



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:41 PM EDT

PDB ID : 7FSB / pdb_00007fsb
Title : Structure of liver pyruvate kinase in complex with allosteric modulator 41
Authors : Lulla, A.; Nilsson, O.; Brear, P.; Nain-Perez, A.; Grotli, M.; Hyvonen, M.
Deposited on : 2022-12-18
Resolution : 2.50 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:

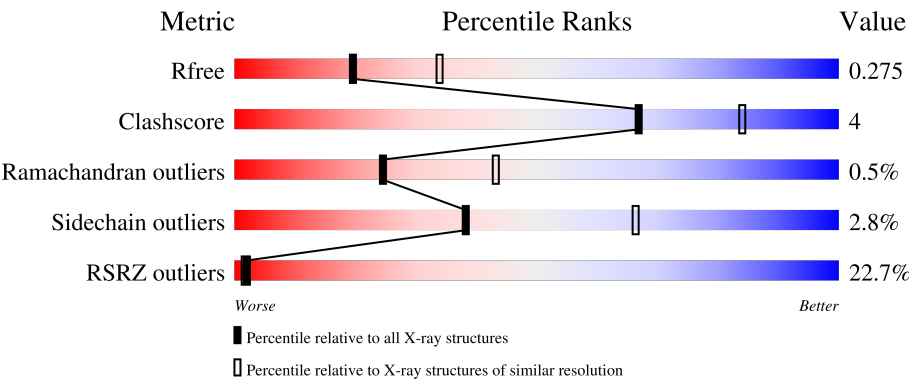
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	447	49% 83% 10% • 6%
1	B	447	29% 88% 9% • •
1	C	447	15% 80% 14% • 5%
1	D	447	3% 84% 9% • 5%
1	E	447	44% 83% 9% • 6%

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Mol	Chain	Length	Quality of chain
1	F	447	
1	G	447	
1	H	447	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	602	-	X	-	-
3	OXL	B	602	-	X	-	-
3	OXL	C	602	-	X	-	-
3	OXL	D	602	-	X	-	-
3	OXL	E	602	-	X	-	-
3	OXL	F	602	-	X	-	-
3	OXL	G	602	-	X	-	-
3	OXL	H	602	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26926 atoms, of which 76 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	422	Total	C	N	O	S	0	6	0
			3236	2034	585	597	20			
1	B	436	Total	C	N	O	S	0	4	0
			3329	2090	604	615	20			
1	C	425	Total	C	N	O	S	0	4	0
			3247	2040	585	603	19			
1	D	425	Total	C	N	O	S	0	6	0
			3252	2042	590	601	19			
1	E	419	Total	C	N	O	S	0	5	0
			3210	2018	579	593	20			
1	F	432	Total	C	N	O	S	0	7	0
			3321	2090	597	614	20			
1	G	421	Total	C	N	O	S	0	6	0
			3231	2031	581	600	19			
1	H	425	Total	C	N	O	S	0	4	0
			3251	2040	594	598	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P30613
A	0	SER	-	expression tag	UNP P30613
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	12	ASP	SER	conflict	UNP P30613
A	130	GLY	-	linker	UNP P30613
A	131	SER	-	linker	UNP P30613
A	132	GLY	-	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression tag	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	12	ASP	SER	conflict	UNP P30613

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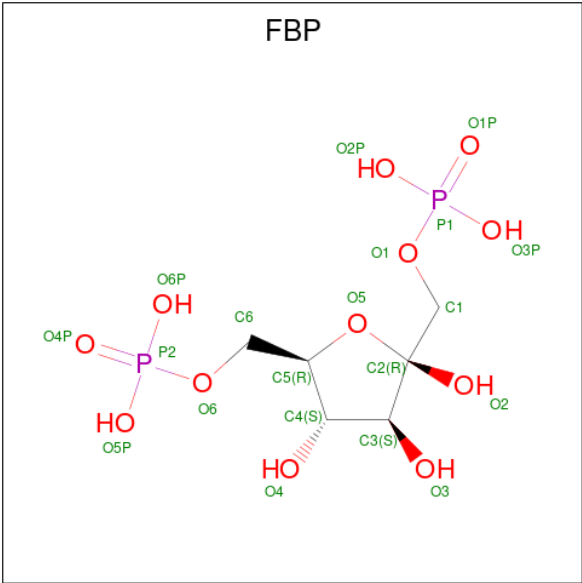
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	GLY	-	linker	UNP P30613
B	131	SER	-	linker	UNP P30613
B	132	GLY	-	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	130	GLY	-	linker	UNP P30613
C	131	SER	-	linker	UNP P30613
C	132	GLY	-	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	UNP P30613
D	130	GLY	-	linker	UNP P30613
D	131	SER	-	linker	UNP P30613
D	132	GLY	-	linker	UNP P30613
E	-1	GLY	-	expression tag	UNP P30613
E	0	SER	-	expression tag	UNP P30613
E	1	MET	-	expression tag	UNP P30613
E	2	GLU	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	228	GLY	-	linker	UNP P30613
E	229	SER	-	linker	UNP P30613
E	230	GLY	-	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	1	MET	-	expression tag	UNP P30613
F	2	GLU	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	228	GLY	-	linker	UNP P30613
F	229	SER	-	linker	UNP P30613
F	230	GLY	-	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	1	MET	-	expression tag	UNP P30613
G	2	GLU	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	130	GLY	-	linker	UNP P30613
G	131	SER	-	linker	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	132	GLY	-	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	1	MET	-	expression tag	UNP P30613
H	2	GLU	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	130	GLY	-	linker	UNP P30613
H	131	SER	-	linker	UNP P30613
H	132	GLY	-	linker	UNP P30613

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



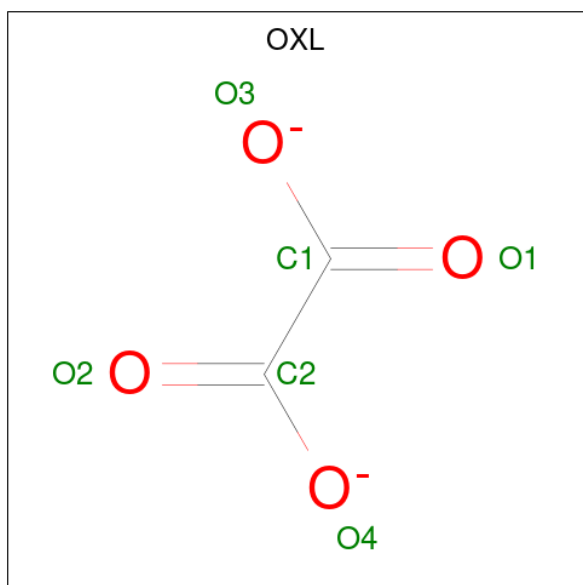
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

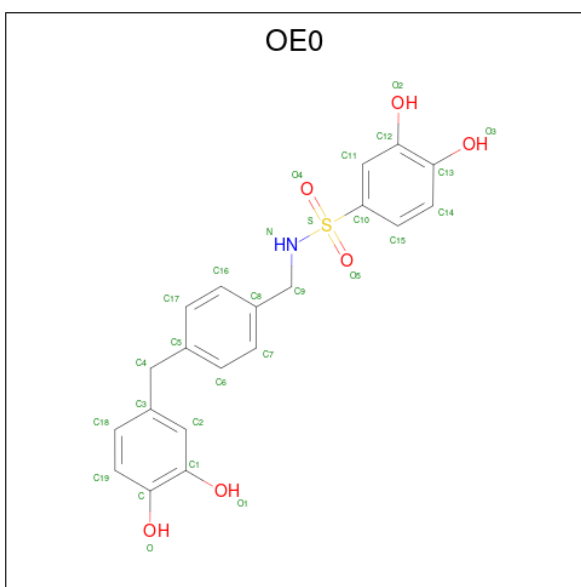
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 6 is N-({4-[(3,4-dihydroxyphenyl)methyl]phenyl}methyl)-3,4-dihydroxybenzene-1-sulfonamide (CCD ID: OE0) (formula: C₂₀H₁₉NO₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 47	C 20	H 19	N 1	O 6	S 1	19	0
6	B	1	Total 47	C 20	H 19	N 1	O 6	S 1	19	0
6	F	1	Total 47	C 20	H 19	N 1	O 6	S 1	19	0
6	G	1	Total 47	C 20	H 19	N 1	O 6	S 1	19	0

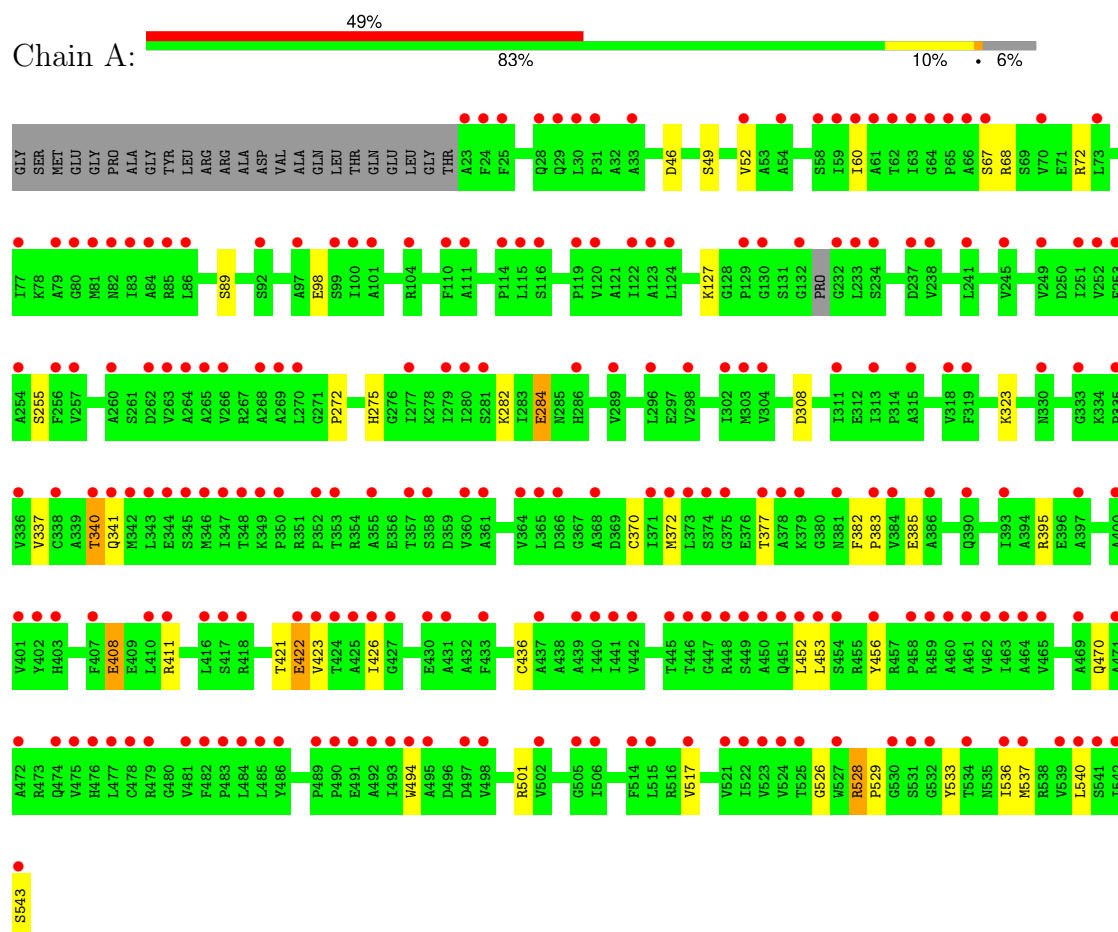
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	12	Total	O	0	0
			12	12		
7	B	18	Total	O	0	0
			18	18		
7	C	50	Total	O	0	0
			50	50		
7	D	123	Total	O	0	0
			123	123		
7	E	17	Total	O	0	0
			17	17		
7	F	30	Total	O	0	0
			30	30		
7	G	56	Total	O	0	0
			56	56		
7	H	131	Total	O	0	0
			131	131		

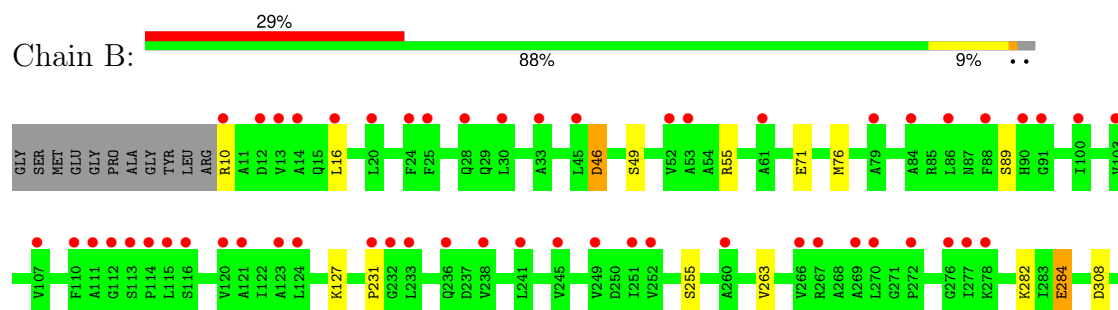
3 Residue-property plots [i](#)

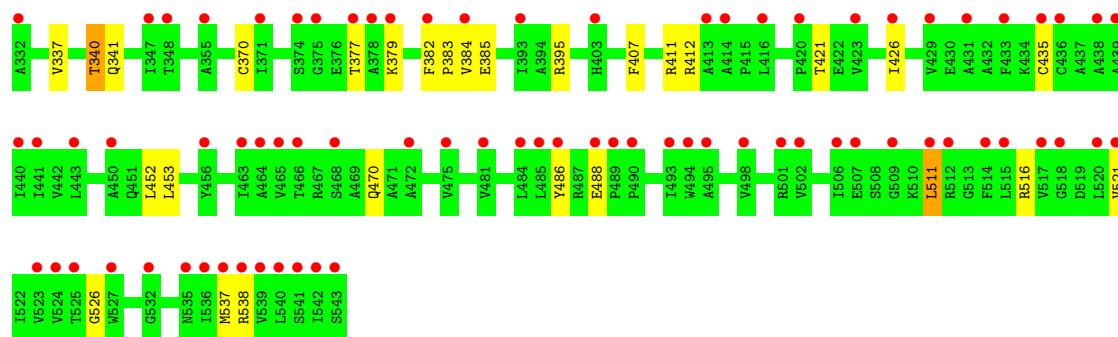
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

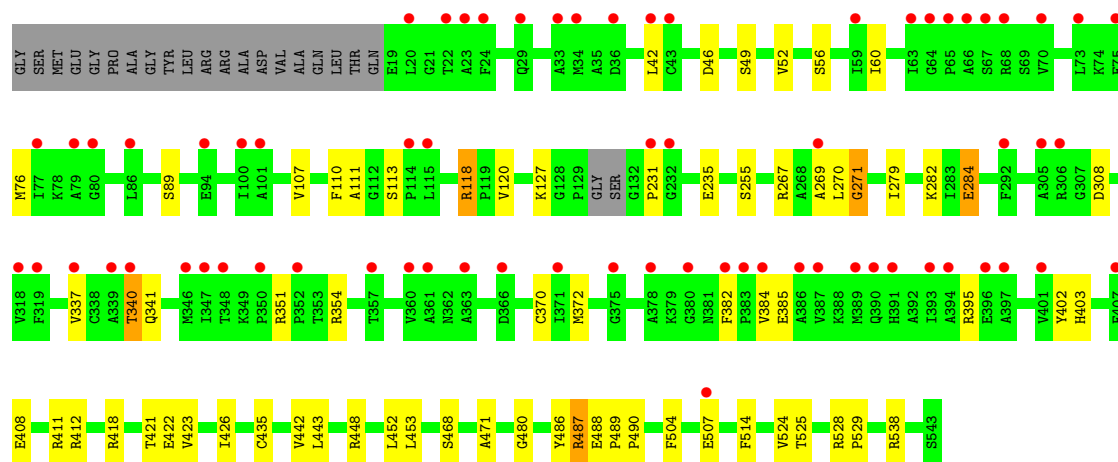
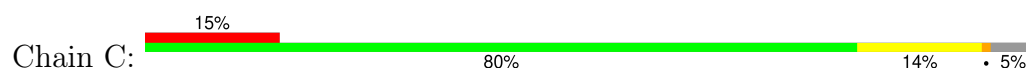


• Molecule 1: Pyruvate kinase PKLR

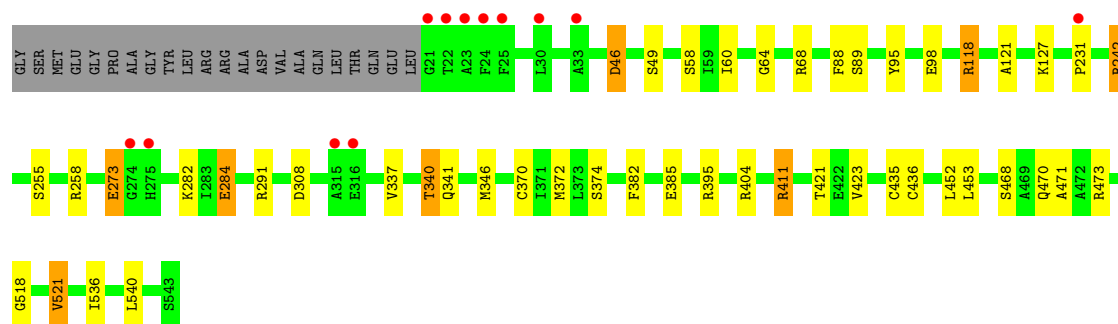
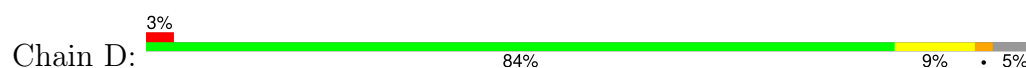




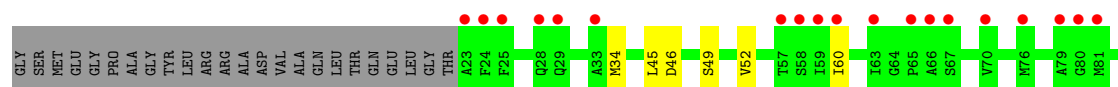
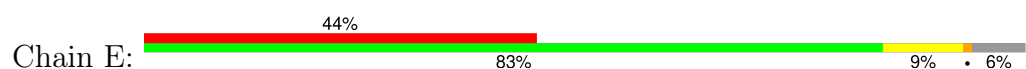
• Molecule 1: Pyruvate kinase PKLR

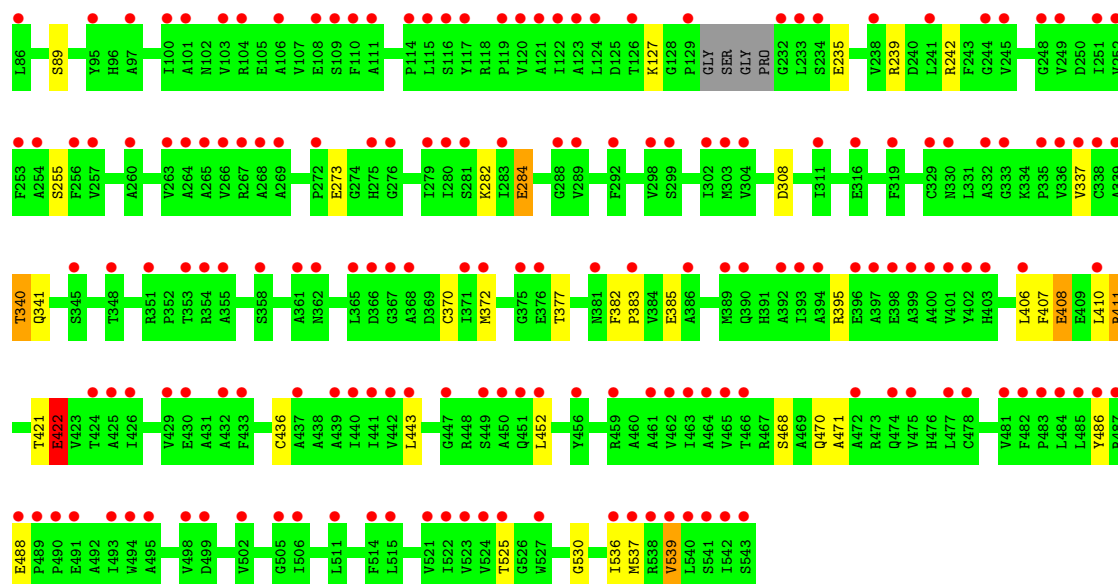


• Molecule 1: Pyruvate kinase PKLR

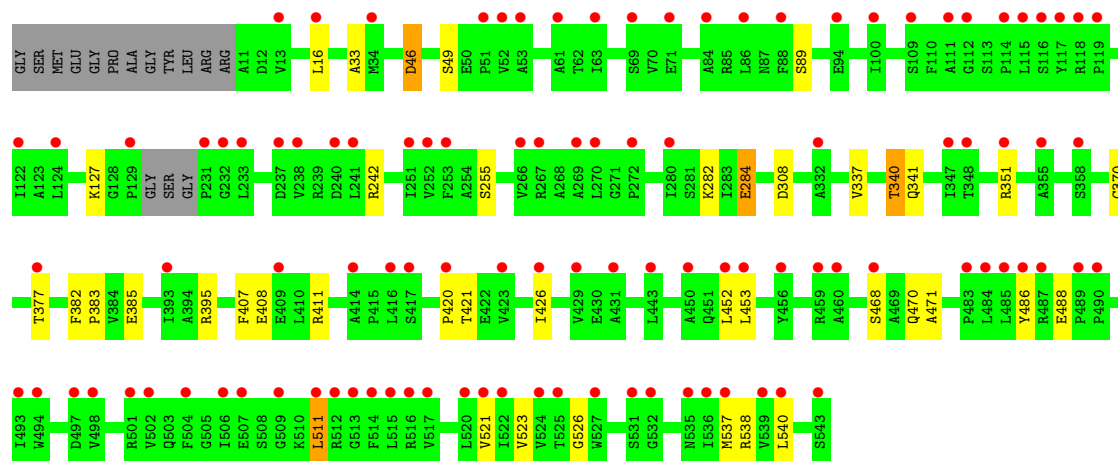
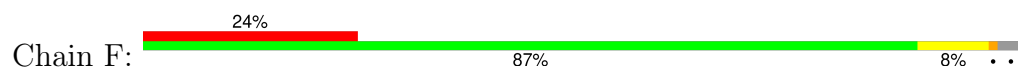


• Molecule 1: Pyruvate kinase PKLR

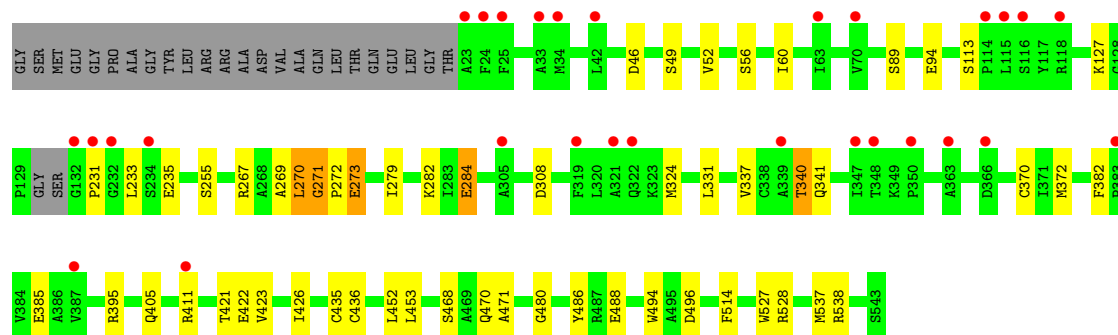
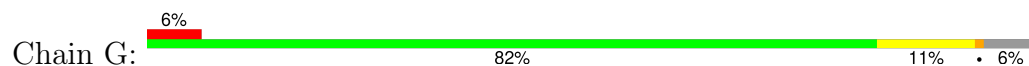




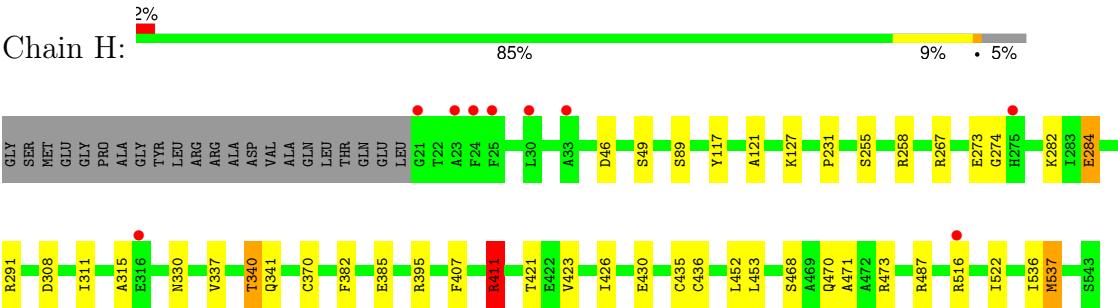
• Molecule 1: Pyruvate kinase PKLR



• Molecule 1: Pyruvate kinase PKLR



● Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.05Å 113.23Å 188.47Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	188.38 – 2.50 188.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	71.3 (188.38-2.50) 71.3 (188.38-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.48Å)	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
R, R_{free}	0.267 , 0.292 0.258 , 0.275	Depositor DCC
R_{free} test set	5205 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26926	wwPDB-VP
Average B, all atoms (Å ²)	94.0	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 92.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1067e-08. 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: OXL, MG, K, FBP, OE0

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	0.65	0/3307	1.08	2/4469 (0.0%)
1	B	0.69	0/3396	1.07	3/4592 (0.1%)
1	C	0.80	0/3313	1.12	8/4479 (0.2%)
1	D	0.84	1/3326 (0.0%)	1.13	4/4497 (0.1%)
1	E	0.66	0/3278	1.08	3/4430 (0.1%)
1	F	0.70	0/3396	1.08	3/4591 (0.1%)
1	G	0.80	0/3303	1.10	6/4465 (0.1%)
1	H	0.82	0/3316	1.12	5/4483 (0.1%)
All	All	0.75	1/26635 (0.0%)	1.10	34/36006 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	374	SER	CA-C	5.93	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	410	LEU	CA-C-N	6.02	128.27	120.44
1	E	410	LEU	C-N-CA	6.02	128.27	120.44
1	F	453	LEU	CA-C-N	5.75	127.99	120.28
1	F	453	LEU	C-N-CA	5.75	127.99	120.28
1	D	453	LEU	CA-C-N	5.74	127.97	120.28
1	D	453	LEU	C-N-CA	5.74	127.97	120.28
1	H	453	LEU	CA-C-N	5.73	128.24	120.38
1	H	453	LEU	C-N-CA	5.73	128.24	120.38
1	B	453	LEU	CA-C-N	5.70	127.91	120.28
1	B	453	LEU	C-N-CA	5.70	127.91	120.28
1	A	453	LEU	CA-C-N	5.62	127.81	120.28
1	A	453	LEU	C-N-CA	5.62	127.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	270	LEU	CA-C-N	5.62	130.69	121.87
1	G	270	LEU	C-N-CA	5.62	130.69	121.87
1	G	514	PHE	CA-CB-CG	5.60	119.40	113.80
1	C	270	LEU	CA-C-N	5.55	130.58	121.87
1	C	270	LEU	C-N-CA	5.55	130.58	121.87
1	C	453	LEU	CA-C-N	5.54	127.70	120.28
1	C	453	LEU	C-N-CA	5.54	127.70	120.28
1	D	88	PHE	CA-CB-CG	-5.53	108.28	113.80
1	C	507	GLU	CB-CG-CD	5.50	121.94	112.60
1	G	453	LEU	CA-C-N	5.45	127.58	120.28
1	G	453	LEU	C-N-CA	5.45	127.58	120.28
1	E	422	GLU	CB-CG-CD	5.43	121.83	112.60
1	F	46	ASP	CA-CB-CG	5.42	118.03	112.60
1	H	411	ARG	N-CA-CB	5.30	118.01	110.16
1	C	504	PHE	CA-C-N	5.25	125.78	120.00
1	C	504	PHE	C-N-CA	5.25	125.78	120.00
1	C	514	PHE	CA-CB-CG	5.25	119.05	113.80
1	D	46	ASP	CA-CB-CG	5.23	117.83	112.60
1	H	311	ILE	CB-CA-C	5.17	115.61	111.06
1	B	46	ASP	CA-CB-CG	5.12	117.72	112.60
1	G	496	ASP	CA-CB-CG	5.09	117.69	112.60
1	H	330	ASN	CA-CB-CG	5.00	117.60	112.60

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	3236	0	3299	27	0
1	B	3329	0	3394	20	1
1	C	3247	0	3300	45	0
1	D	3252	0	3310	28	0
1	E	3210	0	3270	25	0
1	F	3321	0	3393	22	1
1	G	3231	0	3285	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3251	0	3306	26	0
2	A	20	0	10	2	0
2	B	20	0	10	1	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	1	0
2	G	20	0	10	0	0
2	H	20	0	10	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	28	19	0	1	0
6	B	28	19	0	0	0
6	F	28	19	0	0	0
6	G	28	19	0	2	0
7	A	12	0	0	0	0
7	B	18	0	0	0	0
7	C	50	0	0	2	0
7	D	123	0	0	1	0
7	E	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	30	0	0	1	0
7	G	56	0	0	0	0
7	H	131	0	0	0	0
All	All	26850	76	26637	195	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (195) 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:A:272:PRO:HA	1:A:275:HIS:NE2	1.84	0.92
1:C:528:ARG:NH2	1:G:233:LEU:O	2.06	0.89
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.63	0.81
1:G:537:MET:HE3	1:H:537:MET:HG2	1.62	0.81
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.62	0.79
1:F:411:ARG:HG3	1:F:426:ILE:HD11	1.62	0.79
1:C:351:ARG:HH22	1:C:354:ARG:HH22	1.36	0.73
1:G:538:ARG:HG2	1:H:536:ILE:HG12	1.72	0.71
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.57	0.69
1:E:235:GLU:O	1:E:239:ARG:HD3	1.93	0.69
1:G:422[A]:GLU:HG3	1:G:452:LEU:HD13	1.75	0.69
1:C:422[A]:GLU:HG3	1:C:452:LEU:HD13	1.75	0.68
1:B:89:SER:HA	1:B:127:LYS:HG3	1.76	0.68
1:F:89:SER:HA	1:F:127:LYS:HG3	1.75	0.67
1:D:89:SER:HA	1:D:127:LYS:HG3	1.76	0.67
1:E:89:SER:HA	1:E:127:LYS:HG3	1.76	0.67
1:H:89:SER:HA	1:H:127:LYS:HG3	1.76	0.67
1:G:89:SER:HA	1:G:127:LYS:HG3	1.77	0.66
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.76	0.66
1:G:411:ARG:HG2	1:G:426:ILE:HD11	1.77	0.66
1:F:351:ARG:HH21	1:H:315:ALA:HB2	1.60	0.66
1:A:89:SER:HA	1:A:127:LYS:HG3	1.75	0.65
1:C:89:SER:HA	1:C:127:LYS:HG3	1.78	0.64
1:G:340:THR:HG22	1:G:341:GLN:HG3	1.81	0.63
1:C:340:THR:HG22	1:C:341:GLN:HG3	1.81	0.63
1:C:111:ALA:HB1	1:C:487:ARG:NH2	2.14	0.62
1:F:411:ARG:CG	1:F:426:ILE:HD11	2.30	0.62
1:A:340:THR:HG22	1:A:341:GLN:HG3	1.82	0.62
1:A:422:GLU:HG2	1:A:452:LEU:HD13	1.82	0.61
1:E:422:GLU:HG2	1:E:452:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.83	0.61
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.35	0.60
1:E:340:THR:HG22	1:E:341:GLN:HG3	1.84	0.60
1:A:408:GLU:OE2	1:B:411:ARG:NH2	2.34	0.60
1:C:269:ALA:C	1:C:271:GLY:H	2.10	0.60
1:F:340:THR:HG22	1:F:341:GLN:HG3	1.84	0.59
1:G:411:ARG:CG	1:G:426:ILE:HD11	2.33	0.59
1:B:526:GLY:HA3	2:B:601:FBP:O3	2.03	0.59
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.85	0.58
1:B:340:THR:HG22	1:B:341:GLN:HG3	1.83	0.58
1:C:411:ARG:HH12	1:D:411:ARG:HH21	1.52	0.58
1:D:68:ARG:NH2	1:D:95:TYR:O	2.37	0.57
1:E:536:ILE:HG12	1:F:538:ARG:HG2	1.86	0.57
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.86	0.57
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.86	0.57
1:E:408:GLU:OE2	1:F:411:ARG:NH2	2.38	0.56
1:E:539:VAL:HG22	1:F:420:PRO:HB3	1.87	0.56
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.86	0.56
1:D:340:THR:HG22	1:D:341:GLN:HG3	1.88	0.56
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.88	0.56
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.87	0.56
1:G:405:GLN:HB3	6:G:605:OE0:O5	2.05	0.56
1:B:411:ARG:CG	1:B:426:ILE:HD11	2.32	0.56
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.87	0.55
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.87	0.55
1:G:269:ALA:C	1:G:271:GLY:H	2.13	0.55
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.89	0.55
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.88	0.55
1:C:412:ARG:NH2	1:D:404:ARG:HH11	2.05	0.55
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.90	0.54
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.89	0.54
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.22	0.54
1:A:528:ARG:NH1	1:A:533:TYR:CE2	2.75	0.53
1:B:421:THR:HG22	1:B:452:LEU:HD12	1.89	0.53
1:D:64:GLY:O	1:D:68:ARG:HG3	2.09	0.53
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.89	0.53
1:G:421:THR:HG22	1:G:452:LEU:HD12	1.89	0.53
1:A:68:ARG:HH22	1:A:98:GLU:HB3	1.73	0.53
1:C:408:GLU:HG3	1:C:411:ARG:HH12	1.74	0.53
1:E:407:PHE:O	1:E:411:ARG:HB2	2.10	0.52
1:C:408:GLU:HG3	1:C:411:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:382:PHE:HB3	1:H:385:GLU:HB2	1.92	0.52
1:C:411:ARG:NH1	1:D:411:ARG:HH21	2.09	0.51
1:F:407:PHE:CE2	1:F:411:ARG:NH1	2.76	0.51
1:A:517:VAL:HG22	1:A:543:SER:HB3	1.93	0.51
6:A:605:OE0:O5	1:C:402:TYR:HB3	2.11	0.51
1:C:448:ARG:HD3	7:C:710:HOH:O	2.10	0.51
1:B:407:PHE:CE2	1:B:411:ARG:NH1	2.77	0.51
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.92	0.50
1:E:406:LEU:HA	6:G:605:OE0:C18	2.41	0.50
1:G:537:MET:HE3	1:H:537:MET:CG	2.35	0.50
1:C:403:HIS:HE1	7:C:708:HOH:O	1.93	0.49
1:C:107:VAL:HG21	1:C:120:VAL:HB	1.94	0.49
1:A:67:SER:HA	1:A:72:ARG:HG2	1.94	0.49
1:C:411:ARG:NH1	1:D:411:ARG:NH2	2.61	0.49
1:A:494:TRP:NE1	1:A:529:PRO:HG3	2.27	0.49
1:F:526:GLY:HA3	2:F:601:FBP:O3	2.13	0.49
1:H:468:SER:HB3	1:H:471:ALA:HB3	1.95	0.48
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.96	0.48
1:C:529:PRO:HG3	1:G:235:GLU:HG2	1.95	0.48
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.96	0.47
1:A:423:VAL:HG21	1:B:435:CYS:HB3	1.95	0.47
1:C:486:TYR:CE2	1:C:488:GLU:HB2	2.48	0.47
1:G:337:VAL:HG22	1:G:370:CYS:HB2	1.97	0.47
1:A:341:GLN:OE1	1:C:354:ARG:HG2	2.15	0.47
1:A:526:GLY:HA3	2:A:601:FBP:O3	2.15	0.47
1:H:411:ARG:HB3	1:H:426:ILE:HD11	1.97	0.47
1:D:521:VAL:HG12	1:D:540:LEU:HB3	1.97	0.47
1:H:117:TYR:CD2	1:H:487:ARG:NH2	2.83	0.46
1:H:522:ILE:HG23	1:H:537:MET:HE3	1.98	0.46
1:E:443:LEU:HD13	1:E:525:THR:HG22	1.98	0.46
1:G:486:TYR:CZ	1:G:488:GLU:HB2	2.51	0.46
1:B:46:ASP:HB3	1:B:49:SER:HB2	1.98	0.45
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.98	0.45
1:E:337:VAL:HG22	1:E:370:CYS:HB2	1.97	0.45
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.97	0.45
1:G:46:ASP:HB3	1:G:49:SER:HB2	1.97	0.45
1:F:46:ASP:HB3	1:F:49:SER:HB2	1.99	0.45
1:G:435:CYS:HB3	1:H:423:VAL:HG21	1.98	0.45
1:C:46:ASP:HB3	1:C:49:SER:HB2	1.99	0.45
1:D:468:SER:HB3	1:D:471:ALA:HB3	1.99	0.45
1:D:346:MET:HE2	1:D:346:MET:HB3	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ARG:HH11	1:C:118:ARG:H	1.64	0.45
1:G:255:SER:HA	1:G:282:LYS:HD3	1.99	0.45
1:C:435:CYS:HB3	1:D:423:VAL:HG21	1.98	0.44
1:E:46:ASP:HB3	1:E:49:SER:HB2	1.98	0.44
1:E:539:VAL:CG2	1:F:420:PRO:HB3	2.47	0.44
1:C:60:ILE:HB	1:C:372:MET:HG3	2.00	0.44
1:D:46:ASP:HB3	1:D:49:SER:HB2	2.00	0.44
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.00	0.44
1:E:45:LEU:HB2	1:G:324:MET:HB2	1.99	0.44
1:G:60:ILE:HB	1:G:372:MET:HG3	2.00	0.44
1:H:46:ASP:HB3	1:H:49:SER:HB2	2.00	0.44
1:A:46:ASP:HB3	1:A:49:SER:HB2	2.00	0.44
1:C:284:GLU:HB3	1:C:308:ASP:HB2	1.99	0.44
1:H:337:VAL:HG22	1:H:370:CYS:HB2	2.00	0.44
1:D:255:SER:HA	1:D:282:LYS:HD3	2.00	0.44
1:E:255:SER:HA	1:E:282:LYS:HD3	2.00	0.44
1:F:377:THR:HA	1:F:383:PRO:HB3	1.99	0.44
1:C:442:VAL:HG23	1:C:524:VAL:HB	2.00	0.43
1:E:377:THR:HA	1:E:383:PRO:HB3	2.00	0.43
1:A:255:SER:HA	1:A:282:LYS:HD3	1.99	0.43
1:G:411:ARG:HD3	1:H:430:GLU:CD	2.44	0.43
1:D:284:GLU:HB3	1:D:308:ASP:HB2	2.00	0.43
1:H:255:SER:HA	1:H:282:LYS:HD3	2.00	0.43
1:F:255:SER:HA	1:F:282:LYS:HD3	2.00	0.43
1:C:255:SER:HA	1:C:282:LYS:HD3	2.01	0.43
1:F:468:SER:HB3	1:F:471:ALA:HB3	2.01	0.43
1:G:411:ARG:NH2	1:H:411:ARG:CZ	2.81	0.43
1:C:235:GLU:CD	1:G:494:TRP:HB2	2.43	0.43
1:E:242:ARG:HA	7:E:701:HOH:O	2.19	0.43
1:A:377:THR:HA	1:A:383:PRO:HB3	2.00	0.43
1:G:527:TRP:CE2	1:G:528:ARG:HG2	2.54	0.43
1:B:284:GLU:HB3	1:B:308:ASP:HB2	2.01	0.43
1:D:118:ARG:HD2	7:D:776:HOH:O	2.19	0.43
1:G:284:GLU:HB3	1:G:308:ASP:HB2	2.00	0.42
1:H:407:PHE:O	1:H:411:ARG:HG3	2.19	0.42
1:F:523:VAL:HG21	1:F:540[A]:LEU:HD12	2.00	0.42
1:A:60:ILE:HB	1:A:372:MET:HG3	2.01	0.42
1:B:377:THR:HA	1:B:383:PRO:HB3	2.01	0.42
1:C:267:ARG:CZ	1:C:279:ILE:HD12	2.50	0.42
1:G:468:SER:HB3	1:G:471:ALA:HB3	2.02	0.42
1:G:272:PRO:HD2	1:G:273:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:GLU:HB3	1:H:308:ASP:HB2	2.01	0.42
1:C:418:ARG:NH2	1:D:518:GLY:O	2.46	0.42
1:A:411:ARG:NH2	1:B:411:ARG:HH12	2.17	0.42
1:B:55:ARG:HB2	1:B:395:ARG:HG2	2.02	0.42
1:A:284:GLU:HB3	1:A:308:ASP:HB2	2.02	0.42
1:E:284:GLU:HB3	1:E:308:ASP:HB2	2.02	0.42
1:F:284:GLU:HB3	1:F:308:ASP:HB2	2.02	0.42
1:C:468:SER:HB3	1:C:471:ALA:HB3	2.01	0.42
1:E:60:ILE:HB	1:E:372:MET:HG3	2.01	0.42
1:A:528:ARG:NH1	1:A:533:TYR:CZ	2.88	0.42
1:G:56:SER:HB2	1:G:480:GLY:HA2	2.02	0.42
1:H:121:ALA:HA	1:H:473:ARG:HB3	2.02	0.42
1:E:468:SER:HB3	1:E:471:ALA:HB3	2.01	0.41
1:B:255:SER:HA	1:B:282:LYS:HD3	2.00	0.41
1:F:33:ALA:HB1	7:F:704:HOH:O	2.20	0.41
1:D:121:ALA:HA	1:D:473:ARG:HB3	2.02	0.41
1:G:423:VAL:HG21	1:H:435:CYS:HB3	2.03	0.41
1:A:426:ILE:HD13	1:A:456:TYR:CD1	2.55	0.41
1:G:267:ARG:HG2	1:G:279:ILE:CD1	2.51	0.41
1:H:258:ARG:O	1:H:291:ARG:HD3	2.21	0.41
1:A:501:ARG:NH1	2:A:601:FBP:O2P	2.44	0.41
1:E:530:GLY:O	2:E:601:FBP:O4	2.24	0.41
1:H:267[B]:ARG:NH1	1:H:274:GLY:O	2.54	0.41
1:C:56:SER:HB2	1:C:480:GLY:HA2	2.03	0.41
1:C:423:VAL:HG21	1:D:435:CYS:HB3	2.03	0.41
1:C:489:PRO:HA	1:C:490:PRO:HD3	1.88	0.41
1:D:60:ILE:HB	1:D:372:MET:HG3	2.02	0.41
1:F:486:TYR:CE2	1:F:488:GLU:HB2	2.56	0.41
1:C:76[A]:MET:HG2	1:C:384:VAL:HG22	2.03	0.41
1:D:242[A]:ARG:NH2	1:D:273:GLU:OE1	2.45	0.40
1:E:486:TYR:CE2	1:E:488:GLU:HB2	2.55	0.40
1:E:486:TYR:CZ	1:E:488:GLU:HB2	2.56	0.40
1:C:118:ARG:H	1:C:118:ARG:NH1	2.19	0.40
1:G:411:ARG:NH2	1:H:411:ARG:NH2	2.70	0.40
1:H:407:PHE:CE2	1:H:411:ARG:HD3	2.57	0.40
1:C:443:LEU:HD22	1:C:525:THR:HG22	2.04	0.40
1:G:527:TRP:CD1	1:G:527:TRP:H	2.39	0.40
1:A:323:LYS:HB3	1:C:42:LEU:HD22	2.03	0.40
1:B:76[A]:MET:HG2	1:B:384:VAL:HG22	2.03	0.40
1:B:486:TYR:CE2	1:B:488:GLU:HB2	2.56	0.40
1:D:258:ARG:O	1:D:291:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PHE:CB	1:C:118:ARG:HH12	2.35	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:LEU:O	1:B:511:LEU:O[2_555]	1.98	0.22
1:F:511:LEU:O	1:F:511:LEU:O[2_656]	2.11	0.09

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	424/447 (95%)	416 (98%)	7 (2%)	1 (0%)	43 63
1	B	438/447 (98%)	428 (98%)	8 (2%)	2 (0%)	24 43
1	C	425/447 (95%)	414 (97%)	8 (2%)	3 (1%)	18 34
1	D	429/447 (96%)	424 (99%)	3 (1%)	2 (0%)	24 43
1	E	420/447 (94%)	414 (99%)	5 (1%)	1 (0%)	43 63
1	F	435/447 (97%)	427 (98%)	7 (2%)	1 (0%)	43 63
1	G	423/447 (95%)	412 (97%)	7 (2%)	4 (1%)	14 27
1	H	427/447 (96%)	421 (99%)	4 (1%)	2 (0%)	24 43
All	All	3421/3576 (96%)	3356 (98%)	49 (1%)	16 (0%)	24 43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	271	GLY
1	B	231	PRO
1	C	231	PRO

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Mol	Chain	Res	Type
1	D	231	PRO
1	G	231	PRO
1	H	231	PRO
1	A	340	THR
1	G	270	LEU
1	B	340	THR
1	C	340	THR
1	D	340	THR
1	E	340	THR
1	F	340	THR
1	G	340	THR
1	H	340	THR
1	G	271	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/352 (97%)	329 (97%)	11 (3%)	34	62
1	B	349/352 (99%)	336 (96%)	13 (4%)	30	57
1	C	341/352 (97%)	335 (98%)	6 (2%)	51	77
1	D	342/352 (97%)	330 (96%)	12 (4%)	32	58
1	E	338/352 (96%)	325 (96%)	13 (4%)	29	56
1	F	350/352 (99%)	340 (97%)	10 (3%)	37	65
1	G	340/352 (97%)	331 (97%)	9 (3%)	40	68
1	H	340/352 (97%)	332 (98%)	8 (2%)	43	70
All	All	2740/2816 (97%)	2658 (97%)	82 (3%)	38	64

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	284	GLU

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Mol	Chain	Res	Type
1	A	395	ARG
1	A	408	GLU
1	A	422	GLU
1	A	436	CYS
1	A	470	GLN
1	A	528	ARG
1	A	537[A]	MET
1	A	537[B]	MET
1	A	540	LEU
1	B	10	ARG
1	B	16	LEU
1	B	71	GLU
1	B	263	VAL
1	B	284	GLU
1	B	379	LYS
1	B	412	ARG
1	B	470	GLN
1	B	511	LEU
1	B	516	ARG
1	B	521	VAL
1	B	537[A]	MET
1	B	537[B]	MET
1	C	52	VAL
1	C	113	SER
1	C	118	ARG
1	C	284	GLU
1	C	395	ARG
1	C	487	ARG
1	D	58[A]	SER
1	D	58[B]	SER
1	D	118	ARG
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	273	GLU
1	D	284	GLU
1	D	395	ARG
1	D	411	ARG
1	D	436	CYS
1	D	470	GLN
1	D	521	VAL
1	E	34	MET
1	E	52	VAL

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Mol	Chain	Res	Type
1	E	273	GLU
1	E	284	GLU
1	E	395	ARG
1	E	408	GLU
1	E	411	ARG
1	E	422	GLU
1	E	436	CYS
1	E	470	GLN
1	E	537[A]	MET
1	E	537[B]	MET
1	E	539	VAL
1	F	16	LEU
1	F	242	ARG
1	F	284	GLU
1	F	395	ARG
1	F	408	GLU
1	F	470	GLN
1	F	511	LEU
1	F	521	VAL
1	F	537[A]	MET
1	F	537[B]	MET
1	G	52	VAL
1	G	94	GLU
1	G	113	SER
1	G	273	GLU
1	G	284	GLU
1	G	331	LEU
1	G	395	ARG
1	G	436	CYS
1	G	470	GLN
1	H	273	GLU
1	H	284	GLU
1	H	395	ARG
1	H	411	ARG
1	H	436	CYS
1	H	470	GLN
1	H	516	ARG
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	B	87	ASN
1	B	236	GLN
1	C	275	HIS
1	C	390	GLN
1	E	87	ASN
1	F	236	GLN
1	F	403	HIS
1	G	275	HIS
1	H	535	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 16 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	$\# Z > 2$
2	FBP	D	601	-	18,20,20	0.96	1 (5%)	21,32,32	1.05	1 (4%)
3	OXL	A	602	4	5,5,5	2.12	2 (40%)	6,6,6	2.00	2 (33%)
2	FBP	C	601	-	18,20,20	0.68	0	21,32,32	1.07	2 (9%)
3	OXL	C	602	4	5,5,5	1.98	2 (40%)	6,6,6	1.89	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	D	602	4	5,5,5	2.31	2 (40%)	6,6,6	1.89	2 (33%)
3	OXL	E	602	4	5,5,5	2.18	2 (40%)	6,6,6	1.66	2 (33%)
3	OXL	G	602	4	5,5,5	2.12	2 (40%)	6,6,6	1.77	2 (33%)
3	OXL	H	602	4	5,5,5	1.92	2 (40%)	6,6,6	2.09	2 (33%)
2	FBP	G	601	-	18,20,20	0.67	0	21,32,32	1.00	1 (4%)
6	OE0	B	605	-	30,30,30	0.21	0	42,43,43	0.65	1 (2%)
3	OXL	F	602	4	5,5,5	2.84	4 (80%)	6,6,6	2.51	3 (50%)
6	OE0	F	605	-	30,30,30	0.18	0	42,43,43	0.67	1 (2%)
3	OXL	B	602	4	5,5,5	2.23	2 (40%)	6,6,6	1.52	1 (16%)
2	FBP	B	601	-	18,20,20	0.72	0	21,32,32	0.82	1 (4%)
2	FBP	E	601	-	18,20,20	0.47	0	21,32,32	0.80	0
2	FBP	F	601	-	18,20,20	0.70	1 (5%)	21,32,32	0.69	1 (4%)
2	FBP	A	601	-	18,20,20	0.64	0	21,32,32	0.66	0
6	OE0	A	605	-	30,30,30	0.16	0	42,43,43	0.46	0
2	FBP	H	601	-	18,20,20	0.74	1 (5%)	21,32,32	1.25	1 (4%)
6	OE0	G	605	-	30,30,30	0.19	0	42,43,43	0.73	1 (2%)

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	FBP	D	601	-	-	1/13/32/32	0/1/1/1
3	OXL	A	602	4	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	OXL	C	602	4	-	4/4/4/4	-
3	OXL	D	602	4	-	4/4/4/4	-
3	OXL	E	602	4	-	4/4/4/4	-
3	OXL	G	602	4	-	4/4/4/4	-
3	OXL	H	602	4	-	4/4/4/4	-
2	FBP	G	601	-	-	7/13/32/32	0/1/1/1
6	OE0	B	605	-	-	0/16/16/16	0/3/3/3
3	OXL	F	602	4	-	4/4/4/4	-
6	OE0	F	605	-	-	3/16/16/16	0/3/3/3
3	OXL	B	602	4	-	4/4/4/4	-
2	FBP	B	601	-	-	7/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1
2	FBP	F	601	-	-	6/13/32/32	0/1/1/1
2	FBP	A	601	-	-	4/13/32/32	0/1/1/1
6	OE0	A	605	-	-	3/16/16/16	0/3/3/3
2	FBP	H	601	-	-	2/13/32/32	0/1/1/1
6	OE0	G	605	-	-	0/16/16/16	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	OXL	O2-C2	4.24	1.33	1.22
3	D	602	OXL	O2-C2	3.87	1.32	1.22
3	E	602	OXL	O1-C1	3.83	1.32	1.22
3	F	602	OXL	O2-C2	3.70	1.31	1.22
3	A	602	OXL	O2-C2	3.54	1.31	1.22
3	G	602	OXL	O1-C1	3.49	1.31	1.22
3	H	602	OXL	O2-C2	3.25	1.30	1.22
3	C	602	OXL	O1-C1	3.24	1.30	1.22
3	F	602	OXL	O3-C1	-3.18	1.21	1.30
3	F	602	OXL	O1-C1	3.17	1.30	1.22
3	G	602	OXL	O3-C1	-3.11	1.22	1.30
2	D	601	FBP	P2-O5P	-3.11	1.43	1.54
3	D	602	OXL	O4-C2	-2.85	1.22	1.30
3	C	602	OXL	O3-C1	-2.81	1.22	1.30
3	E	602	OXL	O3-C1	-2.79	1.23	1.30
3	A	602	OXL	O4-C2	-2.64	1.23	1.30
3	F	602	OXL	O4-C2	-2.58	1.23	1.30
3	H	602	OXL	O4-C2	-2.56	1.23	1.30
3	B	602	OXL	O4-C2	-2.43	1.23	1.30
2	H	601	FBP	P1-O1	-2.05	1.53	1.60
2	F	601	FBP	P2-O6P	-2.03	1.47	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	OXL	O4-C2-C1	4.18	120.94	112.83
2	H	601	FBP	O5P-P2-O6	4.07	117.29	106.67
3	F	602	OXL	O4-C2-C1	3.85	120.30	112.83
3	A	602	OXL	O4-C2-C1	3.81	120.23	112.83
2	D	601	FBP	O5P-P2-O6	3.75	116.45	106.67
3	C	602	OXL	O3-C1-C2	3.72	120.04	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	OXL	O3-C1-C2	3.72	120.04	112.83
6	G	605	OE0	C8-C9-N	3.26	119.20	112.08
3	G	602	OXL	O3-C1-C2	3.25	119.13	112.83
3	D	602	OXL	O4-C2-C1	3.03	118.71	112.83
2	C	601	FBP	O6-P2-O4P	3.02	114.60	106.44
3	D	602	OXL	O3-C1-C2	3.02	118.68	112.83
3	E	602	OXL	O3-C1-C2	3.00	118.64	112.83
6	F	605	OE0	C8-C9-N	2.98	118.58	112.08
3	B	602	OXL	O4-C2-C1	2.88	118.42	112.83
6	B	605	OE0	C8-C9-N	2.65	117.85	112.08
3	H	602	OXL	O2-C2-C1	-2.55	115.31	120.63
3	E	602	OXL	O4-C2-C1	2.36	117.40	112.83
3	F	602	OXL	O2-C2-C1	-2.33	115.77	120.63
3	A	602	OXL	O3-C1-C2	2.30	117.30	112.83
2	B	601	FBP	O5P-P2-O6	2.29	112.64	106.67
3	G	602	OXL	O4-C2-C1	2.26	117.21	112.83
2	G	601	FBP	O5P-P2-O6	2.10	112.16	106.67
2	F	601	FBP	O1-P1-O1P	2.08	112.07	106.44
2	C	601	FBP	O3P-P1-O2P	2.03	115.40	107.80

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	C1-O1-P1-O2P
2	B	601	FBP	C1-O1-P1-O3P
2	B	601	FBP	O1-C1-C2-O2
2	B	601	FBP	O1-C1-C2-O5
2	B	601	FBP	C4-C5-C6-O6
2	E	601	FBP	C1-O1-P1-O1P
2	E	601	FBP	C4-C5-C6-O6
2	F	601	FBP	O1-C1-C2-O2
2	F	601	FBP	O1-C1-C2-O5
2	G	601	FBP	C1-O1-P1-O2P
2	G	601	FBP	O1-C1-C2-O2
2	G	601	FBP	O1-C1-C2-O5
6	A	605	OE0	C9-N-S-C10
6	A	605	OE0	C9-N-S-O4
2	A	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	F	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	601	FBP	C4-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	601	FBP	O5-C5-C6-O6
6	F	605	OE0	C9-N-S-O4
6	A	605	OE0	C9-N-S-O5
6	F	605	OE0	C9-N-S-O5
2	G	601	FBP	O5-C5-C6-O6
2	H	601	FBP	C4-C5-C6-O6
6	F	605	OE0	C9-N-S-C10
2	B	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C1-O1-P1-O3P
2	F	601	FBP	C1-O1-P1-O3P
2	G	601	FBP	C1-O1-P1-O3P
3	A	602	OXL	O3-C1-C2-O4
3	D	602	OXL	O3-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O4
3	F	602	OXL	O3-C1-C2-O4
3	A	602	OXL	O1-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O4
3	B	602	OXL	O1-C1-C2-O2
3	E	602	OXL	O1-C1-C2-O2
3	F	602	OXL	O1-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O2
3	G	602	OXL	O1-C1-C2-O2
2	A	601	FBP	C1-O1-P1-O1P
2	F	601	FBP	C1-O1-P1-O1P
2	G	601	FBP	C1-O1-P1-O1P
2	H	601	FBP	C6-O6-P2-O4P
3	D	602	OXL	O3-C1-C2-O2
3	A	602	OXL	O1-C1-C2-O4
3	A	602	OXL	O3-C1-C2-O2
3	B	602	OXL	O1-C1-C2-O4
3	C	602	OXL	O3-C1-C2-O2
3	D	602	OXL	O1-C1-C2-O4

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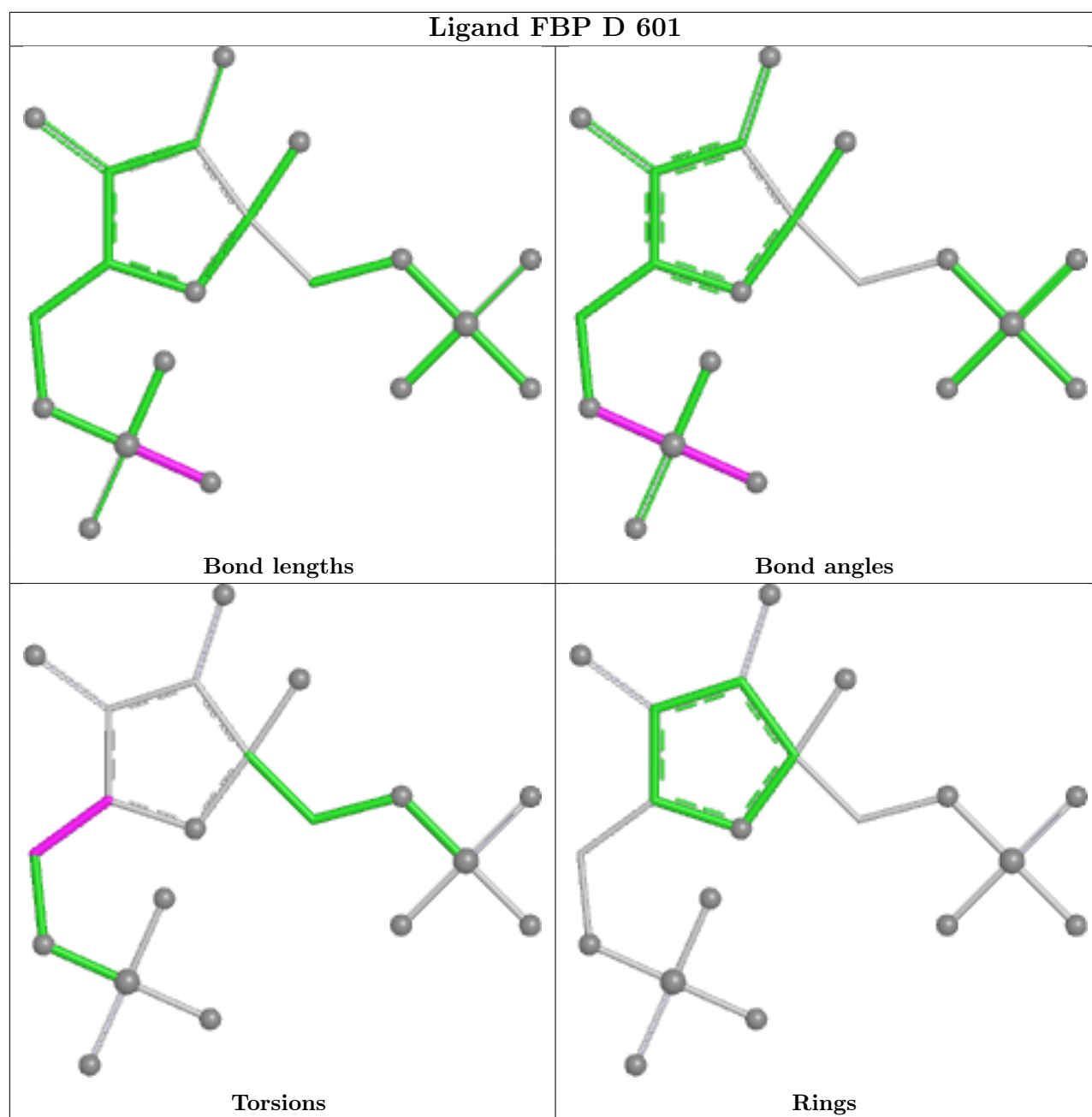
Mol	Chain	Res	Type	Atoms
3	E	602	OXL	O1-C1-C2-O4
3	E	602	OXL	O3-C1-C2-O2
3	F	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O1-C1-C2-O4
3	B	602	OXL	O3-C1-C2-O2
3	C	602	OXL	O1-C1-C2-O4
3	F	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O1-C1-C2-O4
3	G	602	OXL	O3-C1-C2-O2
3	H	602	OXL	O3-C1-C2-O2

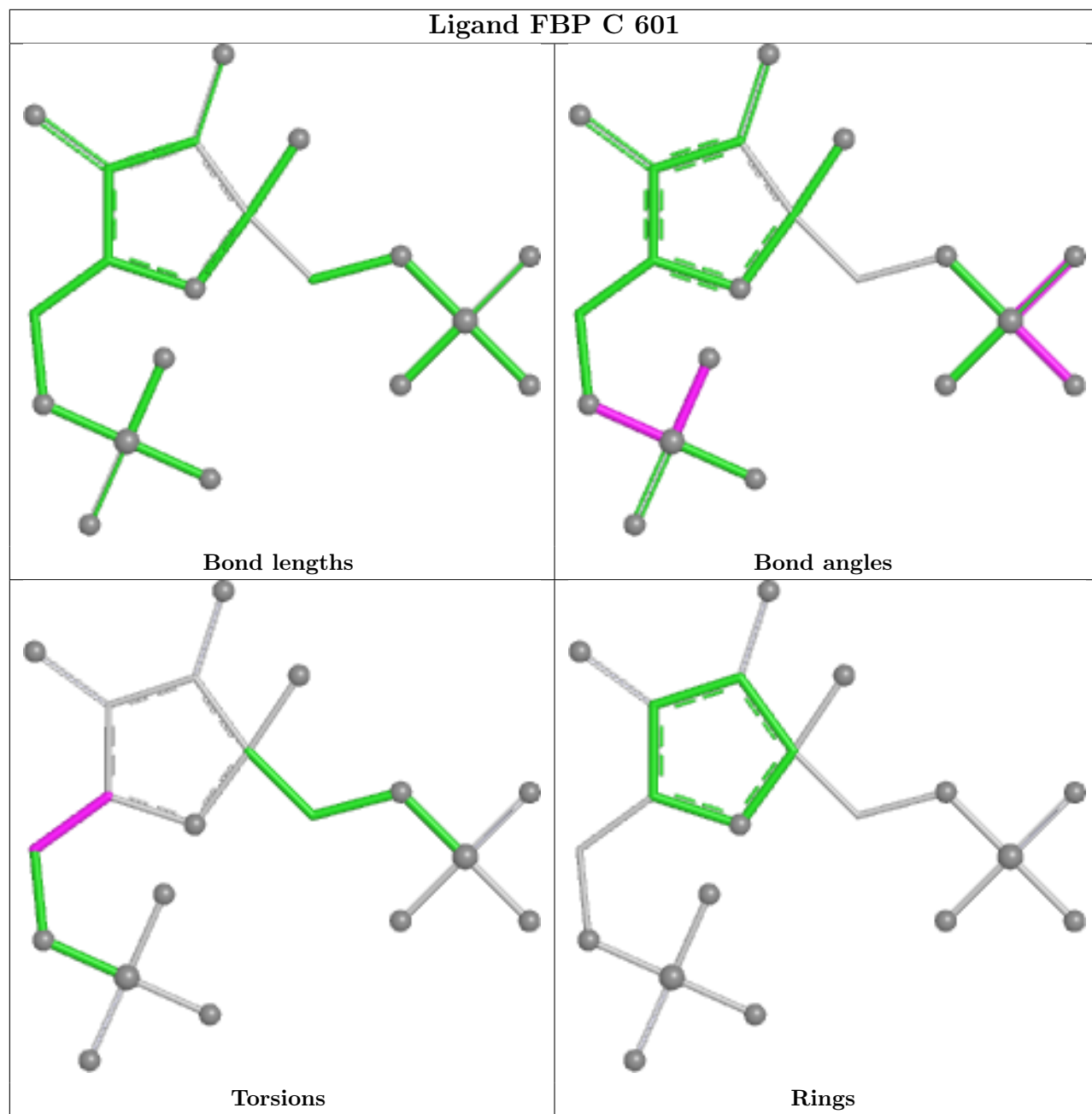
There are no ring outliers.

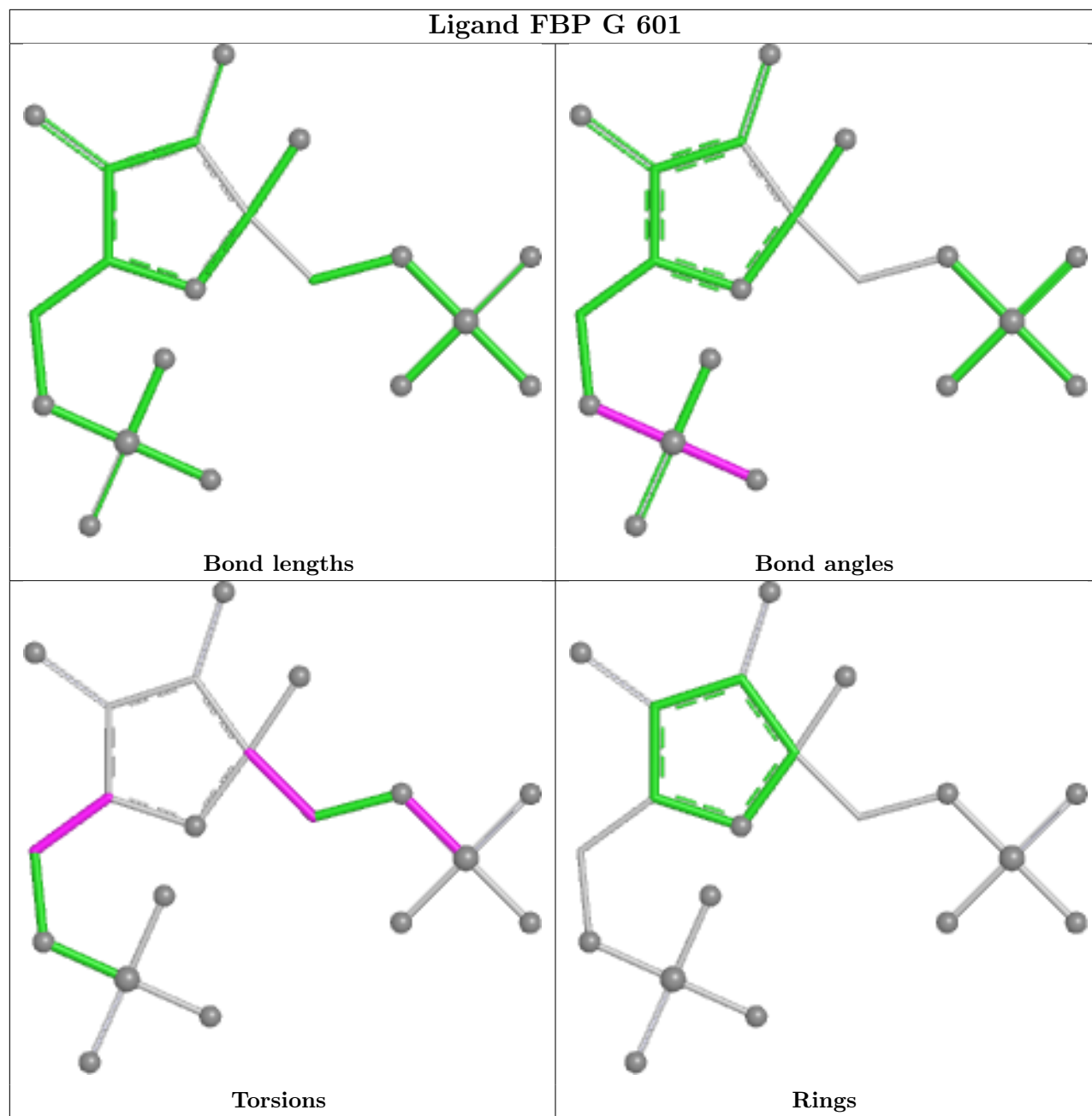
6 monomers are involved in 8 short contacts:

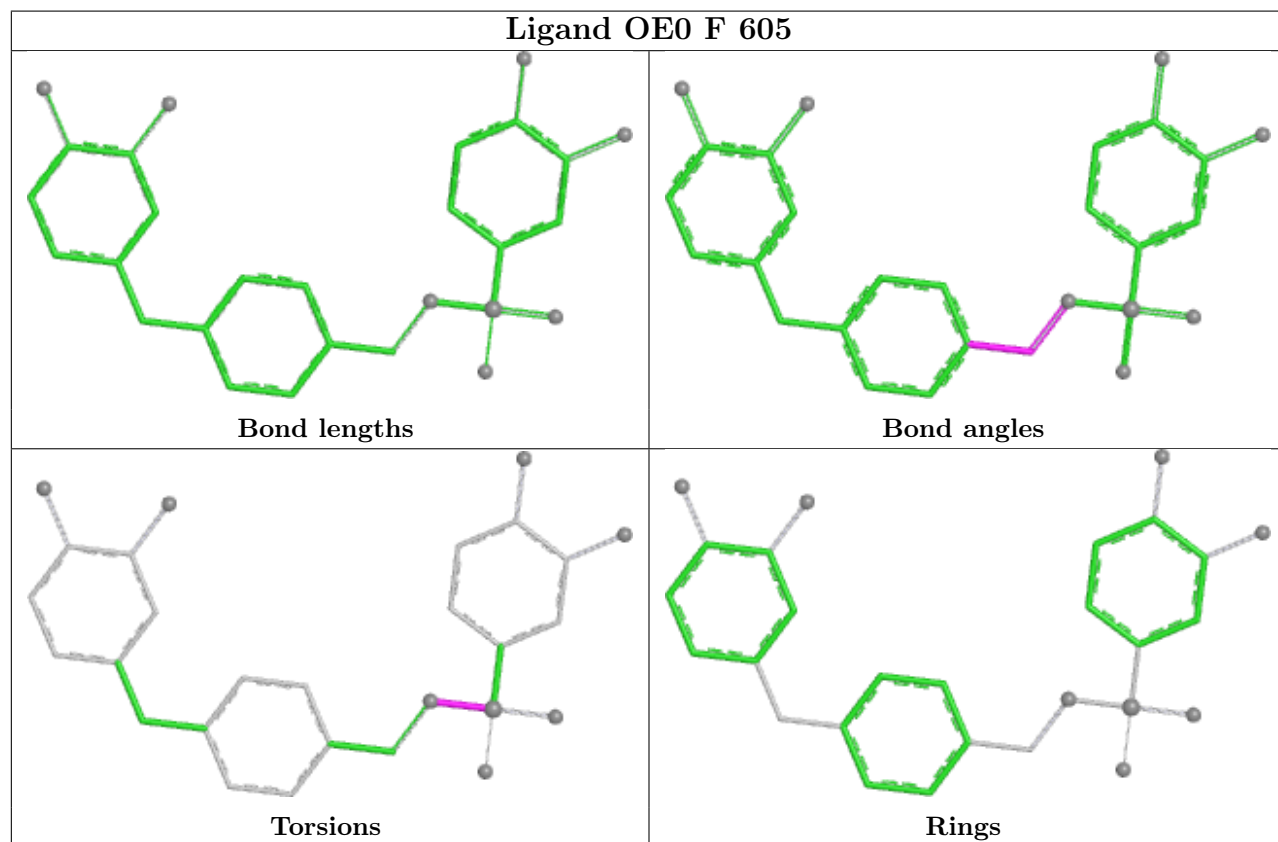
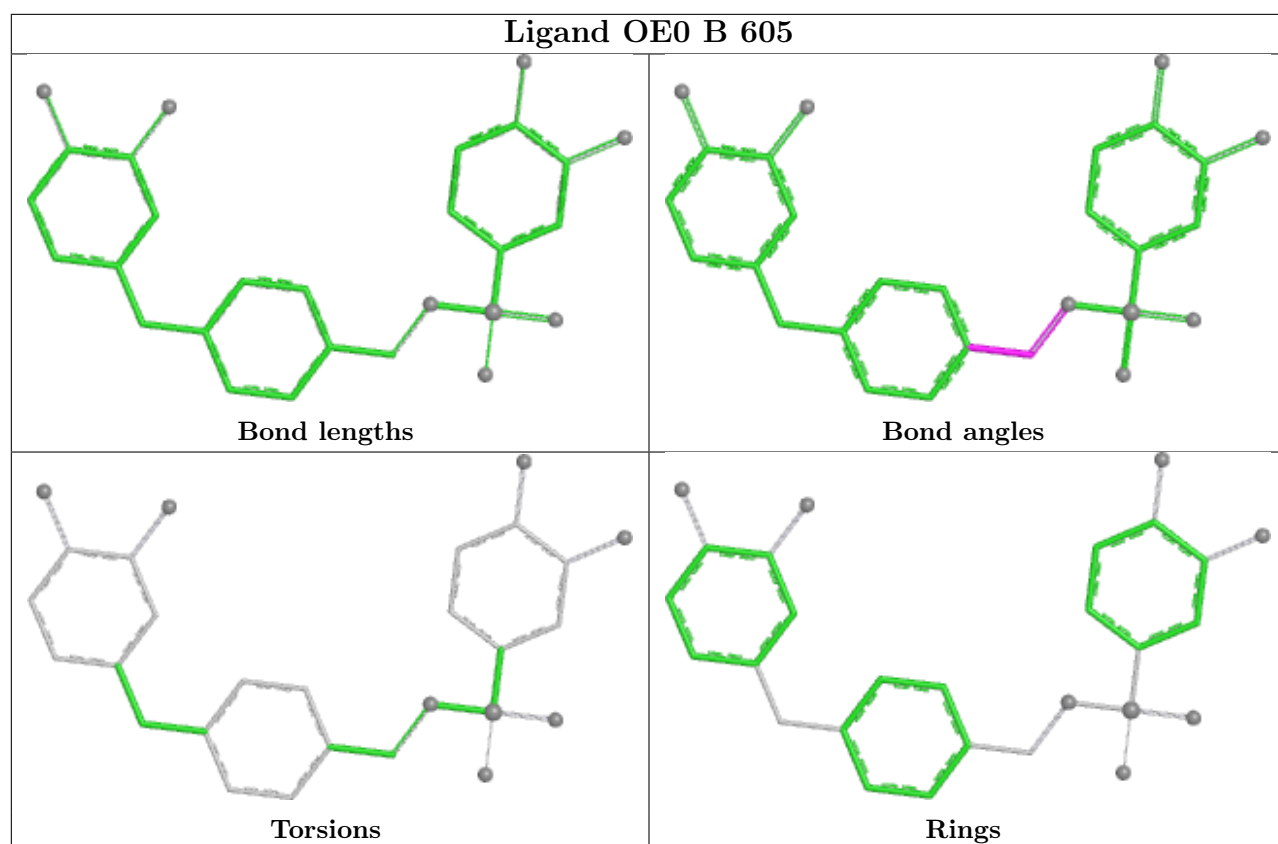
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FBP	1	0
2	E	601	FBP	1	0
2	F	601	FBP	1	0
2	A	601	FBP	2	0
6	A	605	OE0	1	0
6	G	605	OE0	2	0

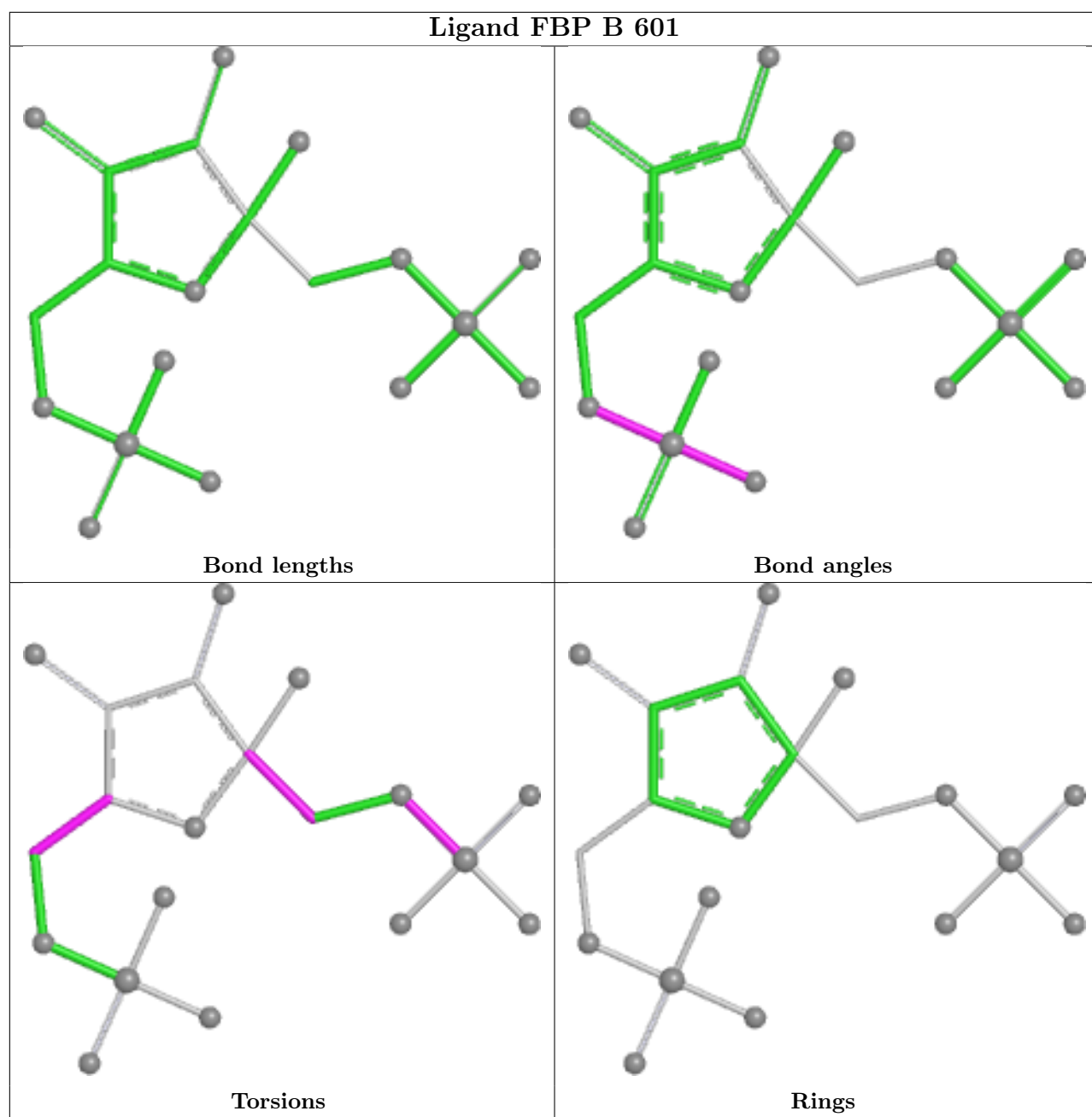
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



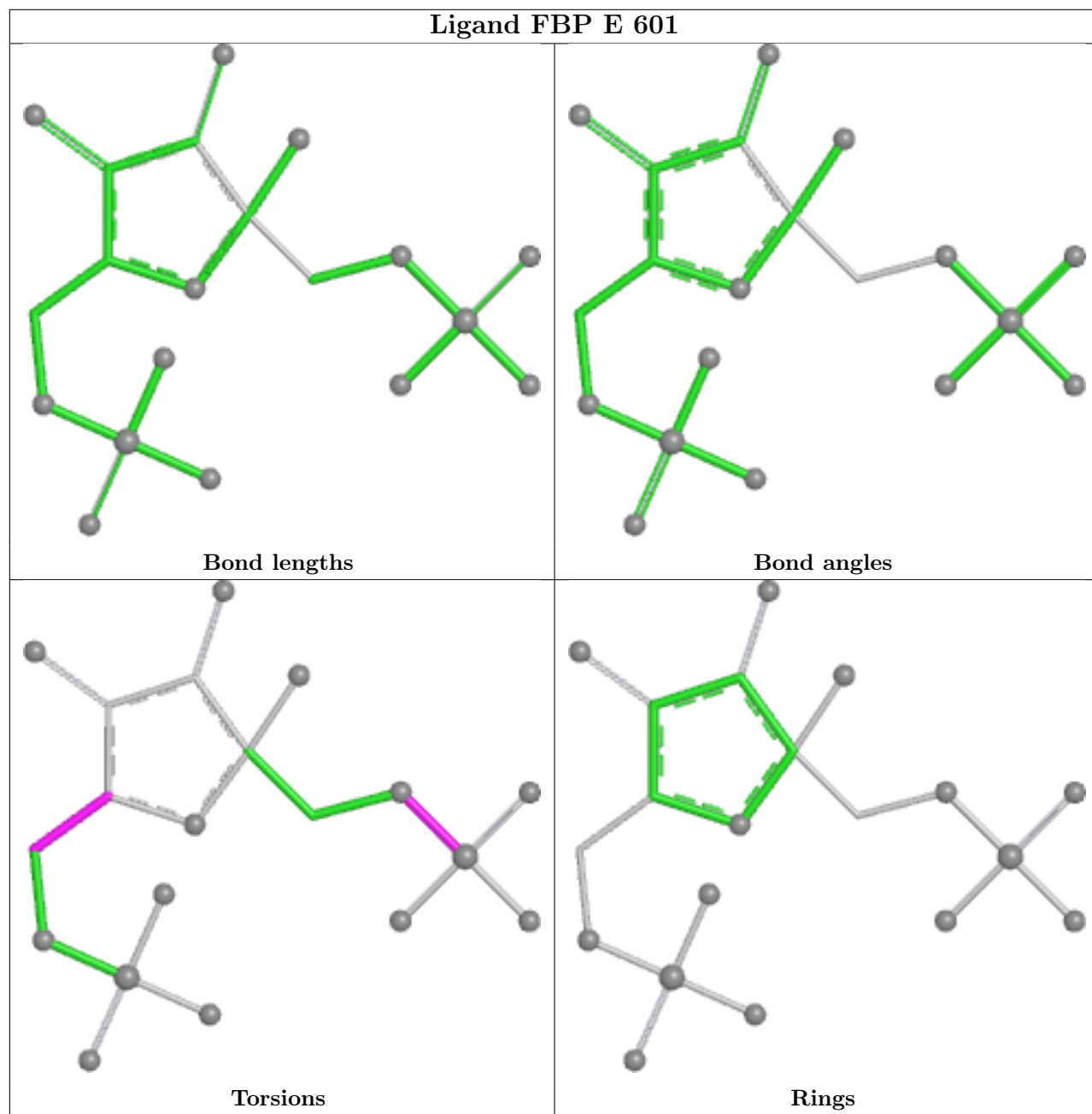




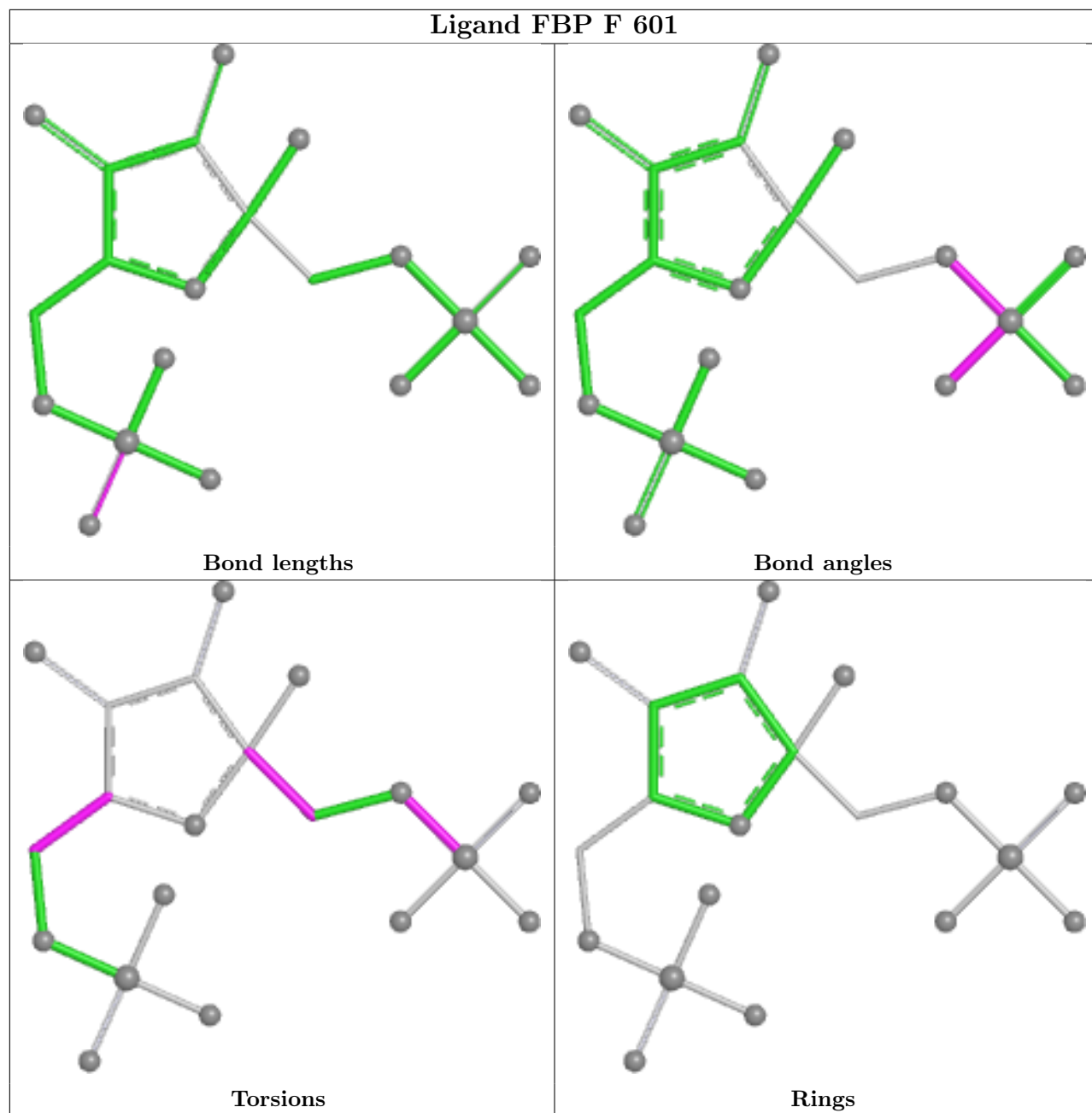


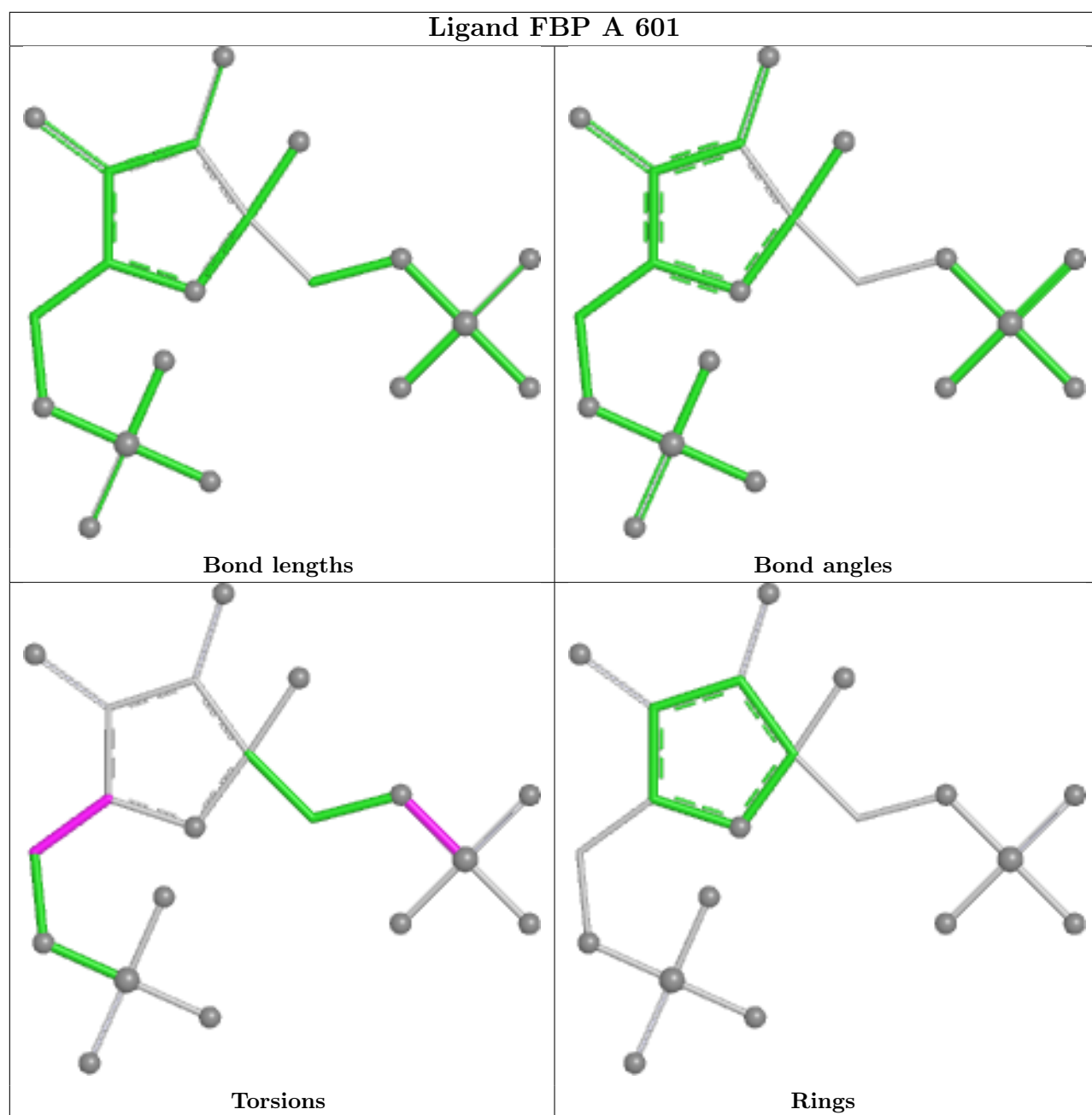


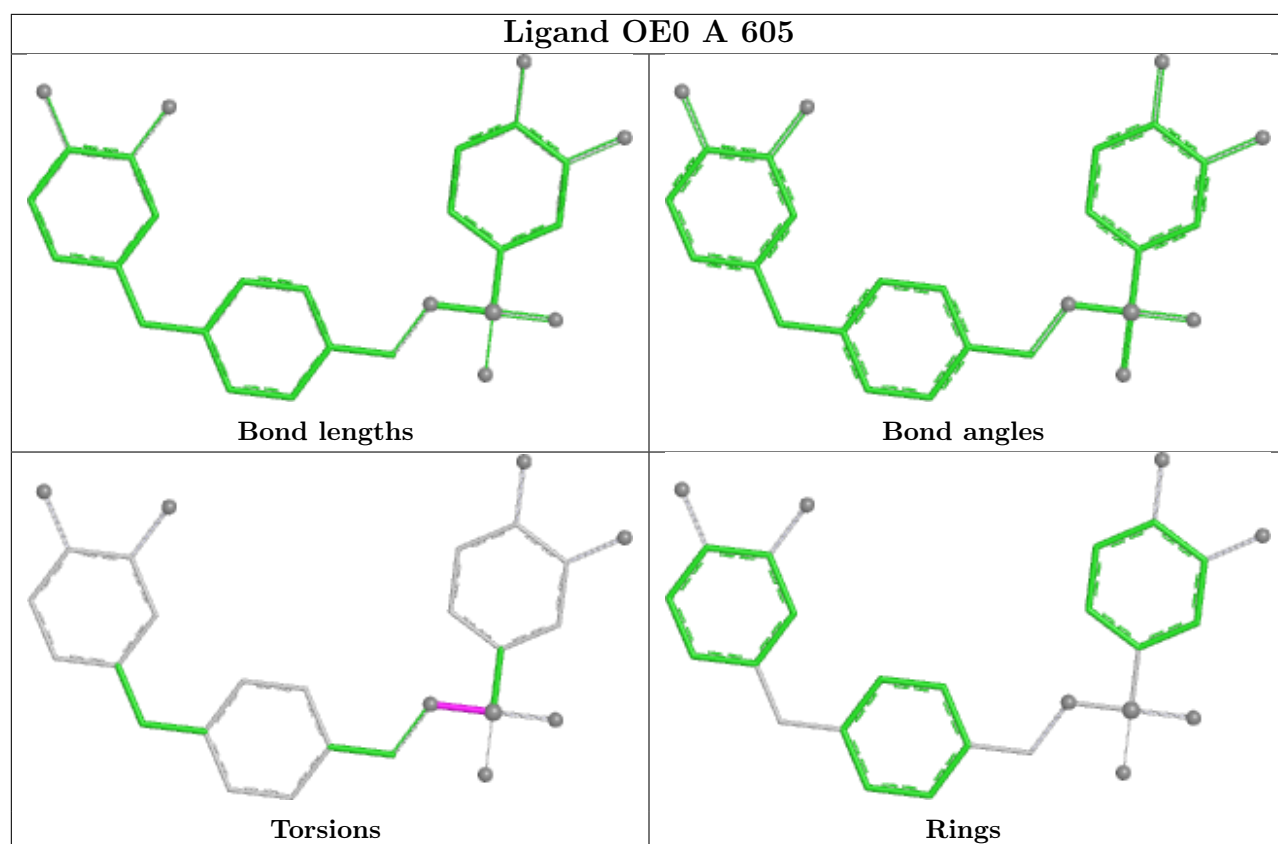
Ligand FBP E 601

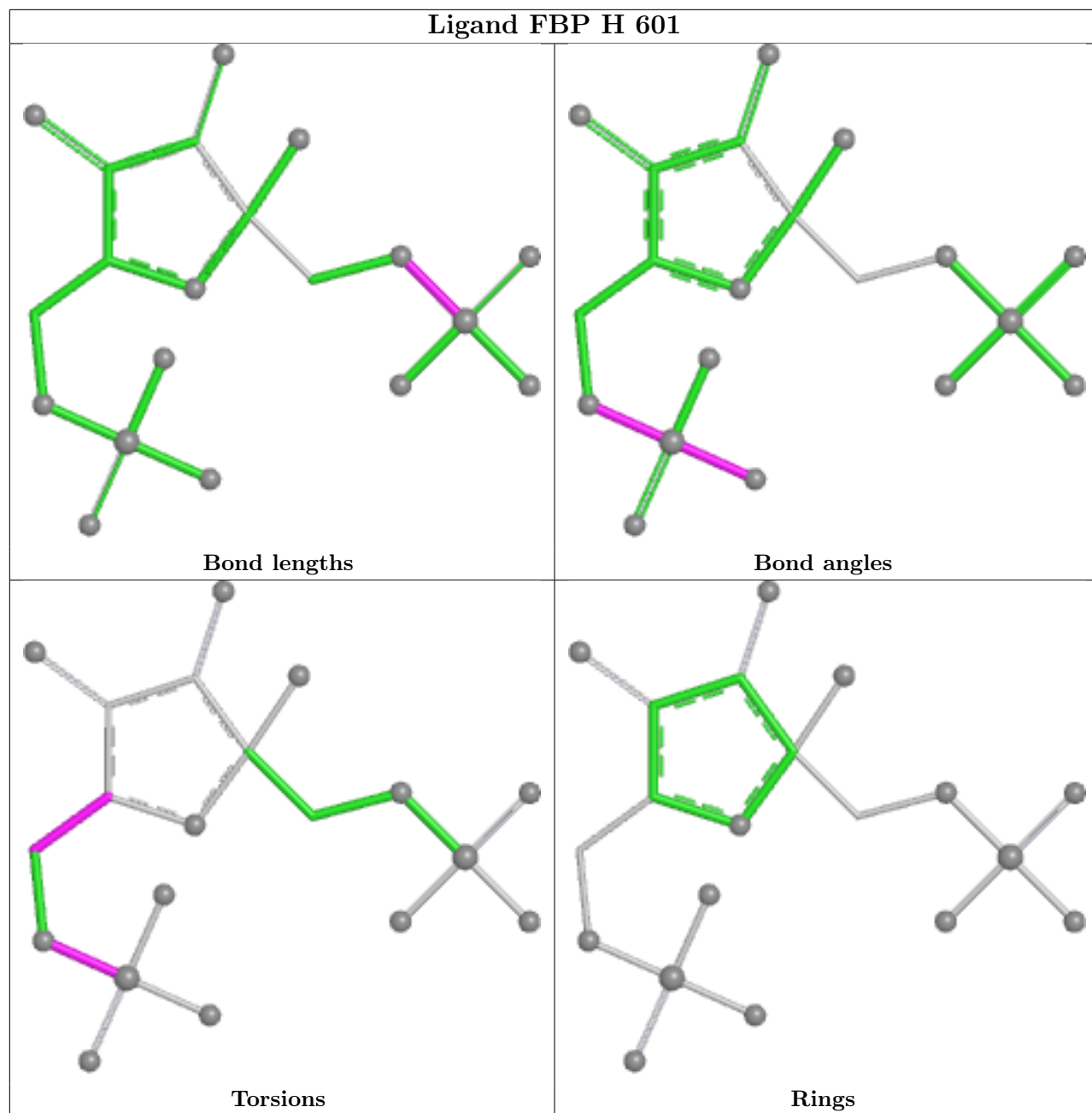


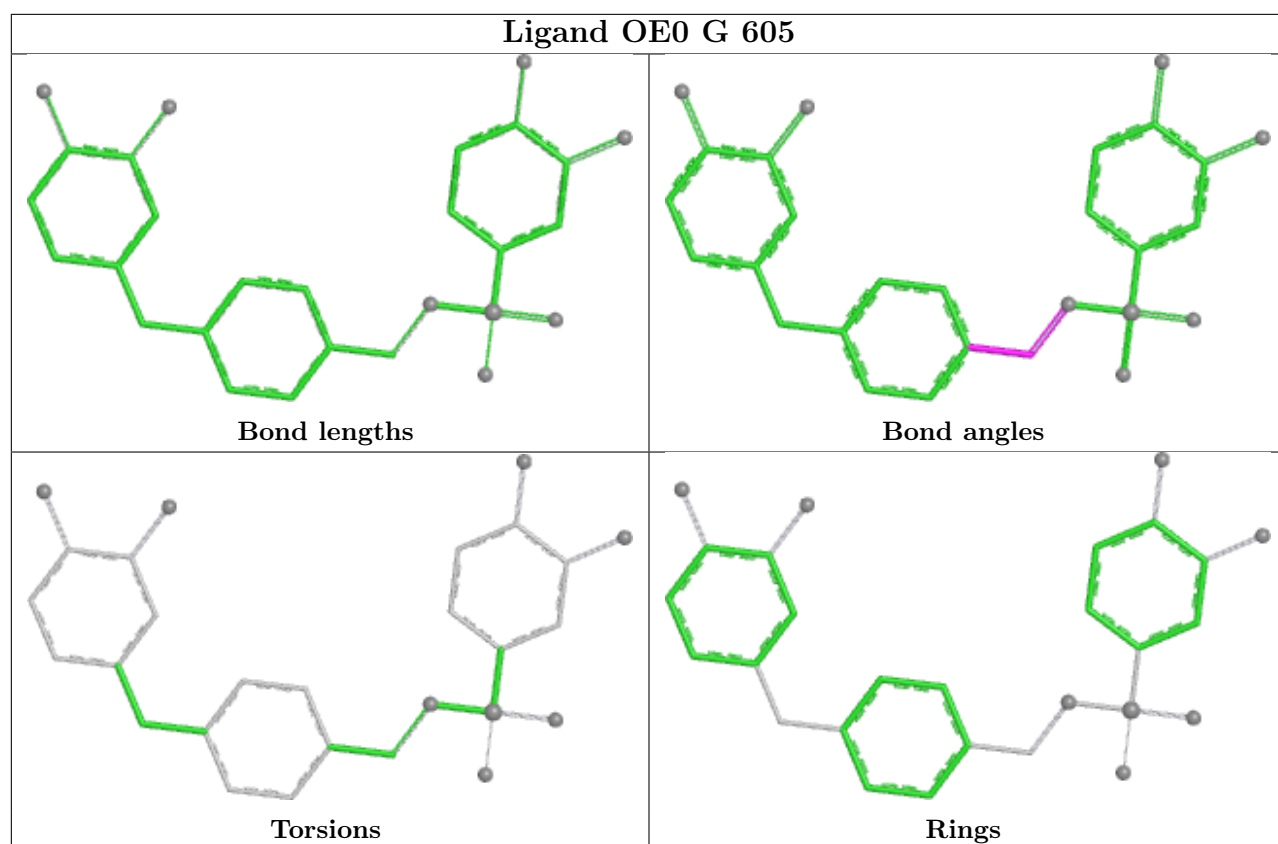
Ligand FBP F 601











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	422/447 (94%)	2.27	221 (52%) 0 0	72, 138, 177, 191	6 (1%)
1	B	436/447 (97%)	1.53	131 (30%) 1 1	61, 107, 148, 159	4 (0%)
1	C	425/447 (95%)	1.00	69 (16%) 4 3	34, 82, 131, 163	4 (0%)
1	D	425/447 (95%)	0.25	12 (2%) 55 50	24, 55, 90, 143	6 (1%)
1	E	419/447 (93%)	2.15	195 (46%) 0 0	52, 129, 164, 188	5 (1%)
1	F	432/447 (96%)	1.40	106 (24%) 2 1	56, 97, 138, 153	7 (1%)
1	G	421/447 (94%)	0.67	29 (6%) 23 20	34, 72, 110, 133	7 (1%)
1	H	425/447 (95%)	0.25	9 (2%) 63 59	25, 54, 90, 139	4 (0%)
All	All	3405/3576 (95%)	1.19	772 (22%) 2 2	24, 91, 158, 191	43 (1%)

All (772) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	442	VAL	9.1
1	A	482	PHE	7.4
1	A	361	ALA	7.3
1	A	453	LEU	6.9
1	A	450	ALA	6.9
1	E	522	ILE	6.8
1	E	120	VAL	6.8
1	A	463	ILE	6.7
1	A	522	ILE	6.7
1	B	511	LEU	6.4
1	A	543	SER	6.1
1	B	517	VAL	6.1
1	A	423	VAL	6.0
1	E	502	VAL	6.0
1	F	511	LEU	5.9
1	F	231	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	539	VAL	5.7
1	A	502	VAL	5.7
1	A	441	ILE	5.7
1	E	400	ALA	5.6
1	A	357	THR	5.5
1	E	464	ALA	5.4
1	E	505	GLY	5.4
1	E	129	PRO	5.4
1	E	489	PRO	5.4
1	E	238	VAL	5.2
1	E	540	LEU	5.2
1	A	238	VAL	5.2
1	A	365	LEU	5.2
1	F	540[A]	LEU	5.1
1	E	521	VAL	5.1
1	E	524	VAL	5.1
1	B	540[A]	LEU	5.1
1	E	397	ALA	5.1
1	G	363	ALA	5.0
1	A	132	GLY	5.0
1	E	542	ILE	4.9
1	E	463	ILE	4.9
1	E	440	ILE	4.9
1	B	543	SER	4.9
1	E	539	VAL	4.9
1	D	25	PHE	4.8
1	H	25	PHE	4.8
1	F	116	SER	4.8
1	E	523	VAL	4.8
1	A	426	ILE	4.7
1	A	63	ILE	4.7
1	E	450	ALA	4.7
1	E	304	VAL	4.6
1	D	24	PHE	4.6
1	E	254	ALA	4.6
1	H	24	PHE	4.6
1	A	232	GLY	4.5
1	A	465	VAL	4.5
1	A	475	VAL	4.5
1	E	393	ILE	4.5
1	E	336	VAL	4.5
1	A	401	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	460	ALA	4.5
1	B	438	ALA	4.5
1	A	484	LEU	4.4
1	E	266	VAL	4.4
1	E	390	GLN	4.4
1	A	523	VAL	4.4
1	E	232	GLY	4.3
1	E	122	ILE	4.3
1	A	464	ALA	4.3
1	A	481	VAL	4.3
1	A	440	ILE	4.3
1	A	524	VAL	4.3
1	B	509	GLY	4.2
1	E	115	LEU	4.2
1	C	59	ILE	4.2
1	A	489	PRO	4.1
1	E	249	VAL	4.1
1	A	123	ALA	4.1
1	E	123	ALA	4.1
1	A	456	TYR	4.1
1	A	343	LEU	4.1
1	E	241	LEU	4.1
1	A	390	GLN	4.0
1	A	80	GLY	4.0
1	E	541[A]	SER	4.0
1	E	465	VAL	4.0
1	F	521	VAL	4.0
1	A	492	ALA	4.0
1	E	365	LEU	4.0
1	E	358	SER	4.0
1	C	20	LEU	4.0
1	E	233	LEU	4.0
1	E	485	LEU	4.0
1	E	252	VAL	4.0
1	A	490	PRO	4.0
1	E	437	ALA	4.0
1	H	21	GLY	4.0
1	E	493	ILE	4.0
1	A	449	SER	4.0
1	A	462	VAL	4.0
1	E	257	VAL	4.0
1	E	29	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	25	PHE	3.9
1	A	251	ILE	3.9
1	A	241	LEU	3.9
1	A	353	THR	3.9
1	A	377	THR	3.9
1	B	249	VAL	3.9
1	E	482	PHE	3.9
1	A	269	ALA	3.9
1	E	319	PHE	3.9
1	E	302	ILE	3.9
1	A	540	LEU	3.8
1	E	452	LEU	3.8
1	A	400	ALA	3.8
1	A	86	LEU	3.8
1	F	543	SER	3.8
1	E	124	LEU	3.8
1	A	81	MET	3.8
1	B	502	VAL	3.8
1	E	514	PHE	3.8
1	D	21	GLY	3.8
1	F	527	TRP	3.8
1	E	426	ILE	3.8
1	E	441	ILE	3.8
1	F	537[A]	MET	3.8
1	C	23	ALA	3.7
1	B	13	VAL	3.7
1	A	536	ILE	3.7
1	F	456	TYR	3.7
1	E	119	PRO	3.7
1	E	353	THR	3.7
1	A	521	VAL	3.7
1	C	33	ALA	3.7
1	F	485	LEU	3.7
1	A	527	TRP	3.7
1	E	126	THR	3.7
1	A	454	SER	3.7
1	A	477	LEU	3.7
1	E	538	ARG	3.7
1	E	456	TYR	3.7
1	E	33	ALA	3.6
1	F	115	LEU	3.6
1	A	424	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	25	PHE	3.6
1	A	452	LEU	3.6
1	F	232	GLY	3.6
1	A	304	VAL	3.6
1	C	94	GLU	3.6
1	A	471	ALA	3.6
1	C	386	ALA	3.6
1	E	101	ALA	3.6
1	A	100	ILE	3.6
1	A	493	ILE	3.6
1	A	120	VAL	3.6
1	A	249	VAL	3.6
1	E	289	VAL	3.6
1	F	502	VAL	3.6
1	B	355	ALA	3.6
1	E	490	PRO	3.6
1	A	442	VAL	3.5
1	B	523	VAL	3.5
1	F	52	VAL	3.5
1	E	537[A]	MET	3.5
1	A	265	ALA	3.5
1	C	363	ALA	3.5
1	E	403	HIS	3.5
1	A	124	LEU	3.5
1	G	33	ALA	3.5
1	B	429	VAL	3.5
1	E	23	ALA	3.5
1	E	80	GLY	3.5
1	E	368	ALA	3.5
1	E	394	ALA	3.5
1	E	425	ALA	3.5
1	A	485	LEU	3.5
1	A	447	GLY	3.5
1	F	129	PRO	3.5
1	B	515	LEU	3.4
1	A	350	PRO	3.4
1	C	383	PRO	3.4
1	A	101	ALA	3.4
1	B	542	ILE	3.4
1	A	537[A]	MET	3.4
1	A	498	VAL	3.4
1	B	348	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	103	VAL	3.4
1	E	424	THR	3.4
1	F	270	LEU	3.4
1	A	114	PRO	3.4
1	E	272	PRO	3.4
1	B	33	ALA	3.4
1	F	460	ALA	3.4
1	A	472	ALA	3.4
1	B	431	ALA	3.4
1	E	251	ILE	3.4
1	E	495	ALA	3.4
1	A	319	PHE	3.4
1	B	232	GLY	3.4
1	E	110	PHE	3.3
1	F	489	PRO	3.3
1	C	63	ILE	3.3
1	E	433	PHE	3.3
1	A	373	LEU	3.3
1	F	515	LEU	3.3
1	B	525	THR	3.3
1	C	22	THR	3.3
1	C	384	VAL	3.3
1	E	104	ARG	3.3
1	A	254	ALA	3.3
1	A	378	ALA	3.3
1	B	536	ILE	3.3
1	E	264	ALA	3.3
1	C	382	PHE	3.3
1	B	435	CYS	3.3
1	A	233	LEU	3.3
1	B	231	PRO	3.3
1	F	520	LEU	3.3
1	A	289	VAL	3.3
1	A	505	GLY	3.3
1	C	77	ILE	3.3
1	G	305	ALA	3.3
1	C	366	ASP	3.3
1	F	118	ARG	3.3
1	E	401	VAL	3.3
1	A	253	PHE	3.2
1	F	266	VAL	3.2
1	A	445	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	413	ALA	3.2
1	A	483	PRO	3.2
1	F	241	LEU	3.2
1	B	52	VAL	3.2
1	A	525	THR	3.2
1	E	260	ALA	3.2
1	E	116	SER	3.2
1	B	490	PRO	3.2
1	F	238	VAL	3.2
1	G	63	ILE	3.2
1	B	116	SER	3.2
1	E	114	PRO	3.2
1	E	477	LEU	3.2
1	A	130	GLY	3.2
1	B	498	VAL	3.2
1	B	539	VAL	3.2
1	C	70	VAL	3.2
1	B	463	ILE	3.2
1	B	267[A]	ARG	3.1
1	E	28	GLN	3.1
1	C	319	PHE	3.1
1	G	319	PHE	3.1
1	F	517	VAL	3.1
1	C	393	ILE	3.1
1	E	59	ILE	3.1
1	A	66	ALA	3.1
1	A	439	ALA	3.1
1	F	267[A]	ARG	3.1
1	A	358	SER	3.1
1	A	418[A]	ARG	3.1
1	A	461	ALA	3.1
1	D	315	ALA	3.1
1	A	360	VAL	3.1
1	E	462	VAL	3.1
1	A	302	ILE	3.1
1	E	474	GLN	3.1
1	A	65	PRO	3.1
1	C	42	LEU	3.1
1	F	124	LEU	3.1
1	E	245	VAL	3.1
1	E	483	PRO	3.0
1	A	252	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	257	VAL	3.0
1	B	107	VAL	3.0
1	E	451	GLN	3.0
1	E	466	THR	3.0
1	E	355	ALA	3.0
1	D	275[A]	HIS	3.0
1	B	272	PRO	3.0
1	B	115	LEU	3.0
1	A	110	PHE	3.0
1	A	478	CYS	3.0
1	E	234	SER	3.0
1	F	509	GLY	3.0
1	A	83	ILE	3.0
1	A	263	VAL	3.0
1	A	371	ILE	3.0
1	F	426	ILE	3.0
1	E	525	THR	3.0
1	B	25	PHE	3.0
1	C	24	PHE	3.0
1	G	24	PHE	3.0
1	A	311	ILE	3.0
1	B	393	ILE	3.0
1	F	493	ILE	3.0
1	F	536	ILE	3.0
1	E	81	MET	3.0
1	A	33	ALA	3.0
1	A	368	ALA	3.0
1	A	119	PRO	3.0
1	A	115	LEU	3.0
1	A	479	ARG	3.0
1	F	522	ILE	2.9
1	A	372	MET	2.9
1	F	539	VAL	2.9
1	A	397	ALA	2.9
1	E	66	ALA	2.9
1	A	335	PRO	2.9
1	B	270	LEU	2.9
1	B	456	TYR	2.9
1	E	402	TYR	2.9
1	F	453	LEU	2.9
1	E	543	SER	2.9
1	B	521	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	66	ALA	2.9
1	F	512	ARG	2.9
1	G	114	PRO	2.9
1	B	520	LEU	2.9
1	B	12	ASP	2.9
1	A	234	SER	2.9
1	E	447	GLY	2.9
1	B	251	ILE	2.9
1	B	506	ILE	2.9
1	F	429	VAL	2.9
1	E	527	TRP	2.9
1	F	514	PHE	2.9
1	A	517	VAL	2.9
1	F	459	ARG	2.9
1	E	511	LEU	2.9
1	H	30	LEU	2.9
1	E	499	ASP	2.9
1	A	116	SER	2.8
1	E	281	SER	2.8
1	E	354	ARG	2.8
1	E	362	ASN	2.8
1	A	446	THR	2.8
1	F	490	PRO	2.8
1	C	305	ALA	2.8
1	C	361	ALA	2.8
1	E	443	LEU	2.8
1	B	507	GLU	2.8
1	C	64	GLY	2.8
1	E	487	ARG	2.8
1	F	516	ARG	2.8
1	G	411	ARG	2.8
1	A	279	ILE	2.8
1	A	280	ILE	2.8
1	B	493	ILE	2.8
1	E	100	ILE	2.8
1	E	263	VAL	2.8
1	A	97	ALA	2.8
1	E	332	ALA	2.8
1	C	507	GLU	2.8
1	C	380	GLY	2.8
1	A	92	SER	2.8
1	E	70	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	23	ALA	2.8
1	A	459	ARG	2.8
1	G	118	ARG	2.8
1	A	433	PHE	2.8
1	B	514	PHE	2.8
1	E	375	GLY	2.8
1	E	283	ILE	2.8
1	C	352	PRO	2.8
1	E	475	VAL	2.8
1	F	524	VAL	2.8
1	A	23	ALA	2.8
1	A	515	LEU	2.8
1	B	485	LEU	2.8
1	A	530	GLY	2.7
1	A	352	PRO	2.7
1	A	541	SER	2.7
1	C	350	PRO	2.7
1	E	396	GLU	2.7
1	F	351	ARG	2.7
1	A	427	GLY	2.7
1	F	513	GLY	2.7
1	A	348	THR	2.7
1	D	23	ALA	2.7
1	E	439	ALA	2.7
1	A	104	ARG	2.7
1	A	403	HIS	2.7
1	B	114	PRO	2.7
1	A	266	VAL	2.7
1	B	379	LYS	2.7
1	E	410	LEU	2.7
1	E	111	ALA	2.7
1	E	348	THR	2.7
1	H	316	GLU	2.7
1	B	518	GLY	2.7
1	E	367	GLY	2.7
1	A	514	PHE	2.7
1	C	371	ILE	2.7
1	A	330	ASN	2.7
1	A	52	VAL	2.7
1	B	537[A]	MET	2.7
1	A	417	SER	2.7
1	C	387	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	86	LEU	2.7
1	F	498	VAL	2.7
1	E	486	TYR	2.7
1	B	236	GLN	2.7
1	E	244	GLY	2.6
1	B	110	PHE	2.6
1	G	25	PHE	2.6
1	G	350	PRO	2.6
1	A	30	LEU	2.6
1	B	423	VAL	2.6
1	A	344	GLU	2.6
1	C	397	ALA	2.6
1	E	97	ALA	2.6
1	B	403	HIS	2.6
1	E	275	HIS	2.6
1	A	262	ASP	2.6
1	E	276	GLY	2.6
1	A	60	ILE	2.6
1	F	251	ILE	2.6
1	B	535	ASN	2.6
1	D	316	GLU	2.6
1	E	58	SER	2.6
1	A	437	ALA	2.6
1	B	123	ALA	2.6
1	B	495	ALA	2.6
1	C	394	ALA	2.6
1	E	386	ALA	2.6
1	F	431	ALA	2.6
1	F	497	ASP	2.6
1	F	487	ARG	2.6
1	G	231	PRO	2.6
1	E	63	ILE	2.6
1	E	372	MET	2.6
1	C	73	LEU	2.6
1	E	498	VAL	2.6
1	F	252	VAL	2.6
1	F	423	VAL	2.6
1	B	374	SER	2.6
1	E	345	SER	2.6
1	A	534	THR	2.6
1	B	61	ALA	2.6
1	C	339	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	527	TRP	2.6
1	A	383	PRO	2.6
1	B	426	ILE	2.6
1	B	45	LEU	2.6
1	A	260	ALA	2.6
1	A	129	PRO	2.5
1	A	333	GLY	2.5
1	B	489	PRO	2.5
1	E	536	ILE	2.5
1	A	410	LEU	2.5
1	E	86	LEU	2.5
1	F	233	LEU	2.5
1	F	484	LEU	2.5
1	A	29	GLN	2.5
1	A	82	ASN	2.5
1	E	298	VAL	2.5
1	E	478	CYS	2.5
1	F	358	SER	2.5
1	F	117	TYR	2.5
1	F	119	PRO	2.5
1	A	73	LEU	2.5
1	B	86	LEU	2.5
1	F	443	LEU	2.5
1	B	266	VAL	2.5
1	F	13	VAL	2.5
1	B	332	ALA	2.5
1	E	472	ALA	2.5
1	F	332	ALA	2.5
1	F	355	ALA	2.5
1	A	62	THR	2.5
1	A	281	SER	2.5
1	A	374	SER	2.5
1	C	389	MET	2.5
1	F	114	PRO	2.5
1	A	64	GLY	2.5
1	E	333	GLY	2.5
1	A	313	ILE	2.5
1	F	63	ILE	2.5
1	F	507	GLU	2.5
1	A	494	TRP	2.5
1	B	30	LEU	2.5
1	B	233	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	2.5
1	E	429	VAL	2.5
1	E	399	ALA	2.5
1	F	501	ARG	2.5
1	B	113	SER	2.5
1	C	43	CYS	2.5
1	B	112	GLY	2.5
1	D	274	GLY	2.5
1	A	122	ILE	2.5
1	A	347	ILE	2.5
1	A	416	LEU	2.5
1	B	241	LEU	2.5
1	B	24	PHE	2.5
1	C	337	VAL	2.5
1	E	459	ARG	2.5
1	B	269	ALA	2.5
1	B	378	ALA	2.5
1	E	361	ALA	2.5
1	F	377	THR	2.5
1	F	525	THR	2.5
1	A	338	CYS	2.4
1	B	277	ILE	2.4
1	F	486	TYR	2.4
1	B	124	LEU	2.4
1	A	256	PHE	2.4
1	A	286	HIS	2.4
1	E	494	TRP	2.4
1	G	387	VAL	2.4
1	A	355	ALA	2.4
1	C	269	ALA	2.4
1	E	265	ALA	2.4
1	F	269	ALA	2.4
1	E	488	GLU	2.4
1	F	532	GLY	2.4
1	C	115	LEU	2.4
1	G	115	LEU	2.4
1	H	516	ARG	2.4
1	A	245	VAL	2.4
1	A	381	ASN	2.4
1	B	53	ALA	2.4
1	B	439	ALA	2.4
1	H	33	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	466	THR	2.4
1	E	57	THR	2.4
1	F	531	SER	2.4
1	G	232	GLY	2.4
1	F	393	ILE	2.4
1	A	315	ALA	2.4
1	A	495	ALA	2.4
1	C	378	ALA	2.4
1	E	432	ALA	2.4
1	F	53	ALA	2.4
1	B	278	LYS	2.4
1	C	65	PRO	2.4
1	C	114	PRO	2.4
1	C	231	PRO	2.4
1	A	375	GLY	2.4
1	A	542	ILE	2.4
1	B	441	ILE	2.4
1	C	347	ILE	2.4
1	F	240	ASP	2.4
1	H	275[A]	HIS	2.4
1	B	436	CYS	2.4
1	E	256	PHE	2.4
1	G	34	MET	2.4
1	B	524	VAL	2.4
1	C	401	VAL	2.4
1	D	33	ALA	2.4
1	C	357	THR	2.3
1	E	65	PRO	2.3
1	G	348	THR	2.3
1	F	112	GLY	2.3
1	A	451	GLN	2.3
1	C	100	ILE	2.3
1	E	484	LEU	2.3
1	G	347	ILE	2.3
1	A	497	ASP	2.3
1	B	252	VAL	2.3
1	C	360	VAL	2.3
1	F	535	ASN	2.3
1	A	430	GLU	2.3
1	B	111	ALA	2.3
1	C	79	ALA	2.3
1	E	461	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	67	SER	2.3
1	E	109	SER	2.3
1	G	234	SER	2.3
1	E	248	GLY	2.3
1	A	277	ILE	2.3
1	E	371	ILE	2.3
1	E	366	ASP	2.3
1	A	31	PRO	2.3
1	B	14	ALA	2.3
1	E	79	ALA	2.3
1	E	383	PRO	2.3
1	C	348	THR	2.3
1	A	448	ARG	2.3
1	B	538	ARG	2.3
1	A	28	GLN	2.3
1	F	468	SER	2.3
1	C	391	HIS	2.3
1	A	270	LEU	2.3
1	D	30	LEU	2.3
1	E	60	ILE	2.3
1	E	515	LEU	2.3
1	A	407	PHE	2.3
1	F	88	PHE	2.3
1	A	364	VAL	2.3
1	A	486	TYR	2.3
1	B	238	VAL	2.3
1	E	481	VAL	2.3
1	A	425	ALA	2.3
1	E	267	ARG	2.3
1	B	91	GLY	2.3
1	C	232	GLY	2.3
1	B	100	ILE	2.3
1	E	506	ILE	2.3
1	F	122	ILE	2.3
1	F	506	ILE	2.3
1	E	108	GLU	2.3
1	F	94	GLU	2.3
1	F	409	GLU	2.3
1	A	70	VAL	2.3
1	A	336	VAL	2.3
1	E	337	VAL	2.3
1	B	10	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	335	PRO	2.3
1	F	272	PRO	2.3
1	A	79	ALA	2.2
1	A	469	ALA	2.2
1	B	472	ALA	2.2
1	E	95	TYR	2.3
1	G	23	ALA	2.2
1	B	377	THR	2.2
1	C	340	THR	2.2
1	A	532	GLY	2.2
1	A	346	MET	2.2
1	A	531	SER	2.2
1	B	416	LEU	2.2
1	B	484	LEU	2.2
1	F	34	MET	2.2
1	F	416	LEU	2.2
1	B	88	PHE	2.2
1	B	481	VAL	2.2
1	B	260	ALA	2.2
1	E	121	ALA	2.2
1	E	381	ASN	2.2
1	A	342	MET	2.2
1	B	16	LEU	2.2
1	C	346	MET	2.2
1	F	16	LEU	2.2
1	B	347	ILE	2.2
1	B	440	ILE	2.2
1	C	67	SER	2.2
1	E	279	ILE	2.2
1	A	491	GLU	2.2
1	A	318	VAL	2.2
1	A	458	PRO	2.2
1	B	465	VAL	2.2
1	A	61	ALA	2.2
1	A	84	ALA	2.2
1	B	79	ALA	2.2
1	B	121	ALA	2.2
1	E	268	ALA	2.2
1	F	61	ALA	2.2
1	A	402	TYR	2.2
1	C	390	GLN	2.2
1	A	303	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	42	LEU	2.2
1	E	280	ILE	2.2
1	B	541	SER	2.2
1	E	376	GLU	2.2
1	B	245	VAL	2.2
1	A	264	ALA	2.2
1	B	84	ALA	2.2
1	E	330	ASN	2.2
1	B	28	GLN	2.2
1	E	389	MET	2.2
1	B	486	TYR	2.2
1	C	375	GLY	2.2
1	E	288	GLY	2.2
1	A	393	ILE	2.2
1	F	417	SER	2.2
1	A	422	GLU	2.2
1	F	71	GLU	2.2
1	F	237	ASP	2.2
1	A	85	ARG	2.2
1	B	512	ARG	2.2
1	A	379	LYS	2.2
1	E	24	PHE	2.2
1	E	292	PHE	2.2
1	F	253	PHE	2.2
1	C	318	VAL	2.1
1	E	339	ALA	2.1
1	F	111	ALA	2.1
1	G	321	ALA	2.1
1	B	532	GLY	2.1
1	E	406	LEU	2.1
1	A	77	ILE	2.1
1	E	117	TYR	2.1
1	E	398	GLU	2.1
1	E	491	GLU	2.1
1	A	237	ASP	2.1
1	F	69	SER	2.1
1	G	116	SER	2.1
1	B	382	PHE	2.1
1	F	494	TRP	2.1
1	A	111	ALA	2.1
1	A	268	ALA	2.1
1	B	464	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	269	ALA	2.1
1	E	392	ALA	2.1
1	F	414	ALA	2.1
1	A	296	LEU	2.1
1	F	452	LEU	2.1
1	F	100	ILE	2.1
1	C	396	GLU	2.1
1	E	329	CYS	2.1
1	A	58	SER	2.1
1	B	468	SER	2.1
1	A	349	LYS	2.1
1	B	433	PHE	2.1
1	C	292	PHE	2.1
1	C	407	PHE	2.1
1	F	504	PHE	2.1
1	A	341	GLN	2.1
1	B	120	VAL	2.1
1	F	84	ALA	2.1
1	A	340	THR	2.1
1	A	411	ARG	2.1
1	C	68	ARG	2.1
1	E	311	ILE	2.1
1	E	316	GLU	2.1
1	F	280	ILE	2.1
1	A	99	SER	2.1
1	E	67	SER	2.1
1	E	449	SER	2.1
1	B	420	PRO	2.1
1	A	24	PHE	2.1
1	B	475	VAL	2.1
1	A	54	ALA	2.1
1	A	431	ALA	2.1
1	B	414	ALA	2.1
1	B	450	ALA	2.1
1	B	494	TRP	2.1
1	B	501	ARG	2.1
1	C	86	LEU	2.1
1	C	306	ARG	2.1
1	D	22	THR	2.1
1	A	59	ILE	2.1
1	A	506	ILE	2.1
1	B	371	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	347	ILE	2.1
1	A	366	ASP	2.1
1	E	338	CYS	2.1
1	F	483	PRO	2.1
1	G	383	PRO	2.1
1	C	34	MET	2.1
1	E	76[A]	MET	2.1
1	A	476	HIS	2.1
1	A	474	GLN	2.0
1	A	384	VAL	2.0
1	B	384	VAL	2.0
1	E	253	PHE	2.0
1	A	386	ALA	2.0
1	F	450	ALA	2.0
1	G	339	ALA	2.0
1	B	20	LEU	2.0
1	B	443	LEU	2.0
1	B	276	GLY	2.0
1	C	75	GLU	2.0
1	C	80	GLY	2.0
1	G	132	GLY	2.0
1	C	36	ASP	2.0
1	G	366	ASP	2.0
1	E	299	SER	2.0
1	F	51	PRO	2.0
1	E	303	MET	2.0
1	F	109	SER	2.0
1	C	29	GLN	2.0
1	G	322	GLN	2.0
1	B	103	VAL	2.0
1	E	351	ARG	2.0
1	G	70	VAL	2.0
1	C	101	ALA	2.0
1	E	106	ALA	2.0
1	B	488	GLU	2.0
1	E	430	GLU	2.0
1	B	375	GLY	2.0
1	F	348	THR	2.0
1	D	231	PRO	2.0
1	F	420	PRO	2.0
1	A	345	SER	2.0
1	B	90	HIS	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
5	K	A	604	1/1	0.45	0.11	289,289,289,289	0
5	K	E	604	1/1	0.52	0.11	299,299,299,299	0
2	FBP	A	601	20/20	0.66	0.17	148,149,152,152	0
2	FBP	F	601	20/20	0.67	0.14	128,131,136,136	0
3	OXL	A	602	6/6	0.67	0.14	195,196,196,196	0
2	FBP	B	601	20/20	0.75	0.13	126,126,128,128	0
5	K	C	604	1/1	0.76	0.13	117,117,117,117	0
2	FBP	E	601	20/20	0.76	0.13	136,136,138,138	0
5	K	G	604	1/1	0.76	0.12	117,117,117,117	0
3	OXL	E	602	6/6	0.78	0.12	156,156,156,156	0
5	K	F	604	1/1	0.81	0.08	152,152,152,152	0
3	OXL	C	602	6/6	0.81	0.14	129,129,129,129	0
6	OE0	A	605	28/28	0.81	0.16	116,117,118,119	19
5	K	B	604	1/1	0.83	0.10	144,144,144,144	0
6	OE0	G	605	28/28	0.84	0.15	104,105,106,106	19
3	OXL	B	602	6/6	0.85	0.12	108,108,109,109	0
3	OXL	F	602	6/6	0.85	0.13	128,128,128,128	0
6	OE0	B	605	28/28	0.86	0.16	90,92,96,97	19
6	OE0	F	605	28/28	0.86	0.18	99,101,103,106	19
3	OXL	G	602	6/6	0.86	0.12	114,115,115,115	0
4	MG	E	603	1/1	0.90	0.06	137,137,137,137	0
4	MG	H	603	1/1	0.90	0.14	63,63,63,63	0
4	MG	D	603	1/1	0.90	0.14	75,75,75,75	0
4	MG	G	603	1/1	0.91	0.08	73,73,73,73	0
3	OXL	H	602	6/6	0.91	0.12	85,86,87,87	0
4	MG	C	603	1/1	0.91	0.11	90,90,90,90	0
4	MG	B	603	1/1	0.92	0.09	88,88,88,88	0

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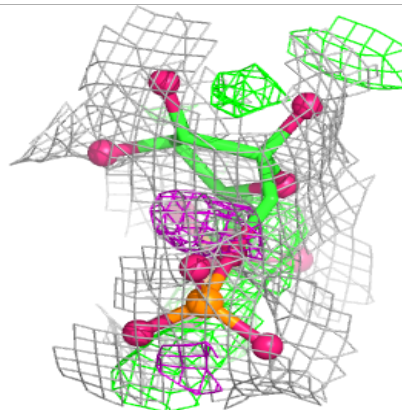
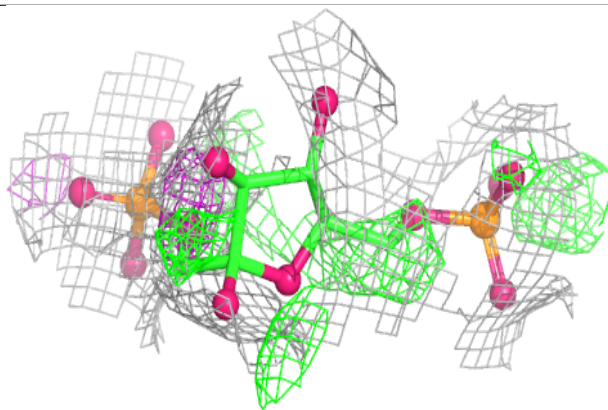
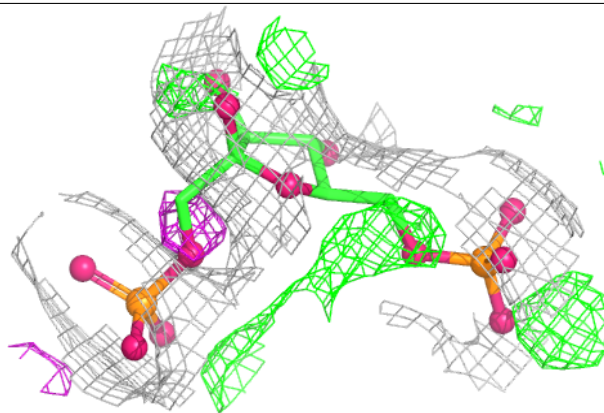
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	603	1/1	0.92	0.06	140,140,140,140	0
3	OXL	D	602	6/6	0.93	0.12	95,95,96,96	0
5	K	H	604	1/1	0.93	0.07	94,94,94,94	0
5	K	D	604	1/1	0.93	0.11	91,91,91,91	0
4	MG	F	603	1/1	0.94	0.08	73,73,73,73	0
2	FBP	C	601	20/20	0.96	0.07	46,48,53,53	0
2	FBP	D	601	20/20	0.97	0.06	41,43,45,46	0
2	FBP	G	601	20/20	0.97	0.06	45,47,55,55	0
2	FBP	H	601	20/20	0.98	0.05	37,40,42,43	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.

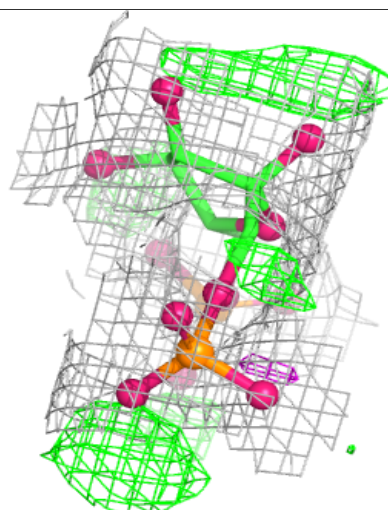
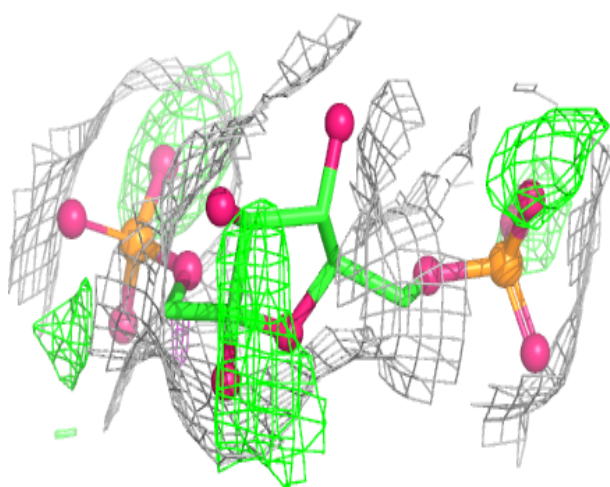
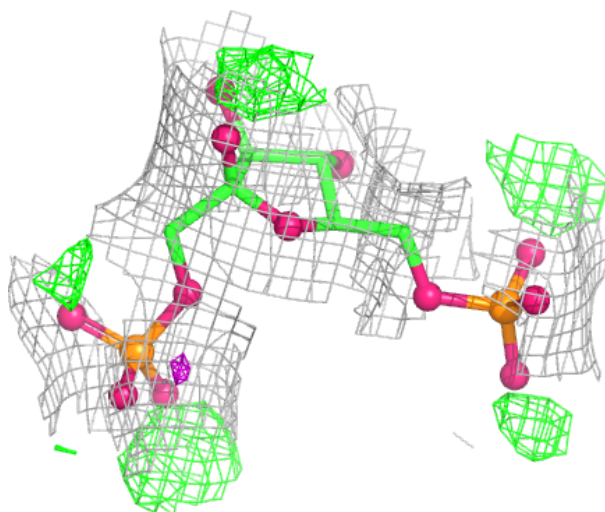
Electron density around FBP A 601:

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



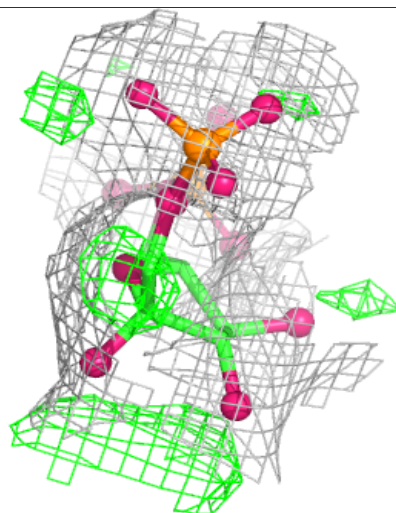
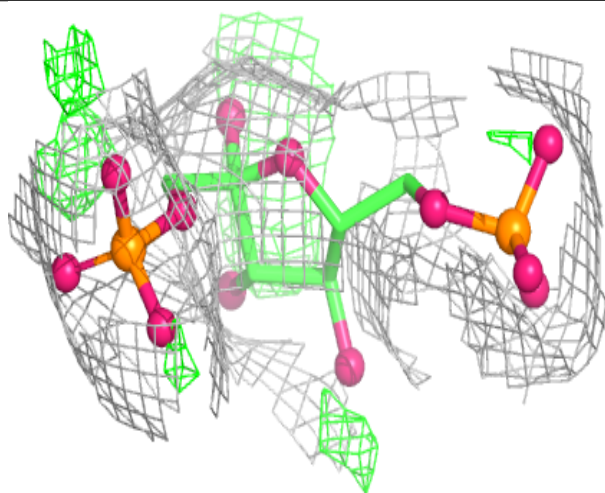
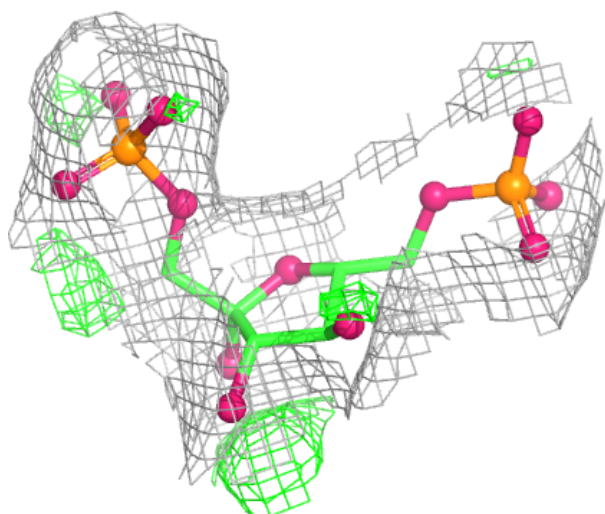
Electron density around FBP F 601:

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



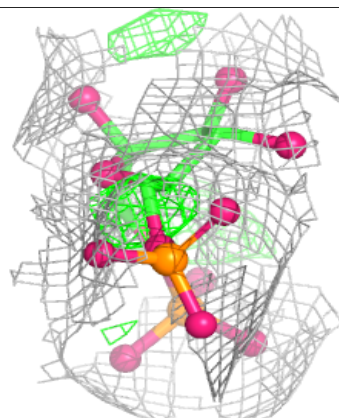
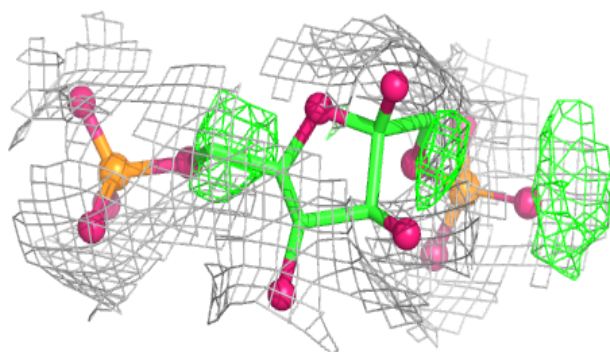
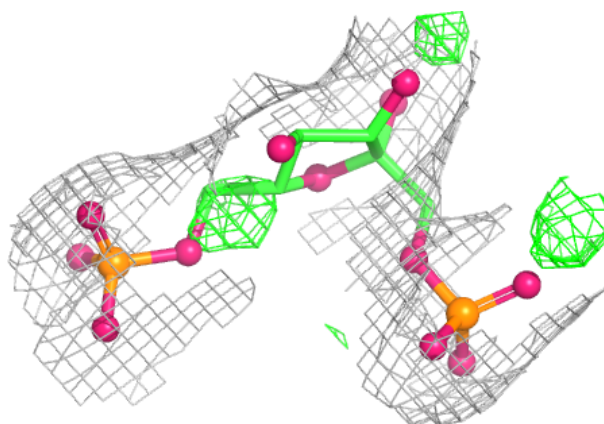
Electron density around FBP B 601:

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

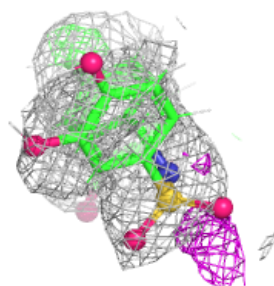
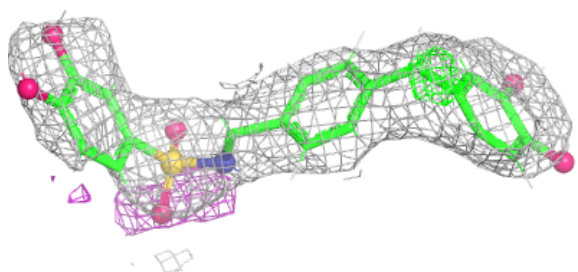
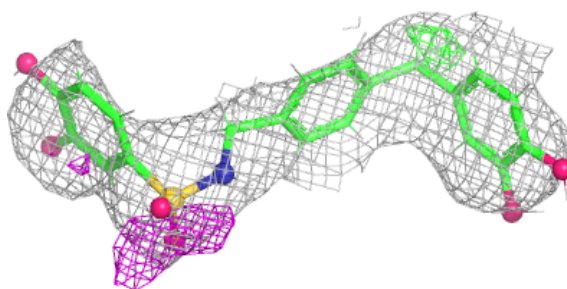


Electron density around FBP E 601:

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

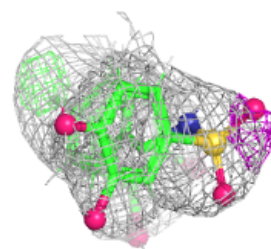
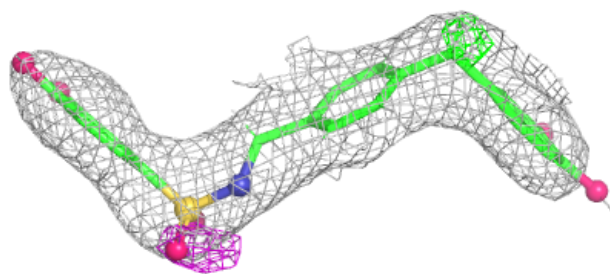
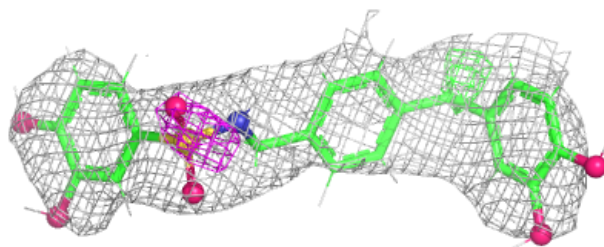
**Electron density around OE0 A 605:**

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

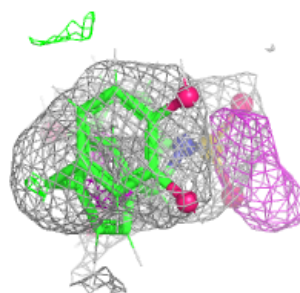
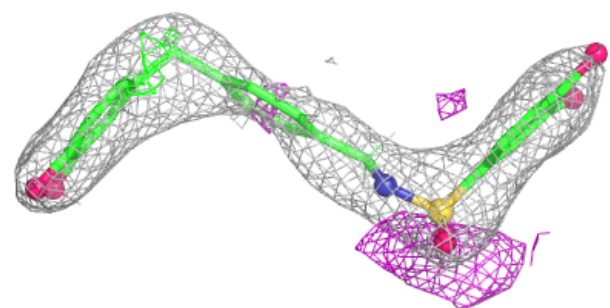
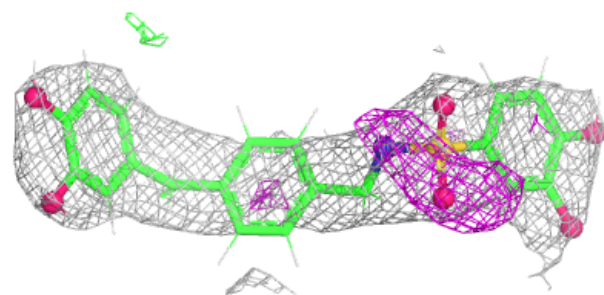


Electron density around OE0 G 605:

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

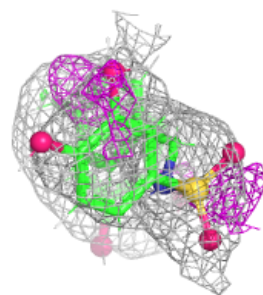
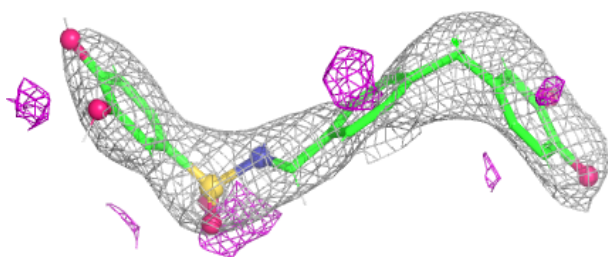
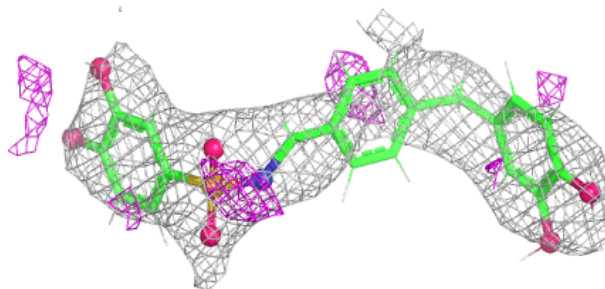
**Electron density around OE0 B 605:**

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

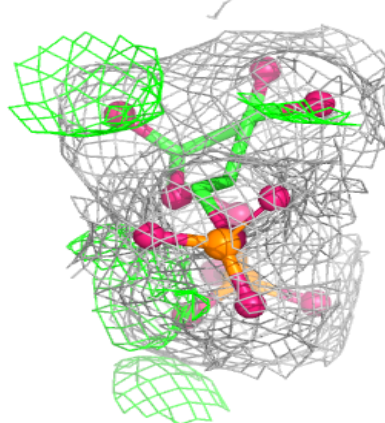
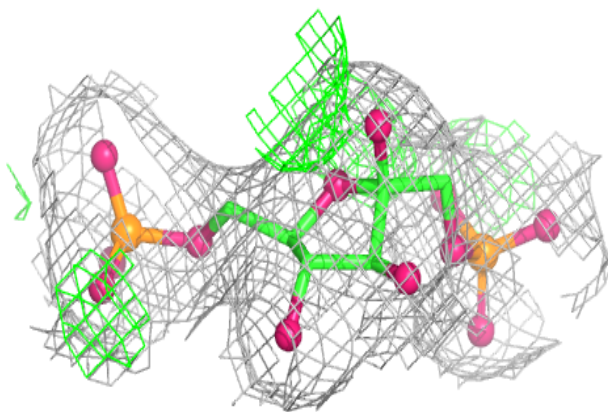
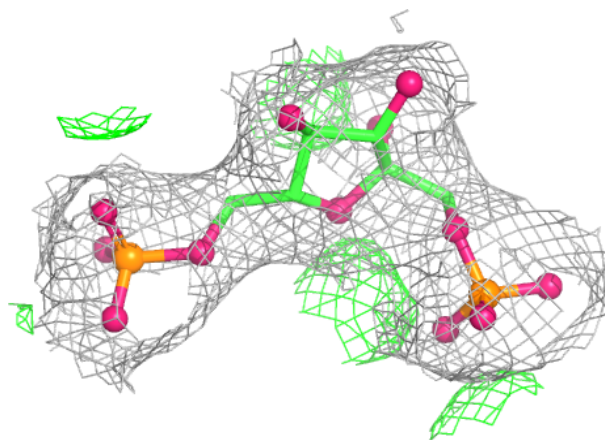


Electron density around OE0 F 605:

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

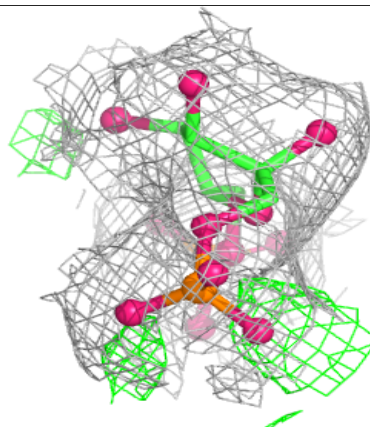
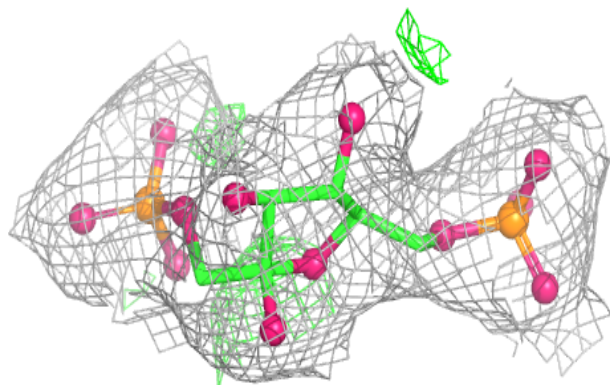
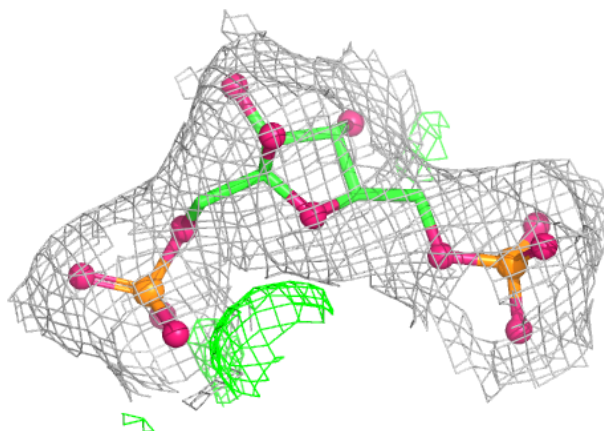
**Electron density around FBP C 601:**

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

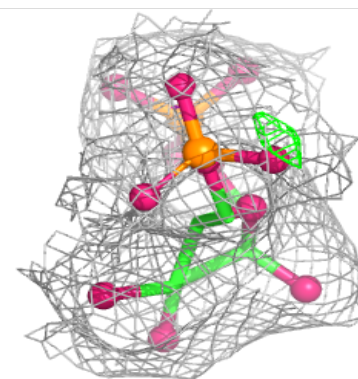
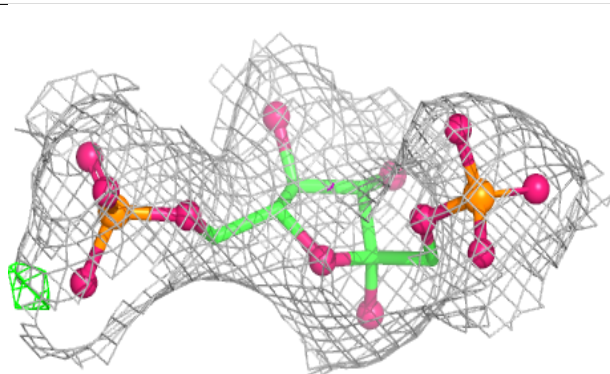
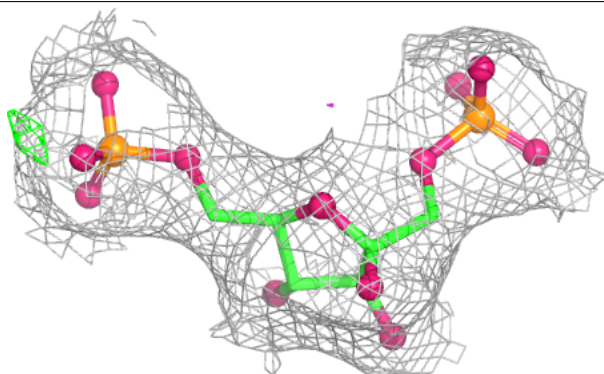


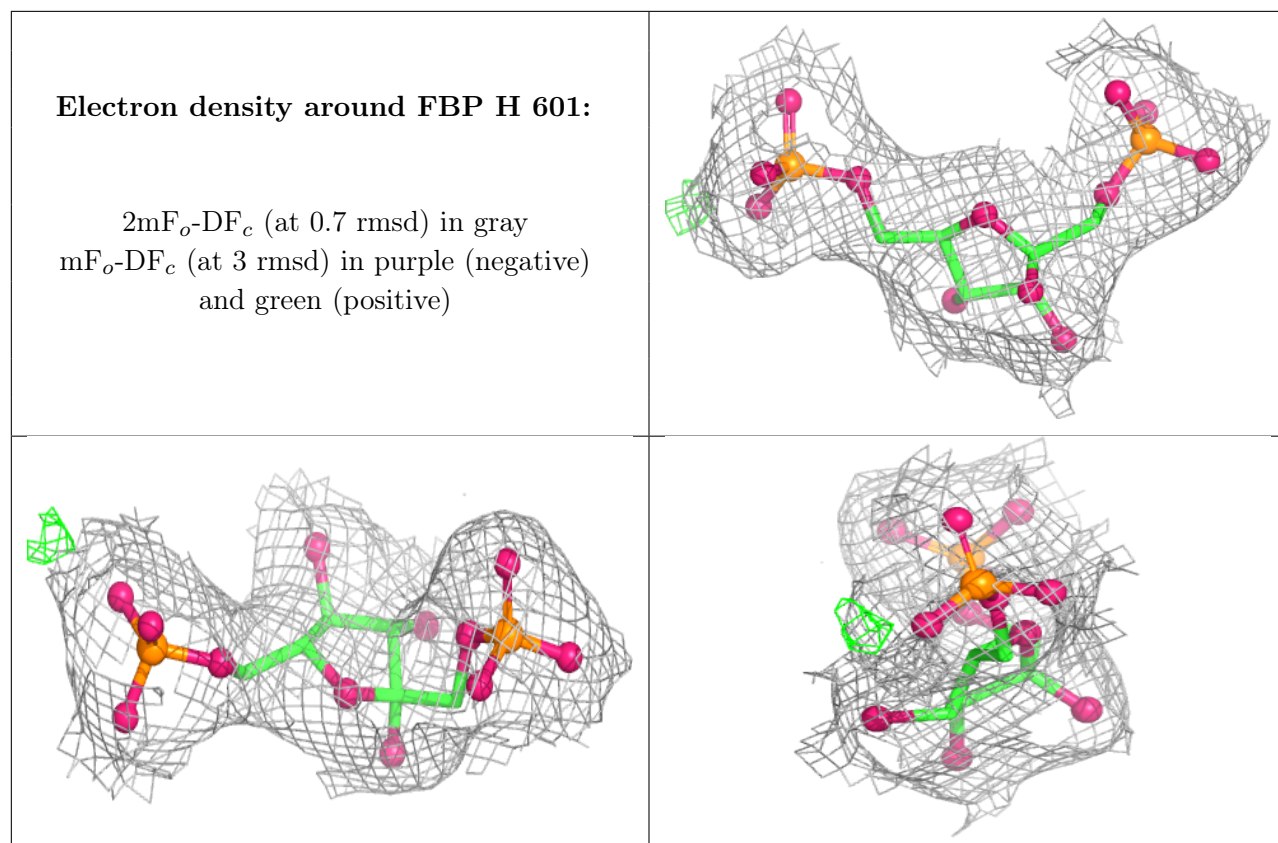
Electron density around FBP D 601:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.