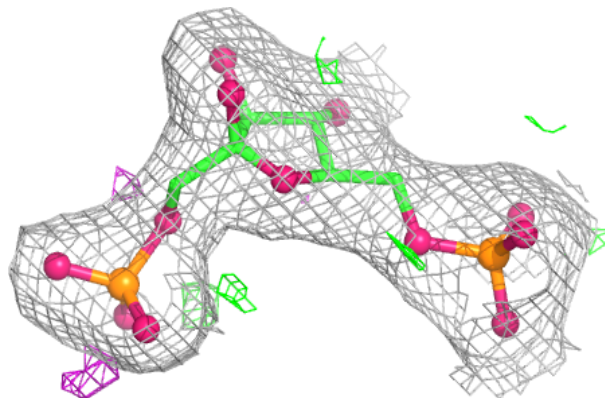


Electron density around FBP C 601:

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

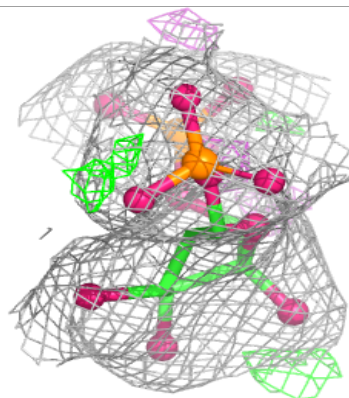
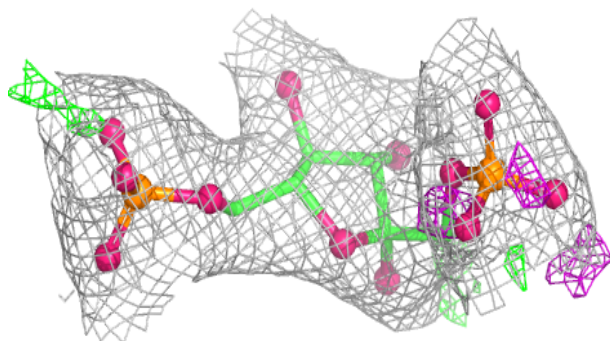
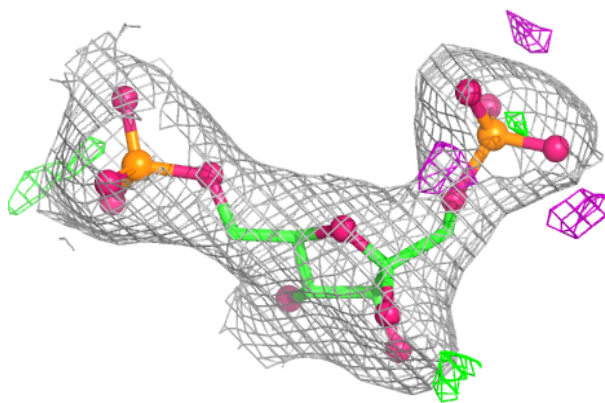
**Electron density around FBP E 601:**

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

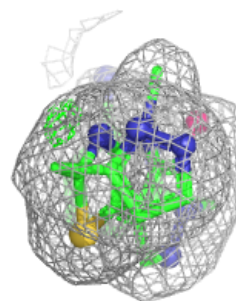
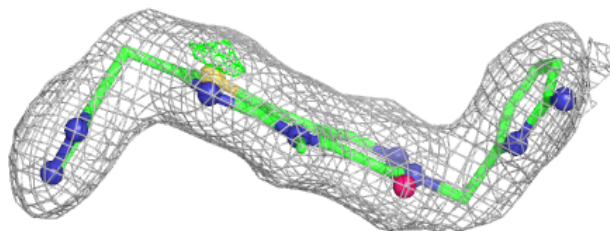
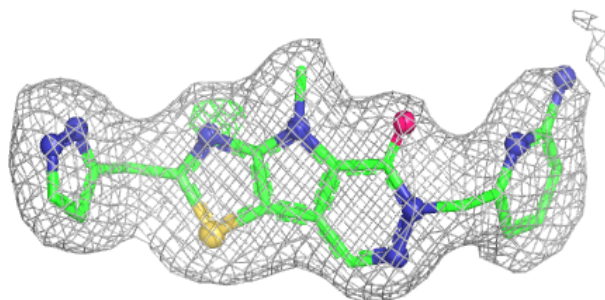


Electron density around FBP G 601:

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

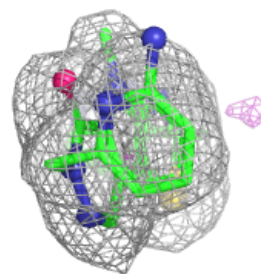
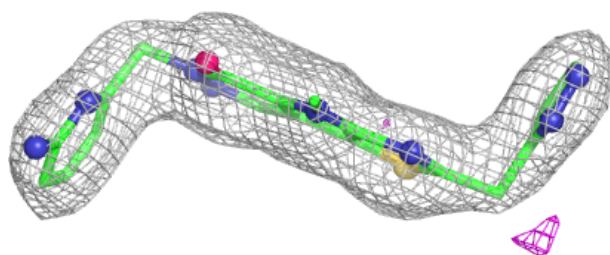
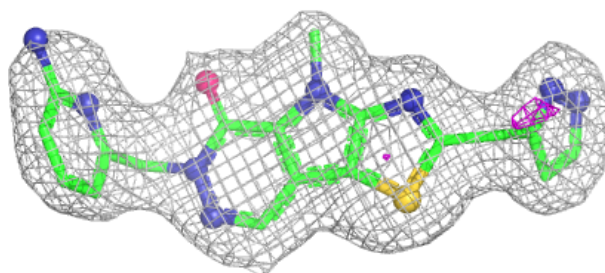
**Electron density around HVI H 601:**

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

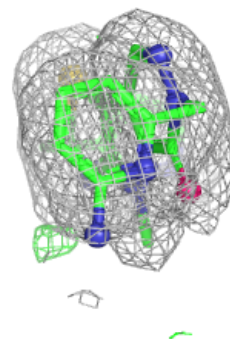
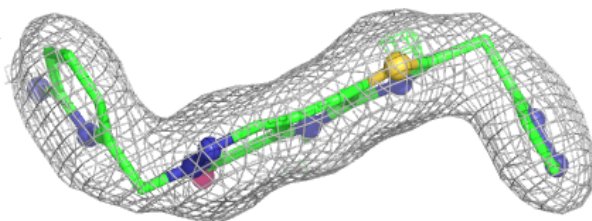
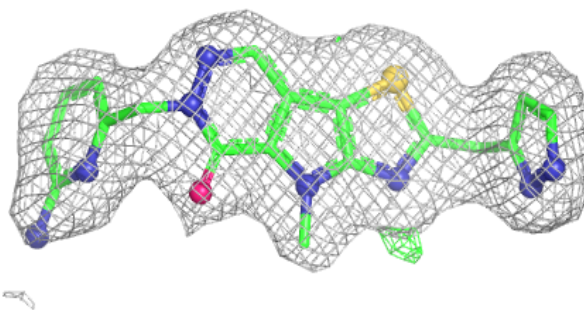


Electron density around HVI D 601:

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

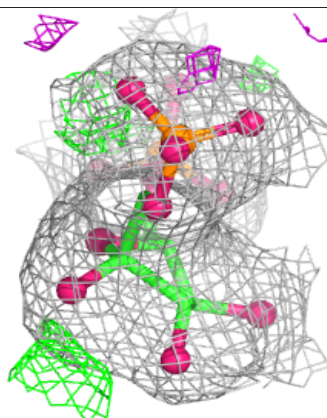
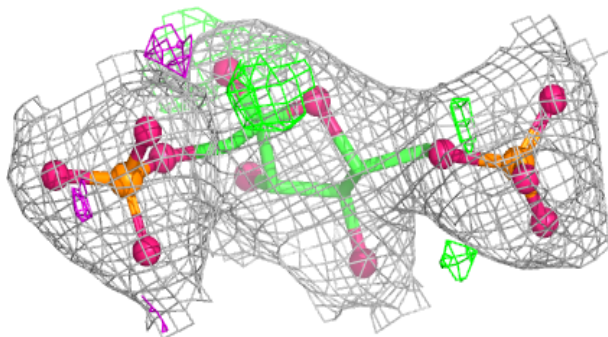
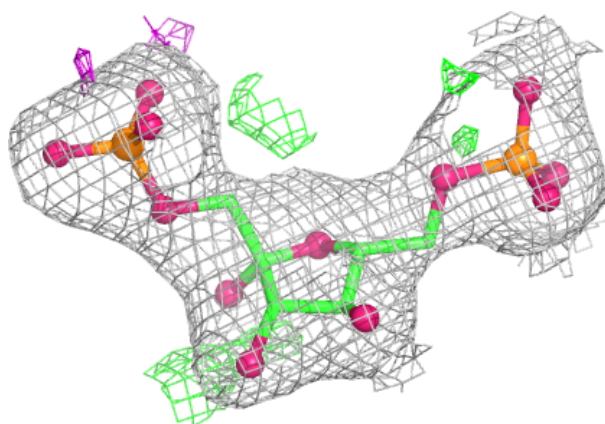
**Electron density around HVI F 601:**

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

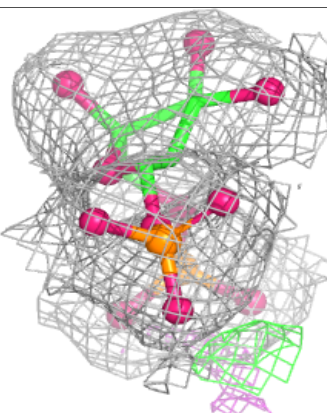
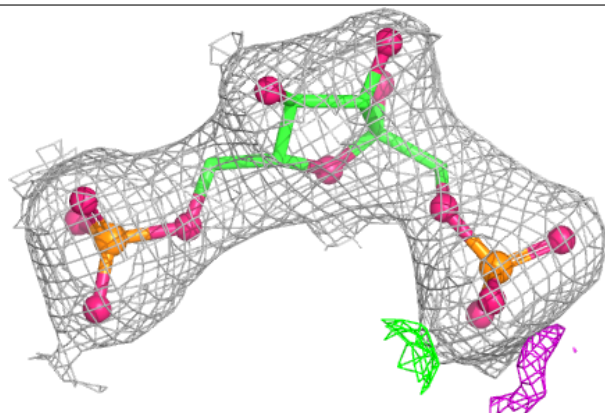


Electron density around FBP D 602:

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

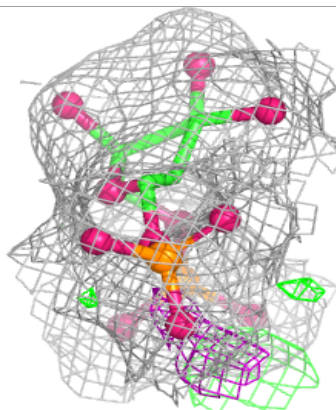
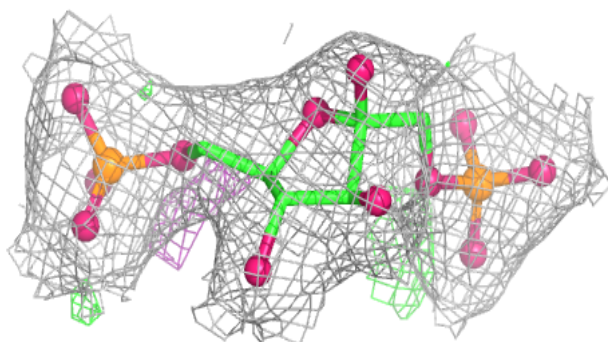
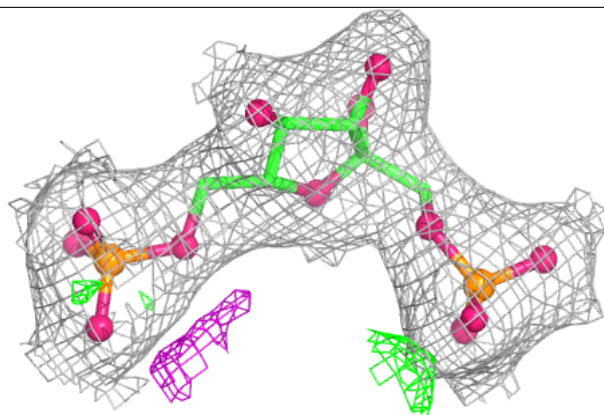
**Electron density around FBP A 601:**

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

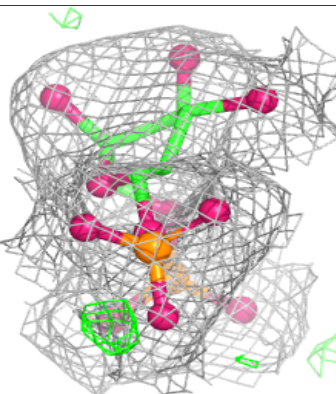
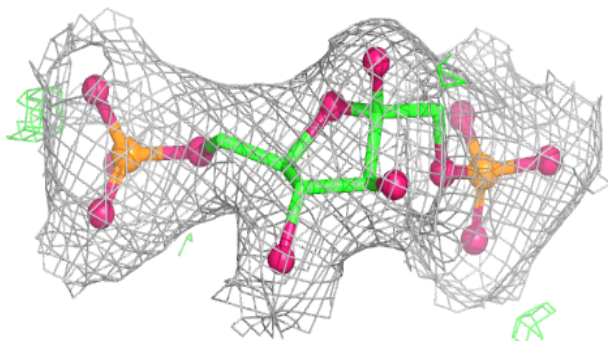
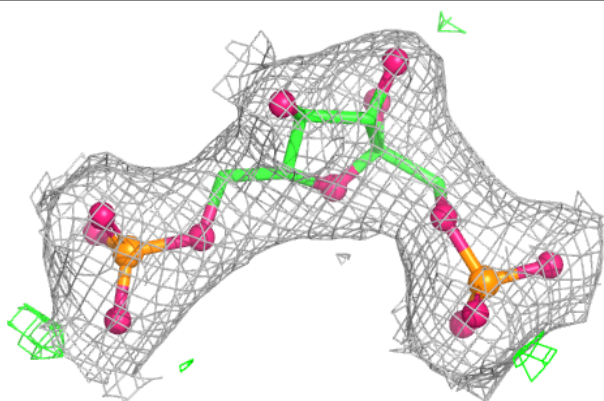


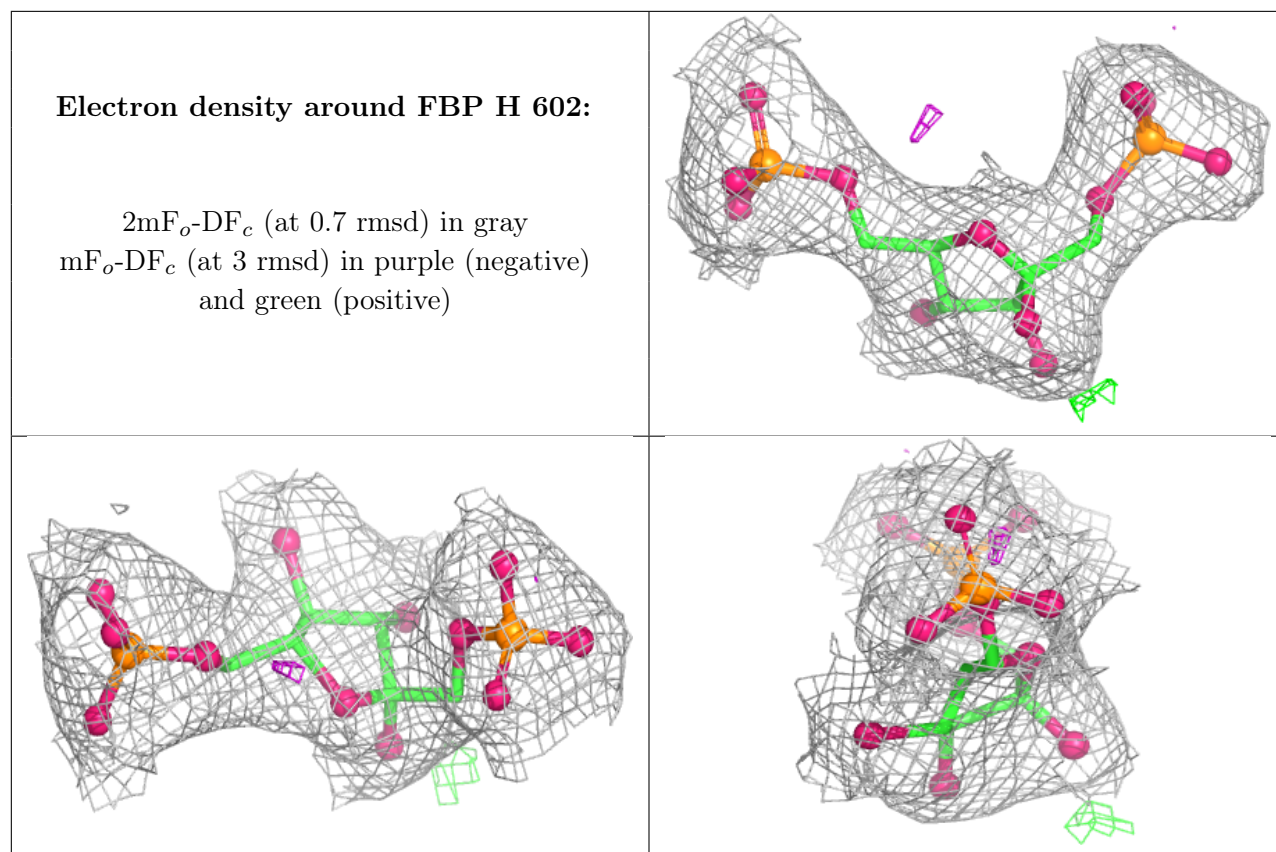
Electron density around FBP F 602:

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

**Electron density around FBP B 602:**

$2mF_o - DF_c$ (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.