



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:15 PM UTC

PDB ID : 8IAU / pdb_00008iau
Title : Crystal structure of Streptococcus pneumoniae pyruvate kinase in complex with oxalate and fructose 1,6-bisphosphate
Authors : Nakashima, R.; Taguchi, A.
Deposited on : 2023-02-09
Resolution : 2.00 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:

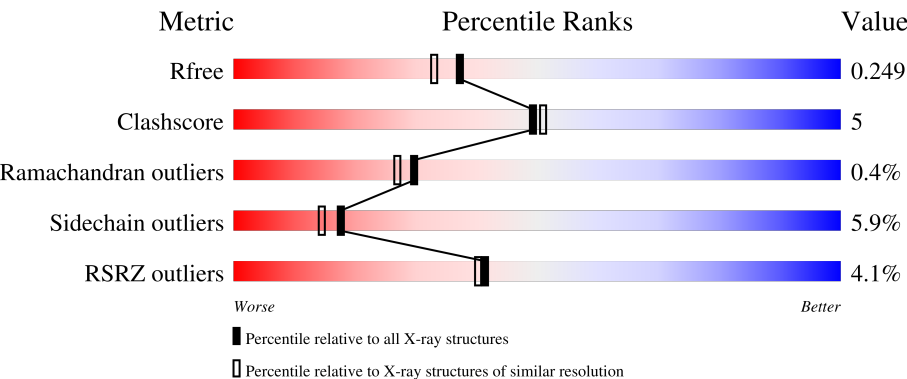
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	521	% 83%11% . .
1	B	521	% 83%11% . .
1	C	521	3% 82%12% . .
1	D	521	% 83%12% . .
1	E	521	12% 76%18% . .

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Mol	Chain	Length	Quality of chain
1	F	521	
1	G	521	
1	H	521	

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
4	OXL	A	603	-	X	-	-
4	OXL	B	603	-	X	-	-
4	OXL	D	603	-	X	-	-
4	OXL	F	603	-	X	-	-
4	OXL	G	603	-	X	-	-
4	OXL	H	603	-	X	-	-
6	PEG	H	605	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31195 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	B	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	C	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	D	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	E	499	Total	C	N	O	S	0	0	0
			3820	2388	659	757	16			
1	F	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	G	500	Total	C	N	O	S	0	0	0
			3828	2393	660	758	17			
1	H	412	Total	C	N	O	S	0	0	0
			3148	1967	546	618	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DQ84
A	-18	GLY	-	expression tag	UNP Q8DQ84
A	-17	SER	-	expression tag	UNP Q8DQ84
A	-16	SER	-	expression tag	UNP Q8DQ84
A	-15	HIS	-	expression tag	UNP Q8DQ84
A	-14	HIS	-	expression tag	UNP Q8DQ84
A	-13	HIS	-	expression tag	UNP Q8DQ84
A	-12	HIS	-	expression tag	UNP Q8DQ84
A	-11	HIS	-	expression tag	UNP Q8DQ84
A	-10	HIS	-	expression tag	UNP Q8DQ84
A	-9	SER	-	expression tag	UNP Q8DQ84
A	-8	SER	-	expression tag	UNP Q8DQ84
A	-7	GLY	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP Q8DQ84
A	-5	VAL	-	expression tag	UNP Q8DQ84
A	-4	PRO	-	expression tag	UNP Q8DQ84
A	-3	ARG	-	expression tag	UNP Q8DQ84
A	-2	GLY	-	expression tag	UNP Q8DQ84
A	-1	SER	-	expression tag	UNP Q8DQ84
A	0	HIS	-	expression tag	UNP Q8DQ84
B	-19	MET	-	initiating methionine	UNP Q8DQ84
B	-18	GLY	-	expression tag	UNP Q8DQ84
B	-17	SER	-	expression tag	UNP Q8DQ84
B	-16	SER	-	expression tag	UNP Q8DQ84
B	-15	HIS	-	expression tag	UNP Q8DQ84
B	-14	HIS	-	expression tag	UNP Q8DQ84
B	-13	HIS	-	expression tag	UNP Q8DQ84
B	-12	HIS	-	expression tag	UNP Q8DQ84
B	-11	HIS	-	expression tag	UNP Q8DQ84
B	-10	HIS	-	expression tag	UNP Q8DQ84
B	-9	SER	-	expression tag	UNP Q8DQ84
B	-8	SER	-	expression tag	UNP Q8DQ84
B	-7	GLY	-	expression tag	UNP Q8DQ84
B	-6	LEU	-	expression tag	UNP Q8DQ84
B	-5	VAL	-	expression tag	UNP Q8DQ84
B	-4	PRO	-	expression tag	UNP Q8DQ84
B	-3	ARG	-	expression tag	UNP Q8DQ84
B	-2	GLY	-	expression tag	UNP Q8DQ84
B	-1	SER	-	expression tag	UNP Q8DQ84
B	0	HIS	-	expression tag	UNP Q8DQ84
C	-19	MET	-	initiating methionine	UNP Q8DQ84
C	-18	GLY	-	expression tag	UNP Q8DQ84
C	-17	SER	-	expression tag	UNP Q8DQ84
C	-16	SER	-	expression tag	UNP Q8DQ84
C	-15	HIS	-	expression tag	UNP Q8DQ84
C	-14	HIS	-	expression tag	UNP Q8DQ84
C	-13	HIS	-	expression tag	UNP Q8DQ84
C	-12	HIS	-	expression tag	UNP Q8DQ84
C	-11	HIS	-	expression tag	UNP Q8DQ84
C	-10	HIS	-	expression tag	UNP Q8DQ84
C	-9	SER	-	expression tag	UNP Q8DQ84
C	-8	SER	-	expression tag	UNP Q8DQ84
C	-7	GLY	-	expression tag	UNP Q8DQ84
C	-6	LEU	-	expression tag	UNP Q8DQ84
C	-5	VAL	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP Q8DQ84
C	-3	ARG	-	expression tag	UNP Q8DQ84
C	-2	GLY	-	expression tag	UNP Q8DQ84
C	-1	SER	-	expression tag	UNP Q8DQ84
C	0	HIS	-	expression tag	UNP Q8DQ84
D	-19	MET	-	initiating methionine	UNP Q8DQ84
D	-18	GLY	-	expression tag	UNP Q8DQ84
D	-17	SER	-	expression tag	UNP Q8DQ84
D	-16	SER	-	expression tag	UNP Q8DQ84
D	-15	HIS	-	expression tag	UNP Q8DQ84
D	-14	HIS	-	expression tag	UNP Q8DQ84
D	-13	HIS	-	expression tag	UNP Q8DQ84
D	-12	HIS	-	expression tag	UNP Q8DQ84
D	-11	HIS	-	expression tag	UNP Q8DQ84
D	-10	HIS	-	expression tag	UNP Q8DQ84
D	-9	SER	-	expression tag	UNP Q8DQ84
D	-8	SER	-	expression tag	UNP Q8DQ84
D	-7	GLY	-	expression tag	UNP Q8DQ84
D	-6	LEU	-	expression tag	UNP Q8DQ84
D	-5	VAL	-	expression tag	UNP Q8DQ84
D	-4	PRO	-	expression tag	UNP Q8DQ84
D	-3	ARG	-	expression tag	UNP Q8DQ84
D	-2	GLY	-	expression tag	UNP Q8DQ84
D	-1	SER	-	expression tag	UNP Q8DQ84
D	0	HIS	-	expression tag	UNP Q8DQ84
E	-19	MET	-	initiating methionine	UNP Q8DQ84
E	-18	GLY	-	expression tag	UNP Q8DQ84
E	-17	SER	-	expression tag	UNP Q8DQ84
E	-16	SER	-	expression tag	UNP Q8DQ84
E	-15	HIS	-	expression tag	UNP Q8DQ84
E	-14	HIS	-	expression tag	UNP Q8DQ84
E	-13	HIS	-	expression tag	UNP Q8DQ84
E	-12	HIS	-	expression tag	UNP Q8DQ84
E	-11	HIS	-	expression tag	UNP Q8DQ84
E	-10	HIS	-	expression tag	UNP Q8DQ84
E	-9	SER	-	expression tag	UNP Q8DQ84
E	-8	SER	-	expression tag	UNP Q8DQ84
E	-7	GLY	-	expression tag	UNP Q8DQ84
E	-6	LEU	-	expression tag	UNP Q8DQ84
E	-5	VAL	-	expression tag	UNP Q8DQ84
E	-4	PRO	-	expression tag	UNP Q8DQ84
E	-3	ARG	-	expression tag	UNP Q8DQ84

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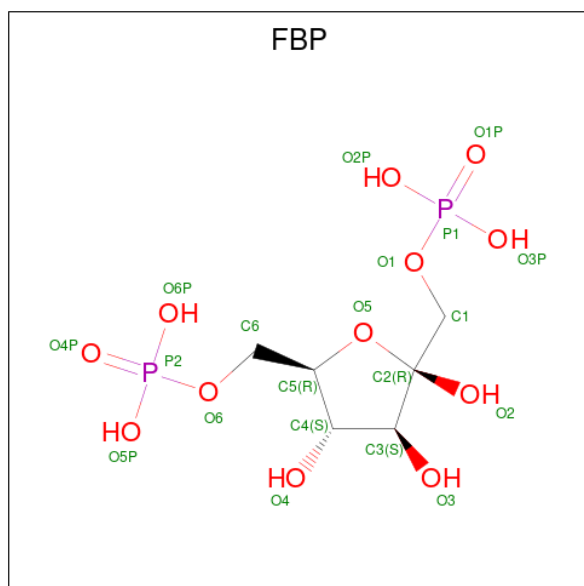
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q8DQ84
E	-1	SER	-	expression tag	UNP Q8DQ84
E	0	HIS	-	expression tag	UNP Q8DQ84
F	-19	MET	-	initiating methionine	UNP Q8DQ84
F	-18	GLY	-	expression tag	UNP Q8DQ84
F	-17	SER	-	expression tag	UNP Q8DQ84
F	-16	SER	-	expression tag	UNP Q8DQ84
F	-15	HIS	-	expression tag	UNP Q8DQ84
F	-14	HIS	-	expression tag	UNP Q8DQ84
F	-13	HIS	-	expression tag	UNP Q8DQ84
F	-12	HIS	-	expression tag	UNP Q8DQ84
F	-11	HIS	-	expression tag	UNP Q8DQ84
F	-10	HIS	-	expression tag	UNP Q8DQ84
F	-9	SER	-	expression tag	UNP Q8DQ84
F	-8	SER	-	expression tag	UNP Q8DQ84
F	-7	GLY	-	expression tag	UNP Q8DQ84
F	-6	LEU	-	expression tag	UNP Q8DQ84
F	-5	VAL	-	expression tag	UNP Q8DQ84
F	-4	PRO	-	expression tag	UNP Q8DQ84
F	-3	ARG	-	expression tag	UNP Q8DQ84
F	-2	GLY	-	expression tag	UNP Q8DQ84
F	-1	SER	-	expression tag	UNP Q8DQ84
F	0	HIS	-	expression tag	UNP Q8DQ84
G	-19	MET	-	initiating methionine	UNP Q8DQ84
G	-18	GLY	-	expression tag	UNP Q8DQ84
G	-17	SER	-	expression tag	UNP Q8DQ84
G	-16	SER	-	expression tag	UNP Q8DQ84
G	-15	HIS	-	expression tag	UNP Q8DQ84
G	-14	HIS	-	expression tag	UNP Q8DQ84
G	-13	HIS	-	expression tag	UNP Q8DQ84
G	-12	HIS	-	expression tag	UNP Q8DQ84
G	-11	HIS	-	expression tag	UNP Q8DQ84
G	-10	HIS	-	expression tag	UNP Q8DQ84
G	-9	SER	-	expression tag	UNP Q8DQ84
G	-8	SER	-	expression tag	UNP Q8DQ84
G	-7	GLY	-	expression tag	UNP Q8DQ84
G	-6	LEU	-	expression tag	UNP Q8DQ84
G	-5	VAL	-	expression tag	UNP Q8DQ84
G	-4	PRO	-	expression tag	UNP Q8DQ84
G	-3	ARG	-	expression tag	UNP Q8DQ84
G	-2	GLY	-	expression tag	UNP Q8DQ84
G	-1	SER	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q8DQ84
H	-19	MET	-	initiating methionine	UNP Q8DQ84
H	-18	GLY	-	expression tag	UNP Q8DQ84
H	-17	SER	-	expression tag	UNP Q8DQ84
H	-16	SER	-	expression tag	UNP Q8DQ84
H	-15	HIS	-	expression tag	UNP Q8DQ84
H	-14	HIS	-	expression tag	UNP Q8DQ84
H	-13	HIS	-	expression tag	UNP Q8DQ84
H	-12	HIS	-	expression tag	UNP Q8DQ84
H	-11	HIS	-	expression tag	UNP Q8DQ84
H	-10	HIS	-	expression tag	UNP Q8DQ84
H	-9	SER	-	expression tag	UNP Q8DQ84
H	-8	SER	-	expression tag	UNP Q8DQ84
H	-7	GLY	-	expression tag	UNP Q8DQ84
H	-6	LEU	-	expression tag	UNP Q8DQ84
H	-5	VAL	-	expression tag	UNP Q8DQ84
H	-4	PRO	-	expression tag	UNP Q8DQ84
H	-3	ARG	-	expression tag	UNP Q8DQ84
H	-2	GLY	-	expression tag	UNP Q8DQ84
H	-1	SER	-	expression tag	UNP Q8DQ84
H	0	HIS	-	expression tag	UNP Q8DQ84

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).

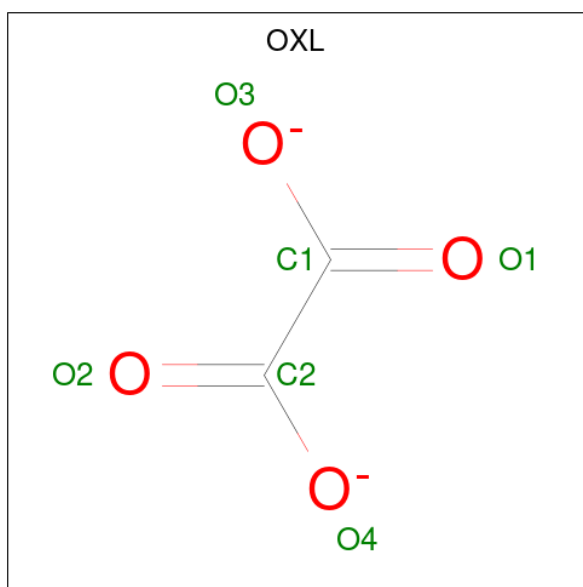


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 20 6 12 2	0	0
2	B	1	Total C O P 20 6 12 2	0	0
2	C	1	Total C O P 20 6 12 2	0	0
2	D	1	Total C O P 20 6 12 2	0	0
2	E	1	Total C O P 20 6 12 2	0	0
2	F	1	Total C O P 20 6 12 2	0	0
2	G	1	Total C O P 20 6 12 2	0	0
2	H	1	Total C O P 20 6 12 2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is OXALATE ION (CCD ID: OXL) (formula: C₂O₄).



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

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

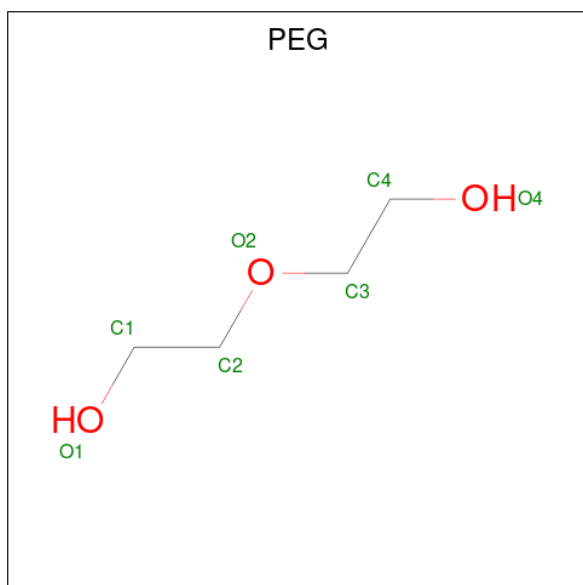
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		
5	F	1	Total	K	0	0
			1	1		

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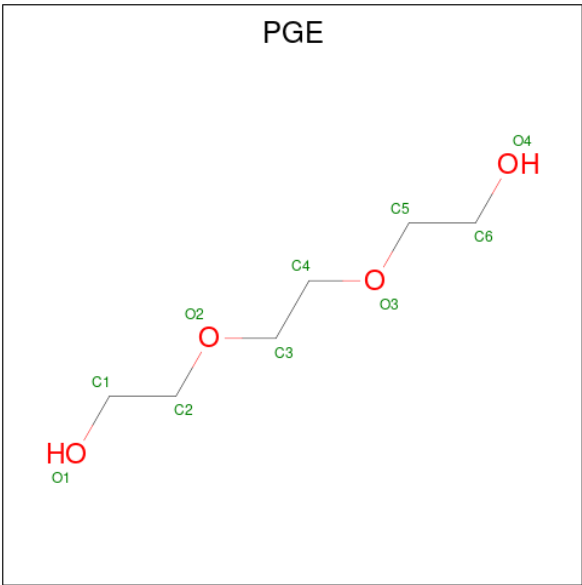
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	K	0	0
			1	1		
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



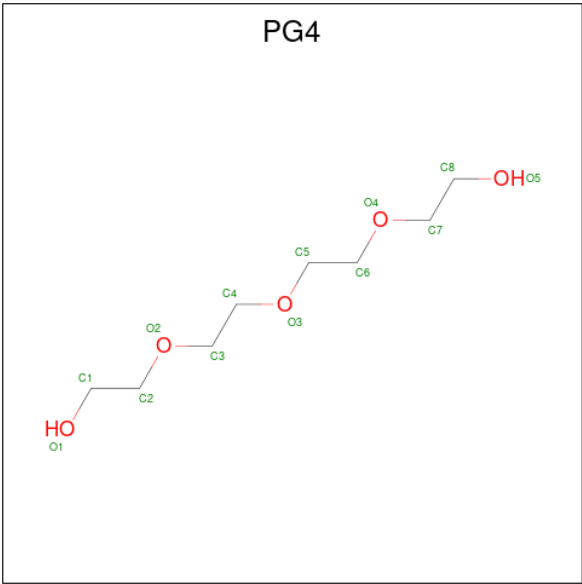
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		
7	D	1	Total	C	O	0	0
			10	6	4		
7	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			13	8	5		

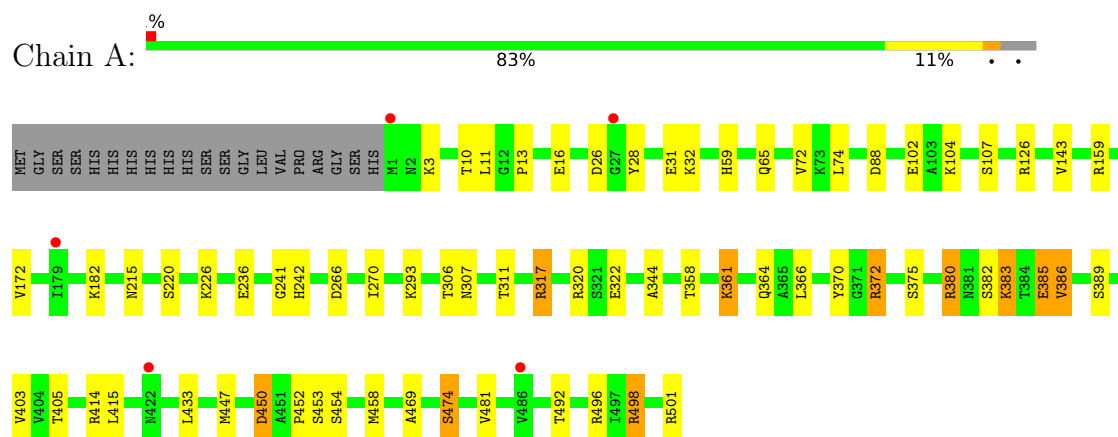
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	169	Total	O	0	0
			169	169		
9	B	139	Total	O	0	0
			139	139		
9	C	103	Total	O	0	0
			103	103		
9	D	147	Total	O	0	0
			147	147		
9	E	56	Total	O	0	0
			56	56		
9	F	101	Total	O	0	0
			101	101		
9	G	129	Total	O	0	0
			129	129		
9	H	72	Total	O	0	0
			72	72		

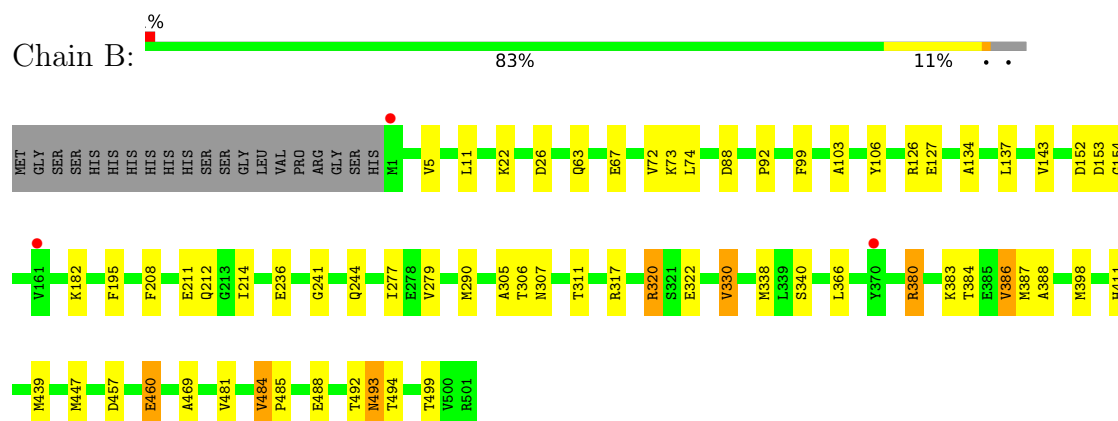
3 Residue-property plots [i](#)

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.

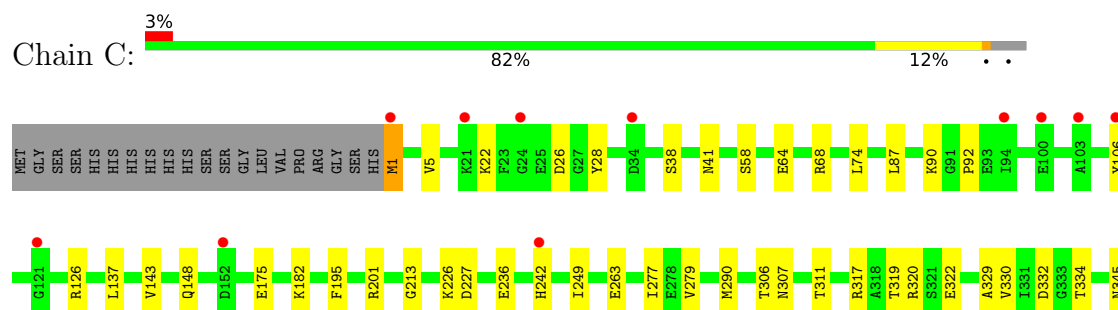
• Molecule 1: Pyruvate kinase

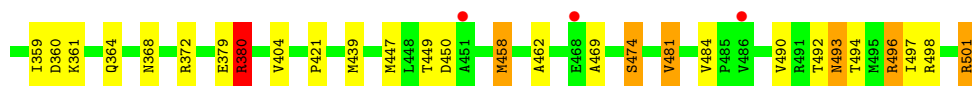


• Molecule 1: Pyruvate kinase

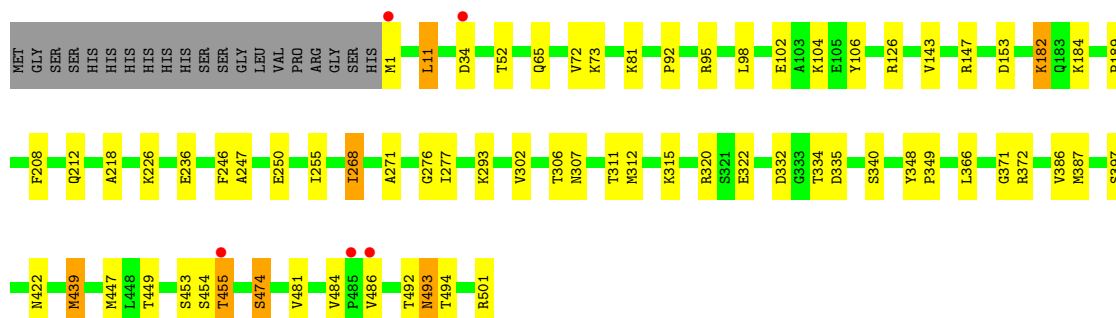
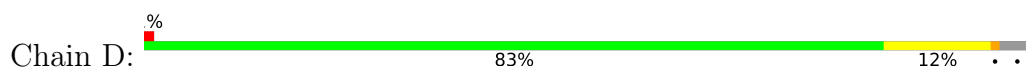


• Molecule 1: Pyruvate kinase

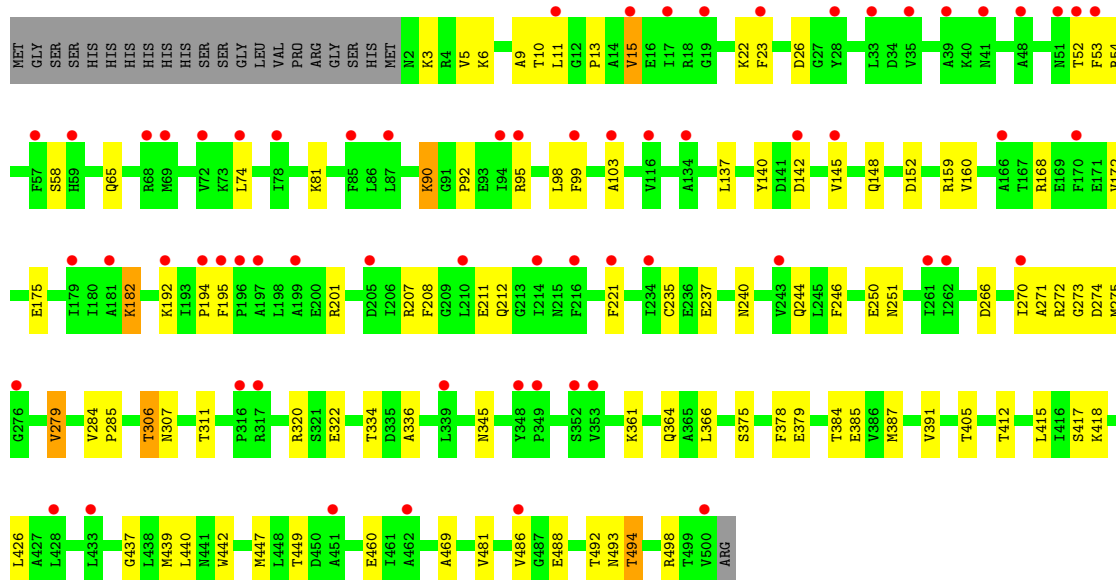
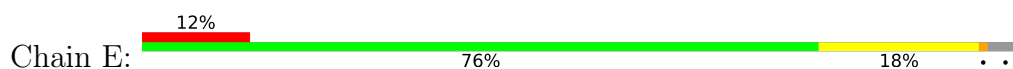




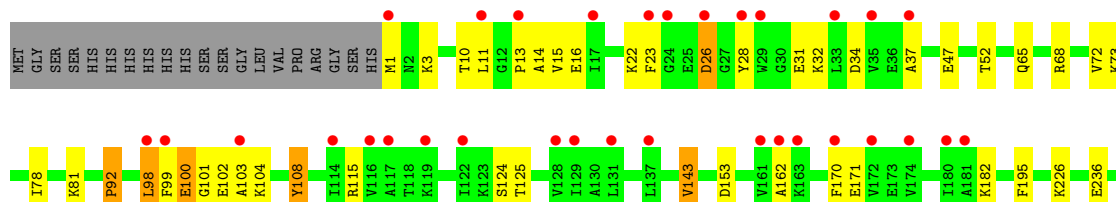
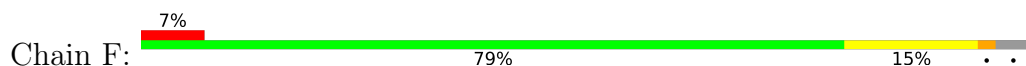
• Molecule 1: Pyruvate kinase

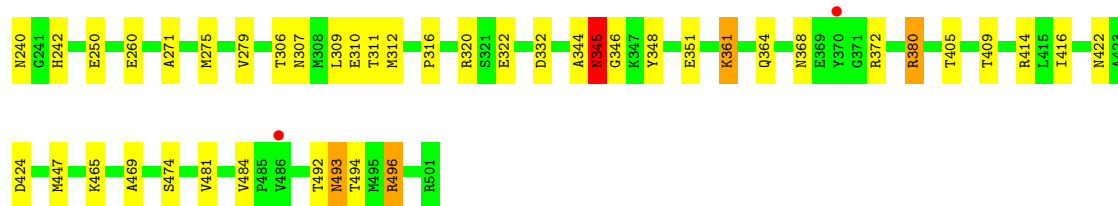


• Molecule 1: Pyruvate kinase

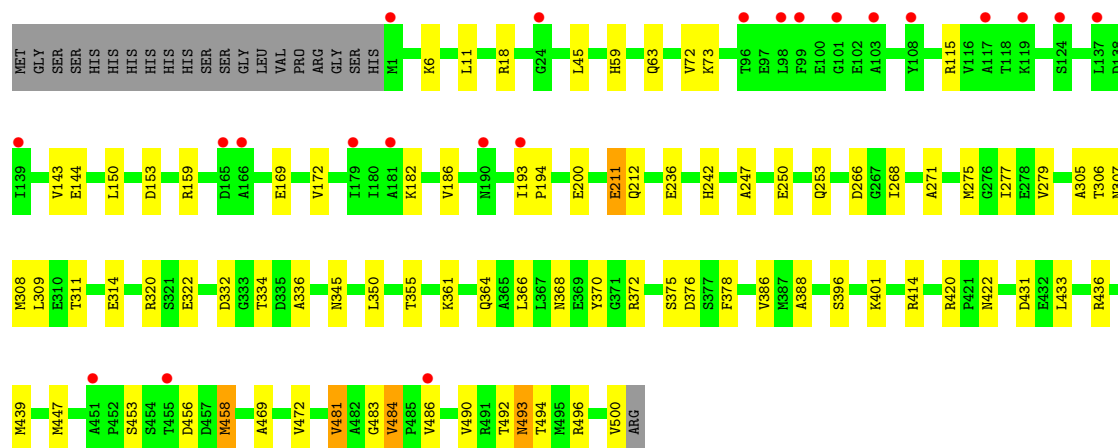
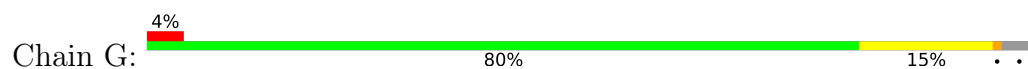


• Molecule 1: Pyruvate kinase

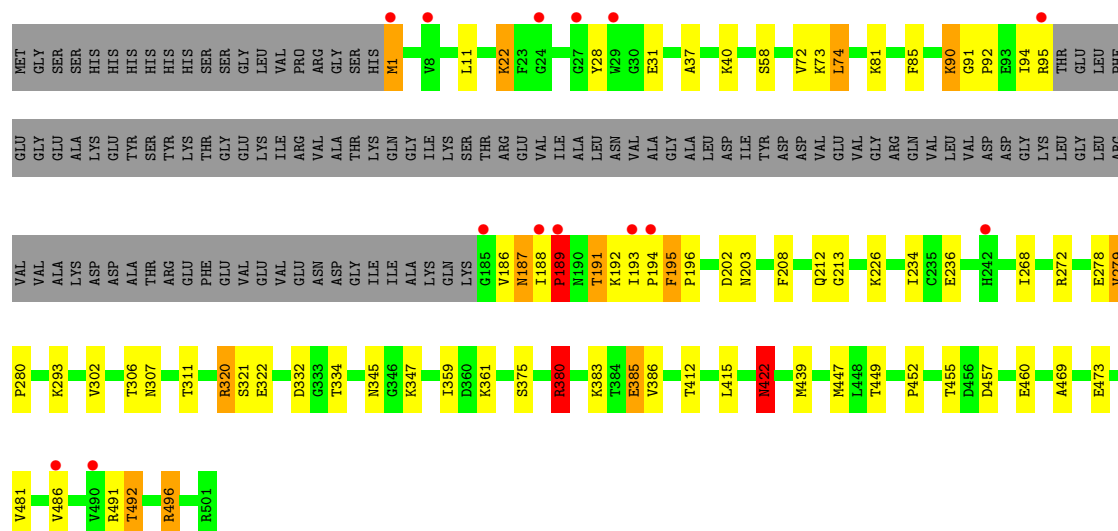




● Molecule 1: Pyruvate kinase



● Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.44Å 114.66Å 140.71Å 88.95° 88.12° 76.52°	Depositor
Resolution (Å)	49.38 – 2.00 49.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.38-2.00) 97.1 (49.38-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.200 , 0.246 0.206 , 0.249	Depositor DCC
R_{free} test set	14695 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31195	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PEG, PG4, MG, FBP, K, OXL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.22	5/3885 (0.1%)	1.51	15/5238 (0.3%)
1	B	1.20	6/3885 (0.2%)	1.50	16/5238 (0.3%)
1	C	1.19	4/3885 (0.1%)	1.46	6/5238 (0.1%)
1	D	1.17	6/3885 (0.2%)	1.47	10/5238 (0.2%)
1	E	1.16	1/3865 (0.0%)	1.53	5/5214 (0.1%)
1	F	1.15	2/3885 (0.1%)	1.52	18/5238 (0.3%)
1	G	1.19	3/3873 (0.1%)	1.50	11/5224 (0.2%)
1	H	1.17	3/3187 (0.1%)	1.59	21/4298 (0.5%)
All	All	1.18	30/30350 (0.1%)	1.51	102/40926 (0.2%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	302	VAL	C-O	7.50	1.32	1.24
1	H	302	VAL	C-O	7.42	1.32	1.24
1	A	242	HIS	CE1-NE2	7.36	1.40	1.32
1	G	420	ARG	N-CA	7.33	1.51	1.46
1	B	411	HIS	CE1-NE2	6.78	1.39	1.32
1	D	92	PRO	C-O	-6.57	1.15	1.23
1	F	78	ILE	C-O	6.27	1.31	1.24
1	D	268	ILE	C-O	6.26	1.30	1.24
1	H	268	ILE	C-O	6.22	1.30	1.24
1	B	380	ARG	CD-NE	-6.01	1.37	1.46
1	D	189	PRO	C-O	-5.95	1.16	1.23
1	B	330	VAL	C-O	5.93	1.30	1.24
1	B	244	GLN	C-O	-5.79	1.17	1.23
1	A	270	ILE	C-O	5.74	1.31	1.23
1	D	439	MET	CG-SD	-5.74	1.66	1.80
1	H	359	ILE	C-O	5.59	1.30	1.24
1	C	249	ILE	C-O	5.55	1.30	1.24
1	A	382	SER	C-O	5.53	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	GLY	C-O	-5.48	1.18	1.23
1	B	214	ILE	C-O	5.37	1.29	1.23
1	C	360	ASP	C-O	5.33	1.30	1.24
1	C	359	ILE	C-O	5.28	1.30	1.24
1	C	242	HIS	CE1-NE2	5.26	1.37	1.32
1	B	388	ALA	C-O	5.11	1.29	1.24
1	G	305	ALA	C-O	5.09	1.30	1.23
1	A	403	VAL	C-O	-5.07	1.18	1.24
1	E	279	VAL	N-CA	5.05	1.50	1.46
1	A	3	LYS	C-O	-5.03	1.17	1.24
1	F	424	ASP	C-O	5.02	1.30	1.23
1	G	388	ALA	C-O	5.02	1.29	1.24

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	189	PRO	CA-N-CD	-10.70	97.03	112.00
1	H	194	PRO	CA-N-CD	-10.51	97.29	112.00
1	C	380	ARG	NE-CZ-NH2	9.47	127.72	119.20
1	H	196	PRO	CA-N-CD	-9.03	99.36	112.00
1	B	380	ARG	NE-CZ-NH2	7.69	126.12	119.20
1	H	194	PRO	N-CA-CB	7.68	107.80	102.35
1	B	320	ARG	CA-C-N	7.30	130.39	120.54
1	B	320	ARG	C-N-CA	7.30	130.39	120.54
1	F	380	ARG	NE-CZ-NH2	7.16	125.64	119.20
1	H	380	ARG	NE-CZ-NH2	7.08	125.58	119.20
1	C	380	ARG	NE-CZ-NH1	-7.05	114.45	121.50
1	G	277	ILE	N-CA-C	-6.77	106.41	111.90
1	E	52	THR	CA-CB-OG1	-6.72	99.52	109.60
1	B	153	ASP	CA-CB-CG	6.49	119.09	112.60
1	D	52	THR	CA-CB-OG1	-6.43	99.95	109.60
1	H	422	ASN	CA-CB-CG	-6.40	106.20	112.60
1	G	500	VAL	CA-C-O	-6.28	110.12	120.80
1	F	65	GLN	CA-C-N	6.26	127.05	120.03
1	F	65	GLN	C-N-CA	6.26	127.05	120.03
1	H	320	ARG	CA-C-N	6.26	129.00	120.54
1	H	320	ARG	C-N-CA	6.26	129.00	120.54
1	A	241	GLY	CA-C-N	6.21	129.76	120.31
1	A	241	GLY	C-N-CA	6.21	129.76	120.31
1	F	380	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	B	134	ALA	CA-C-O	-6.16	115.09	120.88
1	D	340	SER	CA-C-O	-6.10	115.35	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	68	ARG	CA-C-N	6.06	128.68	120.44
1	F	68	ARG	C-N-CA	6.06	128.68	120.44
1	H	196	PRO	N-CA-CB	6.01	110.02	103.23
1	A	215	ASN	N-CA-C	-6.00	106.50	113.88
1	D	65	GLN	CA-C-N	5.89	126.51	119.98
1	D	65	GLN	C-N-CA	5.89	126.51	119.98
1	B	277	ILE	N-CA-C	-5.76	107.23	111.90
1	G	253	GLN	CB-CA-C	-5.75	101.24	110.79
1	A	358	THR	CA-CB-OG1	-5.68	101.07	109.60
1	B	380	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	F	153	ASP	CA-CB-CG	5.62	118.22	112.60
1	F	332	ASP	CA-CB-CG	5.61	118.21	112.60
1	H	380	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	B	340	SER	CA-C-O	-5.56	116.16	119.55
1	G	309	LEU	CA-C-N	5.55	128.03	120.54
1	G	309	LEU	C-N-CA	5.55	128.03	120.54
1	E	65	GLN	CA-C-N	5.48	126.16	120.03
1	E	65	GLN	C-N-CA	5.48	126.16	120.03
1	F	309	LEU	CA-C-N	5.46	129.01	120.82
1	F	309	LEU	C-N-CA	5.46	129.01	120.82
1	D	255	ILE	CA-C-O	-5.45	115.39	121.17
1	A	65	GLN	CA-C-N	5.45	126.15	119.99
1	A	65	GLN	C-N-CA	5.45	126.15	119.99
1	H	452	PRO	CA-N-CD	-5.43	104.39	112.00
1	A	59	HIS	CB-CA-C	5.43	119.74	109.37
1	A	385	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	498	ARG	CB-CA-C	5.37	119.99	109.35
1	C	277	ILE	N-CA-C	-5.36	107.20	111.81
1	H	332	ASP	CA-CB-CG	5.34	117.94	112.60
1	H	452	PRO	N-CA-CB	5.33	108.30	103.34
1	H	195	PHE	CA-C-N	-5.32	115.10	120.31
1	H	195	PHE	C-N-CA	-5.32	115.10	120.31
1	E	426	LEU	CA-C-O	-5.30	115.25	120.98
1	D	34	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	220	SER	CA-C-O	-5.26	115.27	121.16
1	A	88	ASP	CB-CA-C	5.22	118.76	110.19
1	D	184	LYS	CA-C-N	5.22	125.64	120.31
1	D	184	LYS	C-N-CA	5.22	125.64	120.31
1	C	329	ALA	N-CA-C	-5.21	105.68	111.36
1	B	340	SER	O-C-N	5.20	125.39	120.71
1	F	34	ASP	CA-C-N	5.20	129.14	120.62
1	F	34	ASP	C-N-CA	5.20	129.14	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	SER	CA-C-N	5.19	128.20	120.31
1	A	454	SER	C-N-CA	5.19	128.20	120.31
1	D	277	ILE	N-CA-C	-5.19	107.35	111.81
1	D	335	ASP	N-CA-C	-5.17	105.72	112.23
1	C	421	PRO	CB-CA-C	-5.16	104.62	111.23
1	F	346	GLY	CA-C-O	-5.16	116.77	121.47
1	H	85	PHE	CA-C-O	-5.16	114.98	120.40
1	B	236	GLU	CA-C-N	5.15	127.90	120.38
1	B	236	GLU	C-N-CA	5.15	127.90	120.38
1	G	355	THR	CA-CB-OG1	-5.15	101.88	109.60
1	F	15	VAL	N-CA-C	-5.14	107.73	111.90
1	C	380	ARG	CD-NE-CZ	5.14	131.59	124.40
1	E	412	THR	CA-CB-OG1	-5.13	101.90	109.60
1	G	414	ARG	CG-CD-NE	-5.13	100.71	112.00
1	G	453	SER	CA-C-N	5.13	127.15	120.28
1	G	453	SER	C-N-CA	5.13	127.15	120.28
1	H	74	LEU	CA-C-N	5.12	127.40	120.38
1	H	74	LEU	C-N-CA	5.12	127.40	120.38
1	G	308	MET	CA-C-O	-5.12	115.12	120.55
1	A	266	ASP	N-CA-C	-5.12	106.44	113.30
1	H	37	ALA	CA-C-N	5.11	127.09	120.44
1	H	37	ALA	C-N-CA	5.11	127.09	120.44
1	B	241	GLY	CA-C-N	5.11	129.26	120.72
1	B	241	GLY	C-N-CA	5.11	129.26	120.72
1	H	385	GLU	CB-CG-CD	5.09	121.26	112.60
1	B	67	GLU	CB-CA-C	-5.09	102.89	110.88
1	F	37	ALA	CA-C-N	5.09	127.37	120.65
1	F	37	ALA	C-N-CA	5.09	127.37	120.65
1	B	499	THR	CA-CB-OG1	-5.08	101.99	109.60
1	A	28	TYR	CA-C-O	-5.07	115.50	121.07
1	F	416	ILE	CA-C-N	5.05	127.81	120.79
1	F	416	ILE	C-N-CA	5.05	127.81	120.79
1	B	88	ASP	CA-CB-CG	5.04	117.64	112.60
1	G	266	ASP	N-CA-C	-5.04	107.18	113.38

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	3840	0	3887	36	0
1	B	3840	0	3887	32	0
1	C	3840	0	3887	35	0
1	D	3840	0	3887	31	0
1	E	3820	0	3863	57	0
1	F	3840	0	3887	63	0
1	G	3828	0	3874	50	0
1	H	3148	0	3185	44	0
2	A	20	0	10	0	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	0	0
2	F	20	0	10	1	0
2	G	20	0	10	0	0
2	H	20	0	10	0	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	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
4	D	6	0	0	0	0
4	F	6	0	0	0	0
4	G	6	0	0	0	0
4	H	6	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	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	7	0	10	1	0
6	H	7	0	10	5	0
7	B	10	0	14	3	0
7	C	10	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	10	0	14	1	0
7	G	10	0	14	5	0
8	F	13	0	18	5	0
9	A	169	0	0	2	0
9	B	139	0	0	0	0
9	C	103	0	0	4	0
9	D	147	0	0	0	0
9	E	56	0	0	1	0
9	F	101	0	0	2	0
9	G	129	0	0	3	0
9	H	72	0	0	4	0
All	All	31195	0	30531	327	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:LYS:HE3	8:F:605:PG4:H22	1.32	1.11
1:G:368:ASN:HD21	1:G:422:ASN:ND2	1.51	1.06
1:C:1:MET:HE2	1:C:364:GLN:HE21	1.21	1.04
1:A:447:MET:HE1	1:A:469:ALA:HB2	1.41	1.02
1:F:99:PHE:HE2	1:F:125:THR:O	1.48	0.97
1:B:73:LYS:HE3	7:B:605:PGE:H52	1.51	0.93
1:A:311:THR:HG23	1:A:322:GLU:OE1	1.73	0.88
1:A:372:ARG:HG2	1:A:372:ARG:HH11	1.39	0.88
1:F:447:MET:HE1	1:F:469:ALA:HB2	1.59	0.85
1:C:481:VAL:HG13	1:C:492:THR:CG2	2.06	0.84
1:F:481:VAL:CG1	1:F:492:THR:HG21	2.08	0.84
1:H:422:ASN:HB2	9:H:766:HOH:O	1.77	0.82
1:B:481:VAL:CG1	1:B:492:THR:HG21	2.12	0.79
1:A:320:ARG:H	1:D:307:ASN:HD22	1.31	0.79
1:G:368:ASN:ND2	1:G:422:ASN:ND2	2.31	0.79
1:F:73:LYS:CE	8:F:605:PG4:H22	2.12	0.78
1:G:436:ARG:HH12	7:G:605:PGE:H1	1.46	0.78
1:G:481:VAL:HG13	1:G:492:THR:CG2	2.15	0.76
1:E:493:ASN:OD1	1:E:494:THR:HG22	1.86	0.76
1:F:481:VAL:CG1	1:F:492:THR:CG2	2.63	0.76
1:B:307:ASN:HD22	1:C:320:ARG:H	1.34	0.75
1:E:307:ASN:HD22	1:H:320:ARG:H	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:LYS:HE3	8:F:605:PG4:C2	2.14	0.75
1:F:307:ASN:HD22	1:G:320:ARG:H	1.35	0.74
1:A:447:MET:HE1	1:A:469:ALA:CB	2.18	0.73
1:C:481:VAL:HG13	1:C:492:THR:HG21	1.69	0.73
1:G:484:VAL:H	1:G:493:ASN:HD21	1.36	0.73
1:A:307:ASN:HD22	1:D:320:ARG:H	1.37	0.72
1:D:73:LYS:HE3	7:D:605:PGE:H32	1.72	0.72
1:F:320:ARG:H	1:G:307:ASN:HD22	1.37	0.72
1:E:320:ARG:H	1:H:307:ASN:HD22	1.35	0.71
1:H:447:MET:HE1	1:H:469:ALA:HB2	1.72	0.70
1:C:311:THR:HG23	1:C:322:GLU:OE1	1.91	0.70
1:H:92:PRO:HB3	1:H:195:PHE:CG	2.27	0.70
1:F:22:LYS:O	1:F:28:TYR:CD2	2.44	0.69
1:G:73:LYS:HE3	7:G:605:PGE:H4	1.75	0.68
1:G:368:ASN:HD21	1:G:422:ASN:HD21	1.42	0.68
1:C:58:SER:HA	1:C:90:LYS:HG3	1.75	0.68
1:B:481:VAL:HG13	1:B:492:THR:CG2	2.23	0.68
1:F:13:PRO:HB2	1:F:23:PHE:HB2	1.76	0.67
1:H:412:THR:OG1	1:H:492:THR:CG2	2.42	0.67
1:B:320:ARG:H	1:C:307:ASN:HD22	1.43	0.67
1:B:481:VAL:CG1	1:B:492:THR:CG2	2.73	0.66
1:G:311:THR:HG23	1:G:322:GLU:OE1	1.96	0.66
1:F:481:VAL:HG13	1:F:492:THR:CG2	2.25	0.65
1:H:188:ILE:HG22	1:H:191:THR:OG1	1.97	0.65
1:A:372:ARG:HH11	1:A:372:ARG:CG	2.09	0.65
1:A:481:VAL:HG13	1:A:492:THR:CG2	2.27	0.64
1:B:484:VAL:H	1:B:493:ASN:HD21	1.44	0.64
1:E:481:VAL:HG13	1:E:492:THR:CG2	2.27	0.64
1:D:481:VAL:CG1	1:D:492:THR:CG2	2.76	0.64
1:F:73:LYS:CE	8:F:605:PG4:C2	2.73	0.63
1:E:311:THR:HG23	1:E:322:GLU:OE1	1.98	0.63
1:H:457:ASP:OD1	1:H:460:GLU:HG2	1.98	0.63
1:C:447:MET:HE1	1:C:469:ALA:HB2	1.80	0.63
1:A:385:GLU:HG3	1:A:415:LEU:HD22	1.80	0.62
1:B:11:LEU:HD11	1:B:72:VAL:CG2	2.30	0.62
1:H:192:LYS:O	1:H:193:ILE:C	2.42	0.62
1:A:361:LYS:O	1:A:364:GLN:HG2	1.99	0.62
1:B:92:PRO:HB3	1:B:195:PHE:CG	2.35	0.62
1:H:189:PRO:HD2	1:H:189:PRO:O	2.00	0.62
1:F:11:LEU:HD11	1:F:72:VAL:CG2	2.30	0.61
1:F:99:PHE:CE2	1:F:125:THR:O	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:ASN:ND2	1:F:422:ASN:OD1	2.28	0.61
1:F:99:PHE:HE2	1:F:125:THR:C	2.08	0.61
1:F:493:ASN:HD22	1:F:494:THR:N	1.99	0.61
1:C:481:VAL:CG1	1:C:492:THR:HG21	2.31	0.60
1:B:73:LYS:HE3	7:B:605:PGE:C5	2.27	0.60
1:C:496:ARG:HD2	9:C:790:HOH:O	1.99	0.60
1:F:14:ALA:HB2	1:F:345:ASN:HA	1.83	0.60
1:G:481:VAL:HG13	1:G:492:THR:HG21	1.84	0.59
1:E:13:PRO:HB2	1:E:23:PHE:CD1	2.37	0.59
1:G:73:LYS:HE3	7:G:605:PGE:C4	2.31	0.59
1:H:208:PHE:O	1:H:212:GLN:HG2	2.02	0.59
1:E:244:GLN:NE2	1:E:437:GLY:O	2.35	0.59
1:E:208:PHE:O	1:E:212:GLN:HG2	2.03	0.59
1:H:412:THR:OG1	1:H:492:THR:HG21	2.03	0.59
1:F:250:GLU:HG2	1:F:271:ALA:HB3	1.85	0.59
1:B:447:MET:HE1	1:B:469:ALA:HB2	1.85	0.58
1:C:64:GLU:OE2	1:C:68:ARG:NH2	2.36	0.58
1:G:18:ARG:NH2	9:G:702:HOH:O	2.36	0.58
1:A:383:LYS:HA	1:A:386:VAL:HG13	1.84	0.58
1:D:481:VAL:HG13	1:D:492:THR:CG2	2.32	0.58
1:E:148:GLN:HE21	1:E:175:GLU:CD	2.11	0.58
1:H:58:SER:HA	1:H:90:LYS:HG3	1.85	0.58
1:D:481:VAL:HG13	1:D:492:THR:HG23	1.84	0.58
1:E:221:PHE:HD1	1:E:251:ASN:HD22	1.50	0.58
1:D:481:VAL:CG1	1:D:492:THR:HG23	2.33	0.58
1:F:98:LEU:N	1:F:98:LEU:HD23	2.18	0.57
1:D:484:VAL:H	1:D:493:ASN:HD21	1.52	0.57
1:F:493:ASN:HD22	1:F:493:ASN:C	2.12	0.57
1:E:235:CYS:O	1:E:240:ASN:N	2.35	0.57
1:E:90:LYS:HE2	1:E:201:ARG:NH1	2.19	0.57
1:A:11:LEU:HD11	1:A:72:VAL:HG22	1.87	0.57
1:A:481:VAL:CG1	1:A:492:THR:CG2	2.83	0.56
1:E:11:LEU:HD22	1:E:15:VAL:HG21	1.86	0.56
1:H:193:ILE:CG2	1:H:195:PHE:CE2	2.89	0.56
1:F:10:THR:HG22	1:F:344:ALA:HB2	1.87	0.56
1:E:385:GLU:HG3	1:E:415:LEU:HD22	1.86	0.56
1:F:100:GLU:OE1	1:F:125:THR:HG22	2.06	0.56
1:G:368:ASN:ND2	1:G:422:ASN:HD21	1.98	0.56
1:C:458:MET:CE	1:C:484:VAL:HG22	2.36	0.55
1:B:493:ASN:C	1:B:493:ASN:HD22	2.14	0.55
1:A:450:ASP:HB2	1:G:63:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE1	9:C:791:HOH:O	2.05	0.55
1:H:457:ASP:HB3	1:H:460:GLU:HB2	1.89	0.55
1:G:59:HIS:HD2	9:G:807:HOH:O	1.88	0.55
1:C:87:LEU:C	1:C:87:LEU:HD23	2.31	0.55
1:F:447:MET:HE1	1:F:469:ALA:CB	2.33	0.55
1:D:493:ASN:C	1:D:493:ASN:HD22	2.15	0.54
1:F:409:THR:OG1	2:F:601:FBP:O3P	2.21	0.54
1:H:383:LYS:HB3	1:H:491:ARG:CD	2.37	0.54
1:C:481:VAL:HG13	1:C:492:THR:HG23	1.87	0.54
1:A:481:VAL:CG1	1:A:492:THR:HG21	2.38	0.54
1:B:99:PHE:HB2	1:B:103:ALA:O	2.08	0.54
1:E:493:ASN:OD1	1:E:494:THR:CG2	2.54	0.54
1:F:484:VAL:H	1:F:493:ASN:HD21	1.56	0.54
1:D:11:LEU:HD11	1:D:72:VAL:CG2	2.38	0.53
1:F:13:PRO:HA	1:F:16:GLU:HB2	1.91	0.53
1:H:92:PRO:HB3	1:H:195:PHE:CD1	2.42	0.53
1:E:250:GLU:HG3	1:E:271:ALA:HB3	1.90	0.53
1:A:414:ARG:NH2	9:A:703:HOH:O	2.39	0.53
1:E:92:PRO:HB3	1:E:195:PHE:CG	2.42	0.53
1:F:481:VAL:HG12	1:F:492:THR:CG2	2.38	0.53
1:D:250:GLU:HG2	1:D:271:ALA:HB3	1.91	0.53
1:C:106:TYR:CD1	1:C:126:ARG:HG3	2.44	0.52
1:G:159:ARG:O	1:G:172:VAL:HA	2.09	0.52
1:H:412:THR:HG21	1:H:492:THR:HG21	1.90	0.52
1:H:193:ILE:HG21	1:H:195:PHE:CE2	2.44	0.52
1:H:311:THR:HG23	1:H:322:GLU:OE1	2.09	0.52
1:E:481:VAL:CG1	1:E:492:THR:HG21	2.39	0.52
1:G:401:LYS:HG2	1:G:472:VAL:HG12	1.92	0.52
1:D:208:PHE:O	1:D:212:GLN:HG2	2.10	0.52
1:H:213:GLY:C	6:H:605:PEG:H21	2.34	0.52
1:G:481:VAL:HG13	1:G:492:THR:HG23	1.91	0.52
1:F:348:TYR:HB3	1:F:351:GLU:HB2	1.91	0.52
1:G:332:ASP:OD1	1:G:372:ARG:NE	2.40	0.52
1:D:311:THR:HG23	1:D:322:GLU:OE1	2.10	0.51
1:D:332:ASP:OD1	1:D:372:ARG:NE	2.40	0.51
1:E:417:SER:OG	1:E:442:TRP:O	2.27	0.51
1:A:317:ARG:NH1	1:D:276:GLY:O	2.43	0.51
1:H:11:LEU:HD11	1:H:72:VAL:CG2	2.40	0.51
1:G:481:VAL:CG1	1:G:492:THR:HG21	2.41	0.51
1:D:104:LYS:HD3	1:D:182:LYS:HE3	1.93	0.50
1:H:385:GLU:HG3	1:H:415:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:484:VAL:H	1:G:493:ASN:ND2	2.08	0.50
1:G:250:GLU:HG2	1:G:271:ALA:HB3	1.93	0.50
1:G:458:MET:HE2	1:G:486:VAL:HG23	1.94	0.50
1:F:26:ASP:OD2	1:F:26:ASP:N	2.38	0.50
1:F:162:ALA:HB3	1:F:171:GLU:HB2	1.94	0.50
1:C:484:VAL:H	1:C:493:ASN:HD21	1.59	0.50
1:C:493:ASN:C	1:C:493:ASN:HD22	2.19	0.50
1:C:498:ARG:HD3	9:C:790:HOH:O	2.11	0.49
1:E:140:TYR:CE2	1:E:168:ARG:HA	2.47	0.49
1:F:92:PRO:HB3	1:F:195:PHE:CG	2.48	0.49
1:A:474:SER:OG	1:A:501:ARG:OXT	2.30	0.49
1:C:92:PRO:HB3	1:C:195:PHE:CG	2.47	0.49
1:C:497:ILE:HD12	1:D:387:MET:HE2	1.93	0.49
1:B:154:GLY:O	1:C:317:ARG:HD2	2.13	0.49
1:D:481:VAL:CG1	1:D:492:THR:HG21	2.42	0.49
1:G:458:MET:HE1	1:G:483:GLY:O	2.13	0.49
1:E:10:THR:OG1	1:E:54:ARG:NH1	2.41	0.49
1:B:493:ASN:HD22	1:B:494:THR:N	2.10	0.48
1:F:99:PHE:HB3	1:F:103:ALA:HB3	1.95	0.48
1:H:73:LYS:HE3	6:H:605:PEG:C4	2.43	0.48
1:C:474:SER:OG	1:C:501:ARG:OXT	2.31	0.48
1:F:493:ASN:C	1:F:493:ASN:ND2	2.71	0.48
1:G:436:ARG:HH12	7:G:605:PGE:C1	2.21	0.48
1:A:452:PRO:HG2	1:A:458:MET:HE3	1.95	0.48
1:A:481:VAL:HG13	1:A:492:THR:HG23	1.95	0.48
1:G:275:MET:O	1:G:279:VAL:HG22	2.14	0.48
1:H:187:ASN:ND2	1:H:278:GLU:OE1	2.47	0.48
1:B:11:LEU:CD1	1:B:72:VAL:CG2	2.92	0.47
1:H:73:LYS:HE3	6:H:605:PEG:H42	1.96	0.47
1:G:375:SER:HA	1:G:378:PHE:CE2	2.49	0.47
1:C:493:ASN:HD22	1:C:494:THR:N	2.12	0.47
1:B:305:ALA:HB1	1:B:338:MET:HE2	1.97	0.47
1:B:493:ASN:C	1:B:493:ASN:ND2	2.73	0.47
1:F:11:LEU:CD1	1:F:72:VAL:CG2	2.92	0.47
1:F:481:VAL:HG12	1:F:492:THR:HG21	1.90	0.47
1:E:481:VAL:HG13	1:E:492:THR:HG23	1.97	0.46
1:F:275:MET:O	1:F:279:VAL:HG22	2.15	0.46
1:G:242:HIS:CE1	1:G:433:LEU:HD22	2.50	0.46
1:H:375:SER:O	1:H:380:ARG:NH1	2.46	0.46
1:C:380:ARG:HD3	1:D:397:SER:OG	2.14	0.46
1:G:247:ALA:HB3	1:G:268:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:PHE:HD2	1:F:124:SER:O	1.98	0.46
1:G:150:LEU:O	1:G:186:VAL:HA	2.16	0.46
1:E:284:VAL:HB	1:E:285:PRO:HD3	1.98	0.46
1:C:311:THR:HG21	1:C:319:THR:HG23	1.97	0.46
1:C:493:ASN:C	1:C:493:ASN:ND2	2.74	0.46
1:H:1:MET:HB2	9:H:757:HOH:O	2.15	0.46
1:E:384:THR:HG22	1:E:415:LEU:HD12	1.98	0.46
1:A:372:ARG:NH2	1:D:372:ARG:NH2	2.64	0.46
1:E:244:GLN:HA	1:E:266:ASP:OD2	2.16	0.46
1:E:320:ARG:HD3	1:H:272:ARG:C	2.41	0.46
1:H:203:ASN:ND2	1:H:234:ILE:HD11	2.30	0.46
1:B:481:VAL:HG12	1:B:492:THR:HG21	1.95	0.46
1:F:98:LEU:HD23	1:F:98:LEU:H	1.80	0.46
1:F:496:ARG:NH1	9:F:705:HOH:O	2.48	0.46
1:B:106:TYR:CG	1:B:126:ARG:HG3	2.51	0.45
1:E:221:PHE:HD1	1:E:251:ASN:ND2	2.14	0.45
1:H:213:GLY:HA3	6:H:605:PEG:H22	1.98	0.45
1:F:73:LYS:HE2	8:F:605:PG4:C2	2.46	0.45
1:D:247:ALA:HB3	1:D:268:ILE:HD13	1.98	0.45
1:E:6:LYS:O	1:E:336:ALA:HA	2.15	0.45
1:F:143:VAL:HG13	1:F:170:PHE:CZ	2.51	0.45
1:F:345:ASN:HD22	1:F:345:ASN:C	2.22	0.45
1:F:372:ARG:HH11	1:G:372:ARG:NH2	2.14	0.45
1:G:59:HIS:CD2	9:G:807:HOH:O	2.66	0.45
1:H:412:THR:CG2	1:H:492:THR:HG21	2.47	0.45
1:F:99:PHE:CE2	1:F:125:THR:C	2.91	0.45
1:F:108:TYR:N	1:F:108:TYR:CD2	2.84	0.45
1:E:246:PHE:CE2	1:E:440:LEU:HD12	2.51	0.45
1:E:481:VAL:CG1	1:E:492:THR:CG2	2.92	0.45
1:A:159:ARG:O	1:A:172:VAL:HA	2.16	0.45
1:E:58:SER:HA	1:E:90:LYS:HB2	1.99	0.44
1:B:73:LYS:CE	7:B:605:PGE:H52	2.34	0.44
1:F:250:GLU:CG	1:F:271:ALA:HB3	2.47	0.44
1:G:484:VAL:CG2	1:H:496:ARG:NH2	2.80	0.44
1:D:106:TYR:CD1	1:D:126:ARG:HG3	2.53	0.44
1:E:142:ASP:CG	1:E:194:PRO:HD3	2.42	0.44
1:E:207:ARG:O	1:E:211:GLU:HG3	2.17	0.44
1:E:246:PHE:HE2	1:E:440:LEU:CD1	2.30	0.44
1:A:11:LEU:HD11	1:A:72:VAL:CG2	2.47	0.44
1:C:332:ASP:OD1	1:C:372:ARG:NE	2.51	0.44
1:B:311:THR:HG23	1:B:322:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:MET:HE1	1:G:469:ALA:HB2	1.99	0.44
1:G:6:LYS:O	1:G:336:ALA:HA	2.18	0.44
1:A:372:ARG:CG	1:A:372:ARG:NH1	2.75	0.44
1:A:380:ARG:NH2	1:A:389:SER:OG	2.46	0.44
1:E:375:SER:HA	1:E:378:PHE:CE2	2.51	0.44
1:A:383:LYS:HG2	9:A:830:HOH:O	2.17	0.43
1:B:447:MET:HE1	1:B:469:ALA:CB	2.47	0.43
1:F:100:GLU:HG2	1:F:101:GLY:N	2.33	0.43
1:F:414:ARG:NH2	9:F:706:HOH:O	2.49	0.43
1:D:493:ASN:HD22	1:D:494:THR:N	2.16	0.43
1:F:372:ARG:NH1	1:G:372:ARG:NH2	2.66	0.43
1:A:11:LEU:CD1	1:A:72:VAL:CG2	2.96	0.43
1:D:484:VAL:H	1:D:493:ASN:ND2	2.15	0.43
1:E:3:LYS:HG2	1:E:5:VAL:O	2.19	0.43
1:E:246:PHE:HE2	1:E:440:LEU:HD12	1.83	0.43
1:E:250:GLU:OE1	1:E:274:ASP:OD1	2.36	0.43
1:E:415:LEU:HD23	1:E:415:LEU:HA	1.91	0.43
1:E:92:PRO:HB3	1:E:195:PHE:CD1	2.54	0.43
1:A:107:SER:O	1:A:126:ARG:NH1	2.51	0.43
1:C:311:THR:HG21	1:C:319:THR:CG2	2.49	0.43
1:H:94:ILE:HG22	1:H:186:VAL:HB	2.01	0.43
1:H:412:THR:OG1	1:H:492:THR:HG23	2.16	0.43
1:D:312:MET:HA	1:D:315:LYS:O	2.19	0.43
1:F:3:LYS:HE3	1:F:3:LYS:HB3	1.80	0.43
1:G:211:GLU:HG2	1:G:212:GLN:HE21	1.84	0.43
1:C:148:GLN:HE21	1:C:175:GLU:CD	2.26	0.43
1:F:99:PHE:CD2	1:F:124:SER:O	2.72	0.43
1:G:368:ASN:CG	1:G:422:ASN:HD21	2.26	0.43
1:C:213:GLY:CA	7:C:605:PGE:H52	2.49	0.42
1:D:453:SER:C	1:D:455:THR:H	2.27	0.42
1:E:270:ILE:HG23	1:E:275:MET:HE1	2.01	0.42
1:H:492:THR:HG23	9:H:738:HOH:O	2.18	0.42
1:E:272:ARG:CB	1:H:320:ARG:HG2	2.49	0.42
1:G:361:LYS:O	1:G:364:GLN:HG2	2.19	0.42
1:E:148:GLN:NE2	1:E:175:GLU:OE2	2.51	0.42
1:F:115:ARG:HA	1:F:170:PHE:O	2.20	0.42
1:G:73:LYS:CE	7:G:605:PGE:H4	2.47	0.42
1:E:250:GLU:CG	1:E:271:ALA:HB3	2.49	0.42
1:E:275:MET:O	1:E:279:VAL:HG22	2.19	0.42
1:F:311:THR:HG23	1:F:322:GLU:OE1	2.20	0.42
1:G:332:ASP:OD1	1:G:372:ARG:NH1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:SER:OG	1:D:501:ARG:OXT	2.37	0.42
1:F:372:ARG:NH1	1:G:370:TYR:O	2.51	0.42
1:G:115:ARG:NH1	1:G:169:GLU:OE2	2.53	0.42
1:H:22:LYS:O	1:H:28:TYR:CD2	2.73	0.42
1:B:208:PHE:O	1:B:212:GLN:HG2	2.20	0.42
1:C:404:VAL:HG11	1:C:462:ALA:HB1	2.01	0.42
1:D:348:TYR:N	1:D:349:PRO:CD	2.83	0.42
1:F:465:LYS:HA	1:F:465:LYS:HD2	1.91	0.42
1:H:11:LEU:CD1	1:H:72:VAL:CG2	2.97	0.42
1:D:447:MET:HE3	1:D:447:MET:HB2	1.91	0.42
1:G:45:LEU:HD22	1:G:350:LEU:HA	2.02	0.42
1:A:102:GLU:O	1:A:104:LYS:HE3	2.20	0.42
1:A:375:SER:O	1:A:380:ARG:NH1	2.53	0.42
1:B:5:VAL:HG21	1:B:330:VAL:HG13	2.01	0.42
1:E:99:PHE:HB2	1:E:103:ALA:O	2.20	0.42
1:G:144:GLU:OE2	1:G:144:GLU:N	2.52	0.42
1:E:387:MET:O	1:E:391:VAL:HG23	2.19	0.41
1:E:273:GLY:CA	1:E:306:THR:HG21	2.50	0.41
1:E:481:VAL:HG13	1:E:492:THR:HG21	1.99	0.41
1:C:368:ASN:HB2	9:C:754:HOH:O	2.19	0.41
1:E:361:LYS:O	1:E:364:GLN:HG2	2.19	0.41
1:F:240:ASN:HA	1:F:242:HIS:CE1	2.55	0.41
1:G:484:VAL:HG22	1:G:494:THR:OG1	2.19	0.41
1:H:279:VAL:O	1:H:280:PRO:C	2.62	0.41
1:B:383:LYS:HA	1:B:386:VAL:HG13	2.02	0.41
1:B:485:PRO:HD2	1:B:488:GLU:CG	2.50	0.41
1:C:5:VAL:HG21	1:C:330:VAL:HG22	2.03	0.41
1:F:310:GLU:OE1	1:F:310:GLU:HA	2.20	0.41
1:A:372:ARG:HG2	1:A:372:ARG:NH1	2.14	0.41
1:A:433:LEU:HD21	6:A:605:PEG:H41	2.03	0.41
1:G:493:ASN:C	1:G:493:ASN:HD22	2.26	0.41
1:H:383:LYS:HB3	1:H:491:ARG:HD3	2.02	0.41
1:A:10:THR:HG22	1:A:344:ALA:HB2	2.01	0.41
1:A:366:LEU:HD23	1:A:370:TYR:CE2	2.56	0.41
1:C:38:SER:O	1:C:41:ASN:HB2	2.20	0.41
1:E:98:LEU:HA	1:E:182:LYS:HB2	2.02	0.41
1:F:312:MET:HE3	1:F:316:PRO:O	2.20	0.41
1:H:91:GLY:HA2	1:H:202:ASP:OD2	2.21	0.41
1:F:361:LYS:O	1:F:364:GLN:HG2	2.20	0.41
1:B:485:PRO:HD2	1:B:488:GLU:HG2	2.02	0.41
1:E:159:ARG:O	1:E:172:VAL:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ILE:HA	1:G:194:PRO:HD3	1.91	0.41
1:F:11:LEU:HD11	1:F:72:VAL:HG22	2.01	0.41
1:A:13:PRO:HA	1:A:16:GLU:HB2	2.03	0.40
1:D:218:ALA:HA	1:D:246:PHE:O	2.21	0.40
1:E:145:VAL:HA	1:E:160:VAL:HG12	2.03	0.40
1:E:272:ARG:HB3	1:H:320:ARG:CG	2.51	0.40
1:H:193:ILE:HG22	1:H:195:PHE:CE2	2.56	0.40
1:B:384:THR:OG1	2:B:601:FBP:O5P	2.27	0.40
1:E:447:MET:HE1	1:E:469:ALA:HB2	2.03	0.40
6:H:605:PEG:H11	9:H:768:HOH:O	2.21	0.40
1:D:98:LEU:HD23	1:D:182:LYS:HG3	2.03	0.40
1:G:11:LEU:HD11	1:G:72:VAL:CG2	2.52	0.40
1:B:11:LEU:HD11	1:B:72:VAL:HG21	2.02	0.40
1:E:418:LYS:NZ	9:E:703:HOH:O	2.54	0.40
1:A:386:VAL:HG11	1:B:398:MET:SD	2.62	0.40
1:B:457:ASP:HB3	1:B:460:GLU:HB2	2.03	0.40
1:E:9:ALA:O	1:E:53:PHE:HA	2.21	0.40
1:F:368:ASN:HD22	1:F:368:ASN:HA	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/521 (96%)	484 (97%)	14 (3%)	1 (0%)	43	42
1	B	499/521 (96%)	488 (98%)	9 (2%)	2 (0%)	30	27
1	C	499/521 (96%)	482 (97%)	15 (3%)	2 (0%)	30	27
1	D	499/521 (96%)	484 (97%)	14 (3%)	1 (0%)	43	42
1	E	497/521 (95%)	462 (93%)	32 (6%)	3 (1%)	21	17
1	F	499/521 (96%)	468 (94%)	28 (6%)	3 (1%)	21	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	498/521 (96%)	485 (97%)	12 (2%)	1 (0%)	43	42
1	H	408/521 (78%)	392 (96%)	13 (3%)	3 (1%)	18	14
All	All	3898/4168 (94%)	3745 (96%)	137 (4%)	16 (0%)	30	27

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	189	PRO
1	E	237	GLU
1	F	306	THR
1	G	306	THR
1	A	306	THR
1	B	306	THR
1	D	306	THR
1	E	306	THR
1	H	306	THR
1	C	306	THR
1	F	345	ASN
1	H	31	GLU
1	B	152	ASP
1	E	152	ASP
1	C	28	TYR
1	F	92	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/428 (96%)	390 (95%)	21 (5%)	21	19
1	B	411/428 (96%)	391 (95%)	20 (5%)	22	20
1	C	411/428 (96%)	382 (93%)	29 (7%)	13	10
1	D	411/428 (96%)	388 (94%)	23 (6%)	19	16
1	E	409/428 (96%)	387 (95%)	22 (5%)	20	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	411/428 (96%)	387 (94%)	24 (6%)	18	15
1	G	410/428 (96%)	388 (95%)	22 (5%)	20	17
1	H	338/428 (79%)	309 (91%)	29 (9%)	10	6
All	All	3212/3424 (94%)	3022 (94%)	190 (6%)	18	14

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	31	GLU
1	A	32	LYS
1	A	74	LEU
1	A	143	VAL
1	A	182	LYS
1	A	226	LYS
1	A	236	GLU
1	A	293	LYS
1	A	317	ARG
1	A	361	LYS
1	A	372	ARG
1	A	380	ARG
1	A	383	LYS
1	A	386	VAL
1	A	405	THR
1	A	450	ASP
1	A	453	SER
1	A	474	SER
1	A	496	ARG
1	A	498	ARG
1	B	22	LYS
1	B	26	ASP
1	B	63	GLN
1	B	74	LEU
1	B	127	GLU
1	B	137	LEU
1	B	143	VAL
1	B	182	LYS
1	B	211	GLU
1	B	279	VAL
1	B	290	MET
1	B	317	ARG

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Mol	Chain	Res	Type
1	B	366	LEU
1	B	380	ARG
1	B	386	VAL
1	B	387	MET
1	B	439	MET
1	B	460	GLU
1	B	484	VAL
1	B	493	ASN
1	C	1	MET
1	C	22	LYS
1	C	26	ASP
1	C	74	LEU
1	C	137	LEU
1	C	143	VAL
1	C	182	LYS
1	C	201	ARG
1	C	226	LYS
1	C	227	ASP
1	C	236	GLU
1	C	263	GLU
1	C	279	VAL
1	C	290	MET
1	C	334	THR
1	C	345	ASN
1	C	361	LYS
1	C	379	GLU
1	C	380	ARG
1	C	439	MET
1	C	449	THR
1	C	450	ASP
1	C	458	MET
1	C	474	SER
1	C	481	VAL
1	C	490	VAL
1	C	493	ASN
1	C	496	ARG
1	C	501	ARG
1	D	1	MET
1	D	11	LEU
1	D	81	LYS
1	D	95	ARG
1	D	102	GLU

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Mol	Chain	Res	Type
1	D	143	VAL
1	D	147	ARG
1	D	153	ASP
1	D	182	LYS
1	D	226	LYS
1	D	236	GLU
1	D	293	LYS
1	D	334	THR
1	D	366	LEU
1	D	386	VAL
1	D	422	ASN
1	D	439	MET
1	D	449	THR
1	D	454	SER
1	D	455	THR
1	D	474	SER
1	D	486	VAL
1	D	493	ASN
1	E	15	VAL
1	E	22	LYS
1	E	26	ASP
1	E	74	LEU
1	E	81	LYS
1	E	90	LYS
1	E	95	ARG
1	E	137	LEU
1	E	182	LYS
1	E	192	LYS
1	E	334	THR
1	E	345	ASN
1	E	366	LEU
1	E	379	GLU
1	E	405	THR
1	E	439	MET
1	E	449	THR
1	E	460	GLU
1	E	486	VAL
1	E	488	GLU
1	E	494	THR
1	E	498	ARG
1	F	1	MET
1	F	26	ASP

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Mol	Chain	Res	Type
1	F	31	GLU
1	F	32	LYS
1	F	47	GLU
1	F	52	THR
1	F	81	LYS
1	F	98	LEU
1	F	100	GLU
1	F	102	GLU
1	F	104	LYS
1	F	108	TYR
1	F	143	VAL
1	F	182	LYS
1	F	226	LYS
1	F	236	GLU
1	F	260	GLU
1	F	345	ASN
1	F	361	LYS
1	F	380	ARG
1	F	405	THR
1	F	474	SER
1	F	493	ASN
1	F	496	ARG
1	G	143	VAL
1	G	153	ASP
1	G	182	LYS
1	G	200	GLU
1	G	211	GLU
1	G	236	GLU
1	G	314	GLU
1	G	334	THR
1	G	345	ASN
1	G	366	LEU
1	G	376	ASP
1	G	386	VAL
1	G	396	SER
1	G	431	ASP
1	G	439	MET
1	G	456	ASP
1	G	458	MET
1	G	481	VAL
1	G	484	VAL
1	G	490	VAL

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Mol	Chain	Res	Type
1	G	493	ASN
1	G	496	ARG
1	H	1	MET
1	H	22	LYS
1	H	40	LYS
1	H	74	LEU
1	H	81	LYS
1	H	90	LYS
1	H	95	ARG
1	H	187	ASN
1	H	191	THR
1	H	226	LYS
1	H	236	GLU
1	H	279	VAL
1	H	293	LYS
1	H	321	SER
1	H	334	THR
1	H	345	ASN
1	H	347	LYS
1	H	361	LYS
1	H	380	ARG
1	H	386	VAL
1	H	422	ASN
1	H	439	MET
1	H	449	THR
1	H	455	THR
1	H	473	GLU
1	H	481	VAL
1	H	486	VAL
1	H	492	THR
1	H	496	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	A	345	ASN
1	A	368	ASN
1	A	381	ASN
1	B	307	ASN
1	B	362	ASN
1	B	493	ASN

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Mol	Chain	Res	Type
1	C	183	GLN
1	C	190	ASN
1	C	307	ASN
1	C	364	GLN
1	C	381	ASN
1	C	441	ASN
1	C	493	ASN
1	D	187	ASN
1	D	190	ASN
1	D	307	ASN
1	D	345	ASN
1	D	362	ASN
1	D	368	ASN
1	D	381	ASN
1	D	493	ASN
1	E	148	GLN
1	E	307	ASN
1	E	368	ASN
1	E	381	ASN
1	E	441	ASN
1	F	59	HIS
1	F	242	HIS
1	F	253	GLN
1	F	307	ASN
1	F	362	ASN
1	F	493	ASN
1	G	183	GLN
1	G	190	ASN
1	G	212	GLN
1	G	252	GLN
1	G	307	ASN
1	G	422	ASN
1	G	493	ASN
1	H	187	ASN
1	H	190	ASN
1	H	253	GLN
1	H	307	ASN
1	H	381	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 14 are monoatomic - leaving 22 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	B	601	-	18,20,20	0.99	1 (5%)	21,32,32	1.35	2 (9%)
4	OXL	C	603	3	5,5,5	1.57	1 (20%)	6,6,6	1.27	0
4	OXL	A	603	3	5,5,5	2.29	2 (40%)	6,6,6	1.98	2 (33%)
7	PGE	B	605	-	9,9,9	0.25	0	8,8,8	0.35	0
2	FBP	D	601	-	18,20,20	1.12	1 (5%)	21,32,32	1.06	1 (4%)
7	PGE	D	605	-	9,9,9	0.47	0	8,8,8	0.26	0
6	PEG	A	605	-	6,6,6	0.27	0	5,5,5	0.25	0
2	FBP	E	601	-	18,20,20	0.96	1 (5%)	21,32,32	1.33	3 (14%)
4	OXL	D	603	3	5,5,5	2.14	2 (40%)	6,6,6	0.82	0
7	PGE	G	605	-	9,9,9	0.34	0	8,8,8	0.44	0
8	PG4	F	605	-	12,12,12	0.33	0	11,11,11	0.38	0
4	OXL	B	603	3	5,5,5	1.31	0	6,6,6	2.18	4 (66%)
2	FBP	G	601	-	18,20,20	0.83	1 (5%)	21,32,32	1.29	3 (14%)
2	FBP	A	601	-	18,20,20	0.81	0	21,32,32	1.58	5 (23%)
2	FBP	C	601	-	18,20,20	0.92	0	21,32,32	1.42	2 (9%)
2	FBP	H	601	-	18,20,20	0.83	0	21,32,32	1.75	5 (23%)
7	PGE	C	605	-	9,9,9	0.40	0	8,8,8	0.34	0
4	OXL	H	603	3	5,5,5	1.44	1 (20%)	6,6,6	2.16	4 (66%)
4	OXL	F	603	3	5,5,5	1.60	1 (20%)	6,6,6	1.69	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	H	605	-	6,6,6	0.52	0	5,5,5	0.28	0
2	FBP	F	601	-	18,20,20	0.92	0	21,32,32	1.43	3 (14%)
4	OXL	G	603	3	5,5,5	1.74	1 (20%)	6,6,6	1.58	1 (16%)

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	B	601	-	-	3/13/32/32	0/1/1/1
4	OXL	C	603	3	-	4/4/4/4	-
4	OXL	A	603	3	-	4/4/4/4	-
7	PGE	B	605	-	-	5/7/7/7	-
2	FBP	D	601	-	-	6/13/32/32	0/1/1/1
7	PGE	D	605	-	-	4/7/7/7	-
6	PEG	A	605	-	-	3/4/4/4	-
2	FBP	E	601	-	-	3/13/32/32	0/1/1/1
4	OXL	D	603	3	-	4/4/4/4	-
7	PGE	G	605	-	-	4/7/7/7	-
8	PG4	F	605	-	-	5/10/10/10	-
4	OXL	B	603	3	-	4/4/4/4	-
2	FBP	G	601	-	-	5/13/32/32	0/1/1/1
2	FBP	A	601	-	-	5/13/32/32	0/1/1/1
2	FBP	C	601	-	-	4/13/32/32	0/1/1/1
2	FBP	H	601	-	-	5/13/32/32	0/1/1/1
7	PGE	C	605	-	-	6/7/7/7	-
4	OXL	H	603	3	-	4/4/4/4	-
4	OXL	F	603	3	-	4/4/4/4	-
6	PEG	H	605	-	-	3/4/4/4	-
2	FBP	F	601	-	-	4/13/32/32	0/1/1/1
4	OXL	G	603	3	-	4/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	OXL	C2-C1	3.91	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	OXL	O4-C2	-2.83	1.22	1.30
4	D	603	OXL	O4-C2	-2.78	1.23	1.30
2	D	601	FBP	O2-C2	2.76	1.45	1.40
2	B	601	FBP	P1-O3P	-2.60	1.45	1.54
4	D	603	OXL	C2-C1	2.52	1.59	1.54
4	A	603	OXL	O3-C1	-2.49	1.23	1.30
4	H	603	OXL	O3-C1	-2.42	1.24	1.30
2	E	601	FBP	P1-O3P	-2.29	1.46	1.54
2	G	601	FBP	O2-C2	2.18	1.44	1.40
4	F	603	OXL	O3-C1	-2.11	1.24	1.30
4	G	603	OXL	O1-C1	2.09	1.27	1.22

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FBP	O2P-P1-O1	-4.07	96.06	106.67
2	B	601	FBP	O5P-P2-O6	-4.03	96.17	106.67
2	H	601	FBP	O5P-P2-O6	-4.02	96.19	106.67
2	A	601	FBP	O6-P2-O4P	-3.56	96.82	106.44
2	E	601	FBP	O6P-P2-O5P	3.44	120.70	107.80
2	H	601	FBP	O5P-P2-O4P	3.39	124.06	110.83
4	B	603	OXL	O3-C1-C2	3.24	119.11	112.83
2	F	601	FBP	O3P-P1-O2P	3.22	119.88	107.80
2	H	601	FBP	O3P-P1-O1	-3.18	98.36	106.67
4	A	603	OXL	O3-C1-C2	3.06	118.77	112.83
4	H	603	OXL	O4-C2-C1	2.96	118.58	112.83
2	A	601	FBP	O3P-P1-O2P	2.87	118.57	107.80
2	C	601	FBP	O6P-P2-O6	-2.85	99.23	106.67
2	A	601	FBP	O2-C2-O5	-2.85	103.86	109.33
4	A	603	OXL	O4-C2-C1	2.83	118.31	112.83
2	H	601	FBP	O3P-P1-O1P	2.81	121.77	110.83
2	E	601	FBP	O6-P2-O4P	-2.79	98.90	106.44
4	B	603	OXL	O4-C2-C1	2.78	118.22	112.83
4	H	603	OXL	O3-C1-C2	2.61	117.89	112.83
4	H	603	OXL	O2-C2-C1	-2.57	115.28	120.63
2	D	601	FBP	O3P-P1-O2P	2.33	116.55	107.80
4	G	603	OXL	O4-C2-C1	2.33	117.34	112.83
4	F	603	OXL	O3-C1-C2	2.32	117.33	112.83
2	F	601	FBP	O2-C2-O5	-2.31	104.89	109.33
2	A	601	FBP	O6P-P2-O4P	2.31	119.82	110.83
2	G	601	FBP	O5P-P2-O6	2.30	112.66	106.67
4	B	603	OXL	O1-C1-C2	-2.30	115.85	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	FBP	O6P-P2-O6	-2.23	100.85	106.67
2	H	601	FBP	O3-C3-C4	-2.22	105.42	113.25
4	F	603	OXL	O4-C2-C1	2.19	117.07	112.83
2	F	601	FBP	O4-C4-C3	-2.15	105.71	112.16
2	G	601	FBP	O2P-P1-O1	2.11	112.17	106.67
4	B	603	OXL	O2-C2-C1	-2.11	116.24	120.63
2	A	601	FBP	O2P-P1-O1	-2.09	101.22	106.67
4	H	603	OXL	O1-C1-C2	-2.08	116.30	120.63
2	B	601	FBP	O6P-P2-O5P	2.07	115.55	107.80
2	E	601	FBP	O2P-P1-O1	-2.01	101.43	106.67

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	B	601	FBP	O1-C1-C2-C3
2	B	601	FBP	O1-C1-C2-O5
2	C	601	FBP	O1-C1-C2-C3
2	D	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C1-O1-P1-O2P
2	D	601	FBP	O1-C1-C2-C3
2	D	601	FBP	O1-C1-C2-O5
2	E	601	FBP	O1-C1-C2-O2
2	E	601	FBP	O1-C1-C2-C3
2	E	601	FBP	O1-C1-C2-O5
2	F	601	FBP	C1-O1-P1-O2P
2	F	601	FBP	O1-C1-C2-O2
2	F	601	FBP	O1-C1-C2-C3
2	F	601	FBP	O1-C1-C2-O5
2	G	601	FBP	C1-O1-P1-O1P
2	G	601	FBP	O1-C1-C2-C3
2	G	601	FBP	O1-C1-C2-O5
2	H	601	FBP	C1-O1-P1-O2P
2	H	601	FBP	O1-C1-C2-C3
2	H	601	FBP	O1-C1-C2-O5
7	B	605	PGE	O2-C3-C4-O3
8	F	605	PG4	O3-C5-C6-O4
7	G	605	PGE	O2-C3-C4-O3
7	B	605	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	F	603	OXL	O1-C1-C2-O2
7	B	605	PGE	O3-C5-C6-O4
7	D	605	PGE	O2-C3-C4-O3
4	F	603	OXL	O3-C1-C2-O2
7	C	605	PGE	O2-C3-C4-O3
6	A	605	PEG	O1-C1-C2-O2
7	C	605	PGE	O1-C1-C2-O2
4	F	603	OXL	O3-C1-C2-O4
8	F	605	PG4	O2-C3-C4-O3
7	D	605	PGE	O1-C1-C2-O2
4	F	603	OXL	O1-C1-C2-O4
7	D	605	PGE	C4-C3-O2-C2
6	H	605	PEG	O1-C1-C2-O2
7	G	605	PGE	O3-C5-C6-O4
7	C	605	PGE	C1-C2-O2-C3
2	H	601	FBP	C1-O1-P1-O1P
4	C	603	OXL	O3-C1-C2-O4
8	F	605	PG4	C5-C6-O4-C7
6	A	605	PEG	C4-C3-O2-C2
7	C	605	PGE	C4-C3-O2-C2
4	C	603	OXL	O1-C1-C2-O2
4	D	603	OXL	O3-C1-C2-O4
4	H	603	OXL	O3-C1-C2-O4
7	C	605	PGE	C6-C5-O3-C4
6	H	605	PEG	C4-C3-O2-C2
7	B	605	PGE	C4-C3-O2-C2
4	A	603	OXL	O3-C1-C2-O4
4	B	603	OXL	O3-C1-C2-O4
4	G	603	OXL	O3-C1-C2-O4
7	D	605	PGE	C6-C5-O3-C4
4	D	603	OXL	O1-C1-C2-O2
4	H	603	OXL	O1-C1-C2-O2
6	H	605	PEG	C1-C2-O2-C3
8	F	605	PG4	C4-C3-O2-C2
4	G	603	OXL	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-O2
2	B	601	FBP	O1-C1-C2-O2
2	C	601	FBP	O1-C1-C2-O2
2	D	601	FBP	O1-C1-C2-O2
2	G	601	FBP	O1-C1-C2-O2
2	H	601	FBP	O1-C1-C2-O2
4	A	603	OXL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	603	OXL	O1-C1-C2-O2
7	G	605	PGE	C3-C4-O3-C5
2	C	601	FBP	C1-O1-P1-O1P
7	B	605	PGE	C3-C4-O3-C5
7	C	605	PGE	C3-C4-O3-C5
4	C	603	OXL	O1-C1-C2-O4
4	C	603	OXL	O3-C1-C2-O2
4	D	603	OXL	O3-C1-C2-O2
4	B	603	OXL	O1-C1-C2-O4
4	G	603	OXL	O1-C1-C2-O4
4	H	603	OXL	O1-C1-C2-O4
7	G	605	PGE	C1-C2-O2-C3
4	A	603	OXL	O1-C1-C2-O4
4	D	603	OXL	O1-C1-C2-O4
4	H	603	OXL	O3-C1-C2-O2
4	A	603	OXL	O3-C1-C2-O2
4	B	603	OXL	O3-C1-C2-O2
4	G	603	OXL	O3-C1-C2-O2
8	F	605	PG4	C3-C4-O3-C5
2	A	601	FBP	C1-O1-P1-O3P
2	C	601	FBP	C1-O1-P1-O3P
2	D	601	FBP	C1-O1-P1-O3P
2	G	601	FBP	C1-O1-P1-O2P
6	A	605	PEG	O2-C3-C4-O4

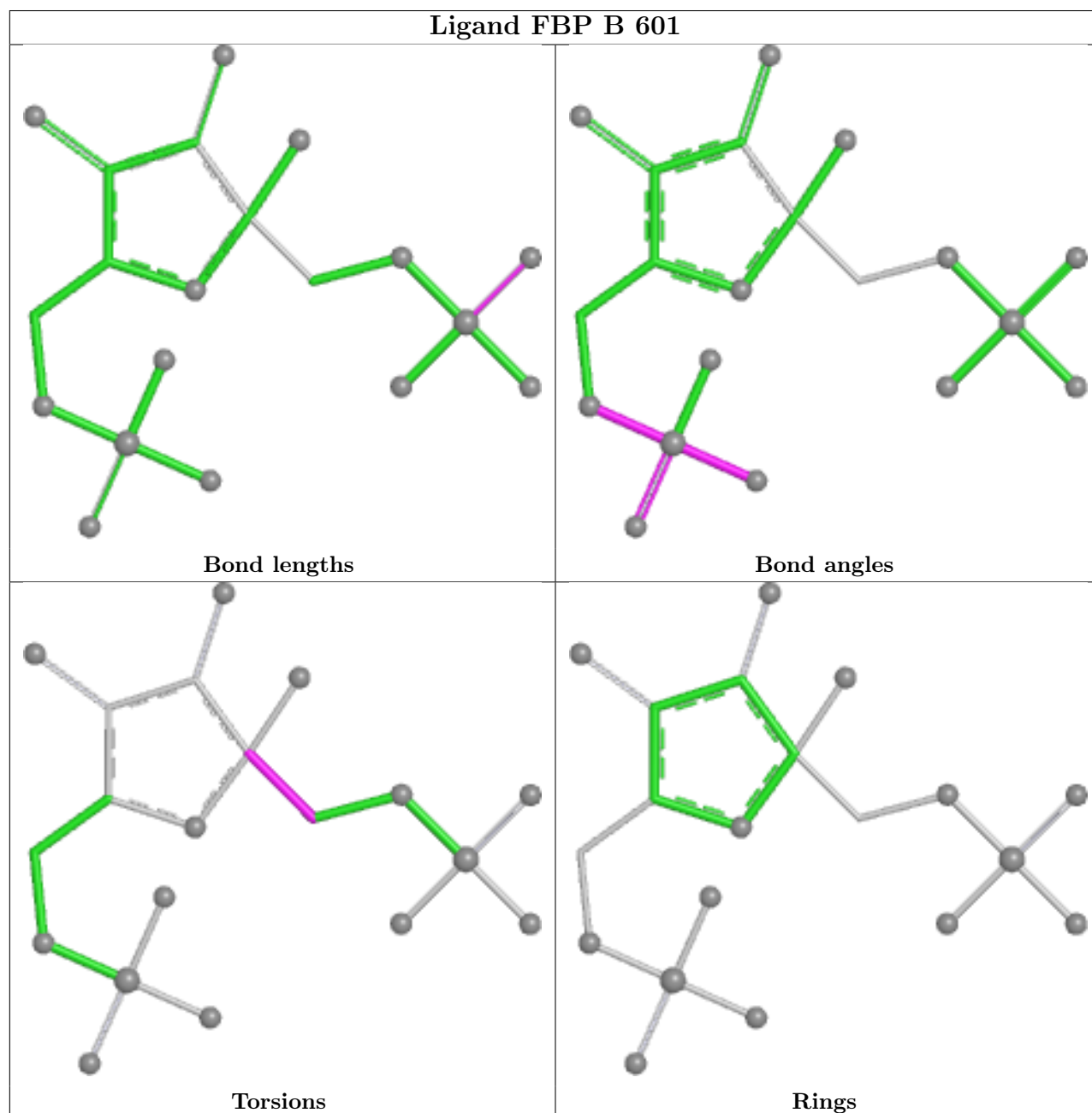
There are no ring outliers.

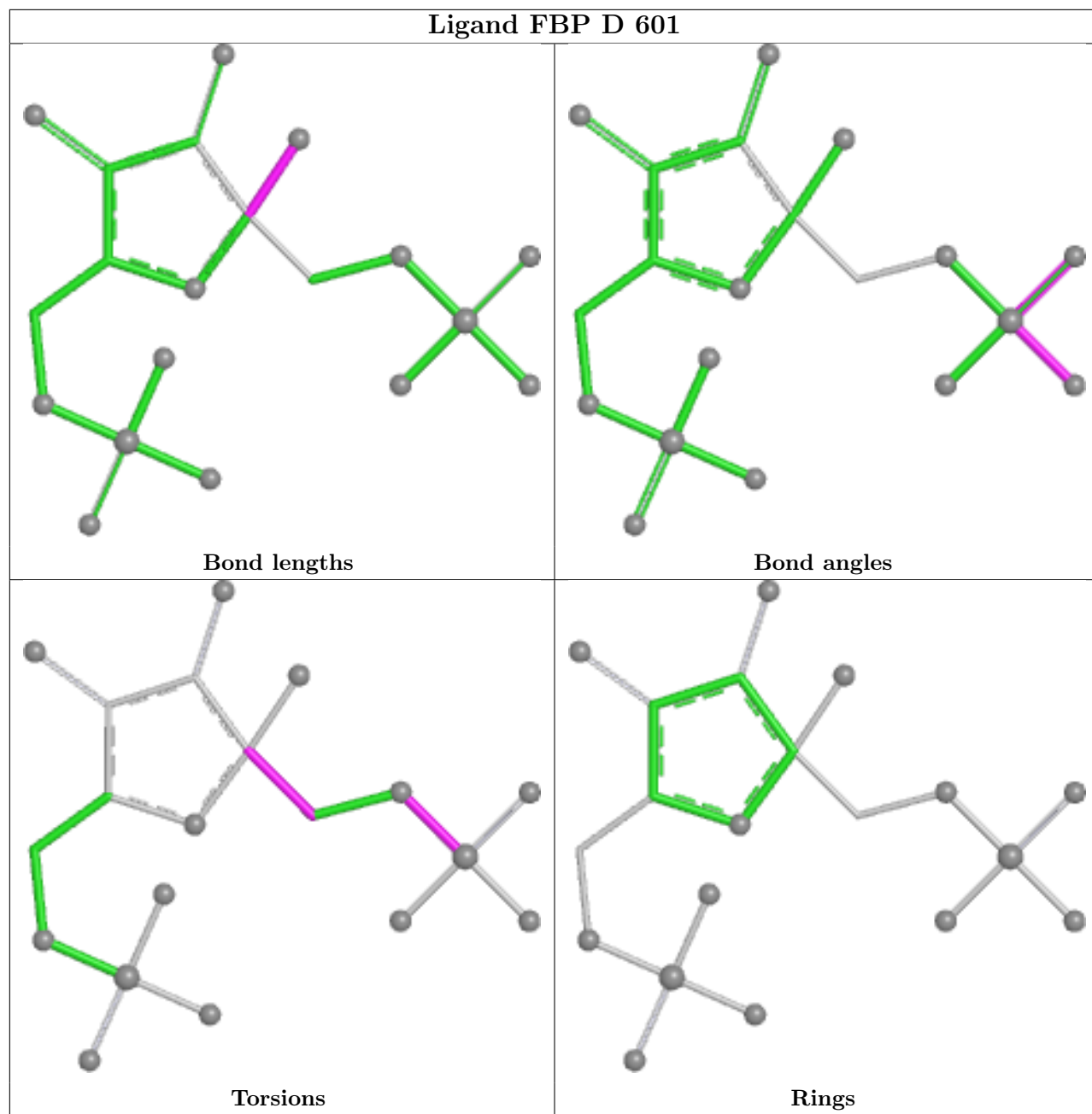
9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FBP	1	0
7	B	605	PGE	3	0
7	D	605	PGE	1	0
6	A	605	PEG	1	0
7	G	605	PGE	5	0
8	F	605	PG4	5	0
7	C	605	PGE	1	0
6	H	605	PEG	5	0
2	F	601	FBP	1	0

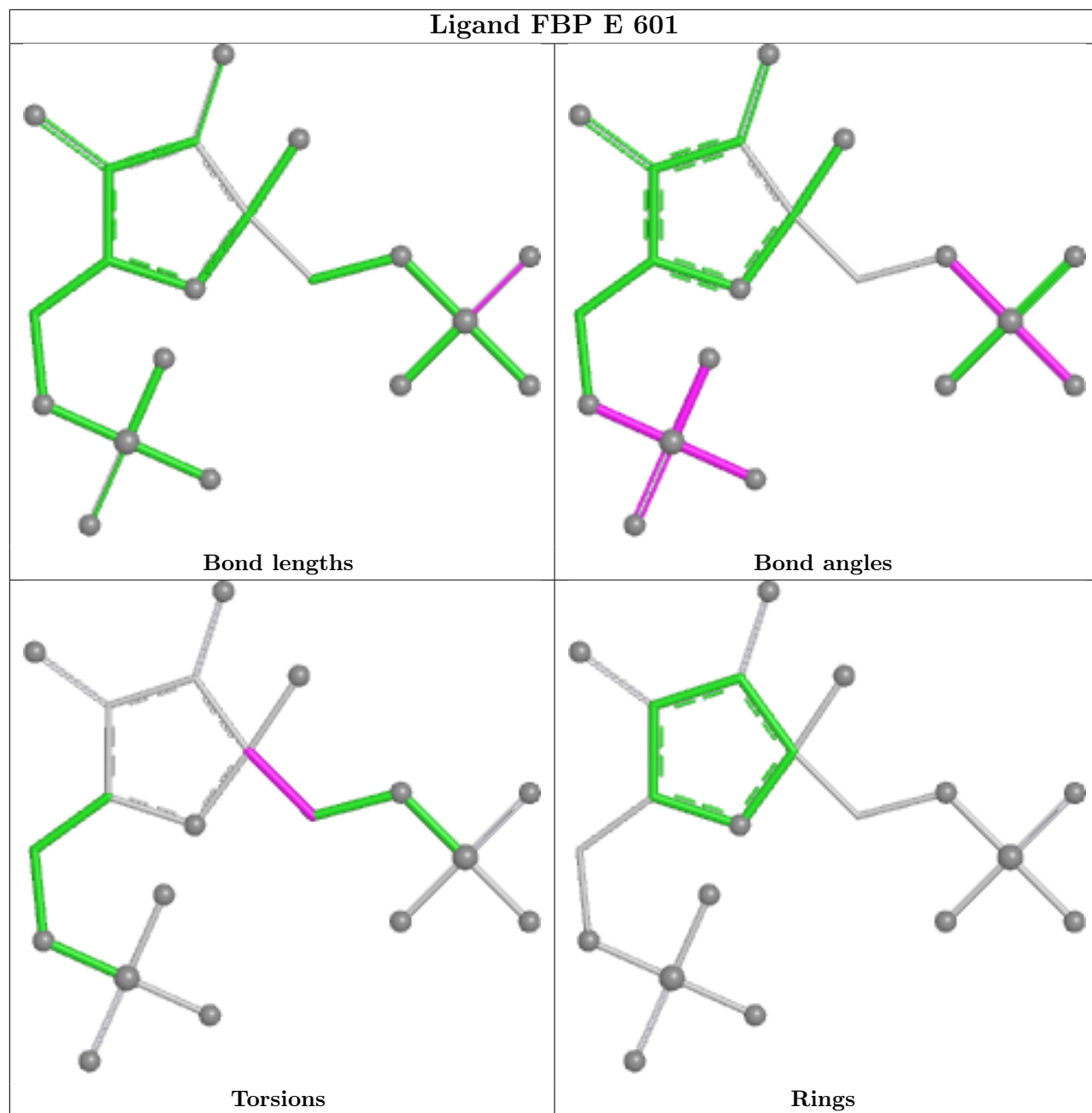
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

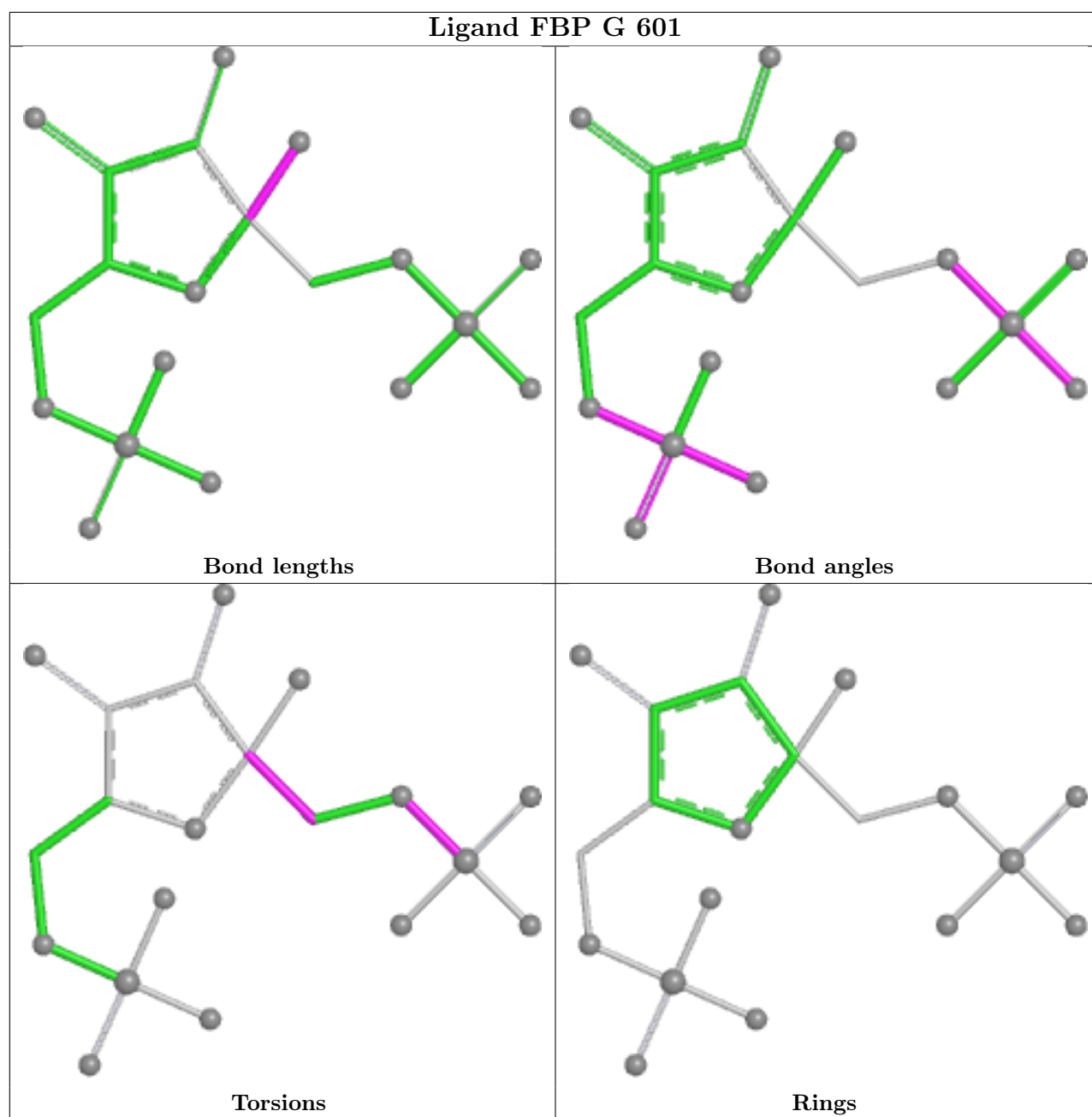
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

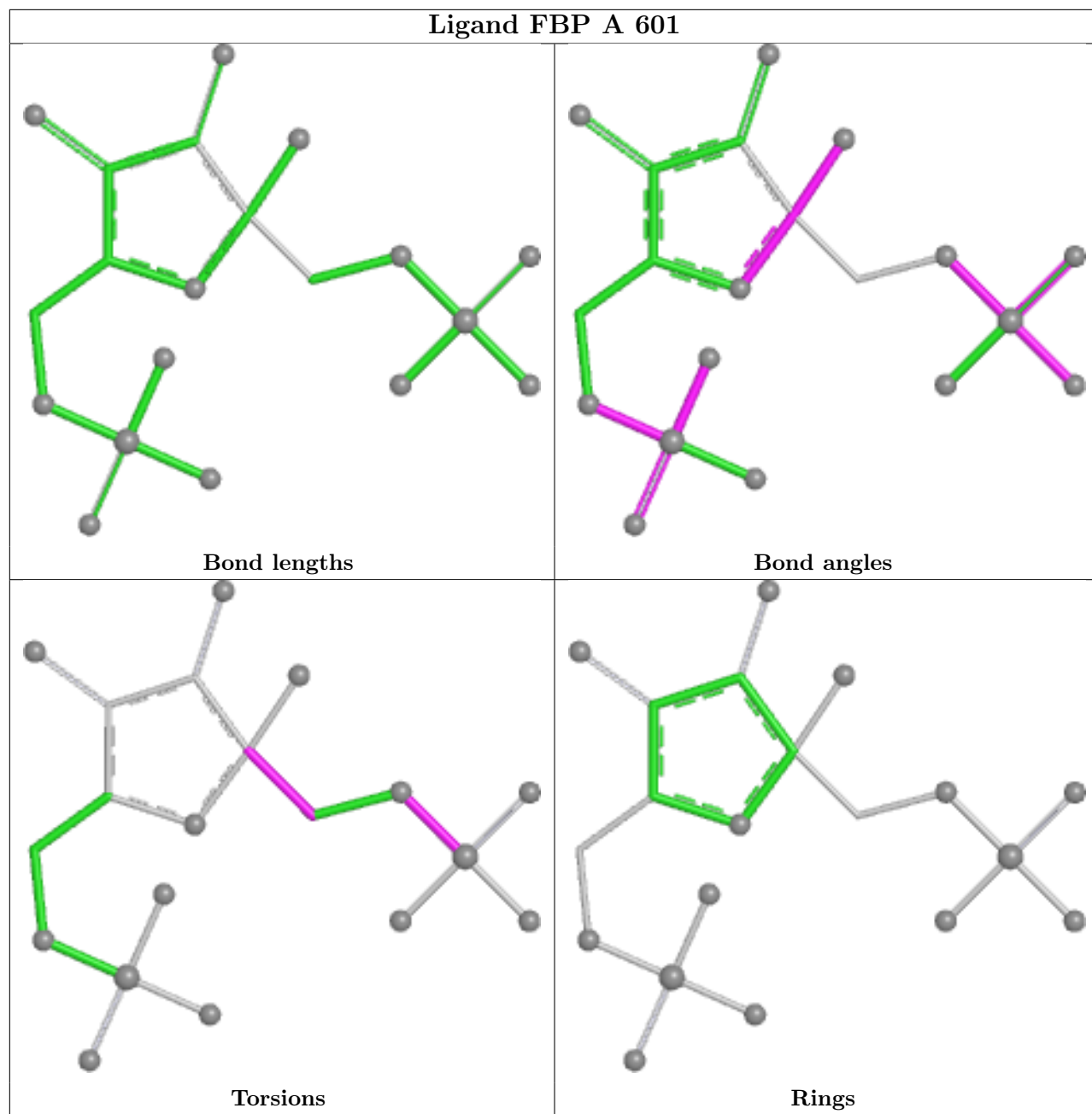


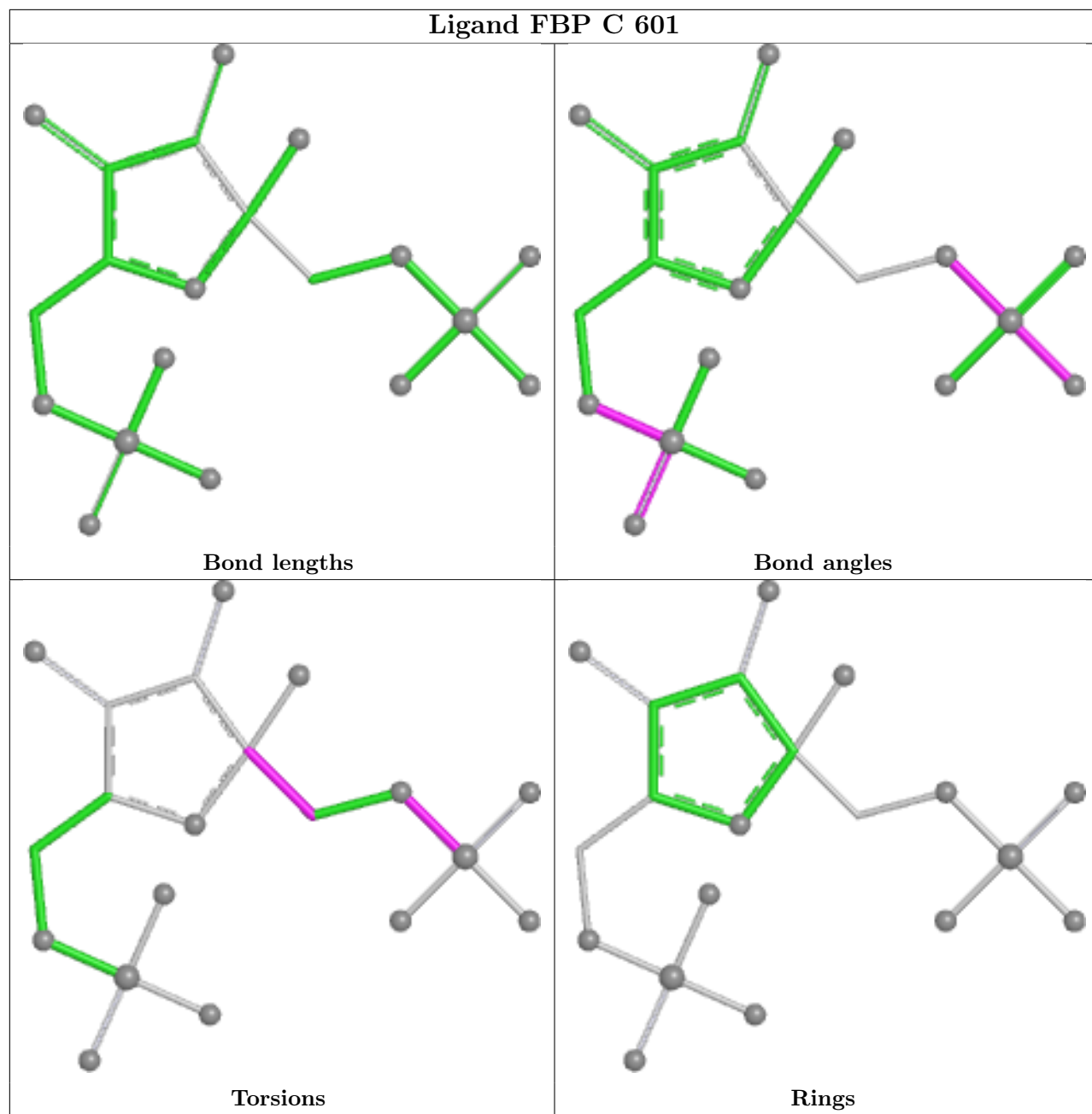


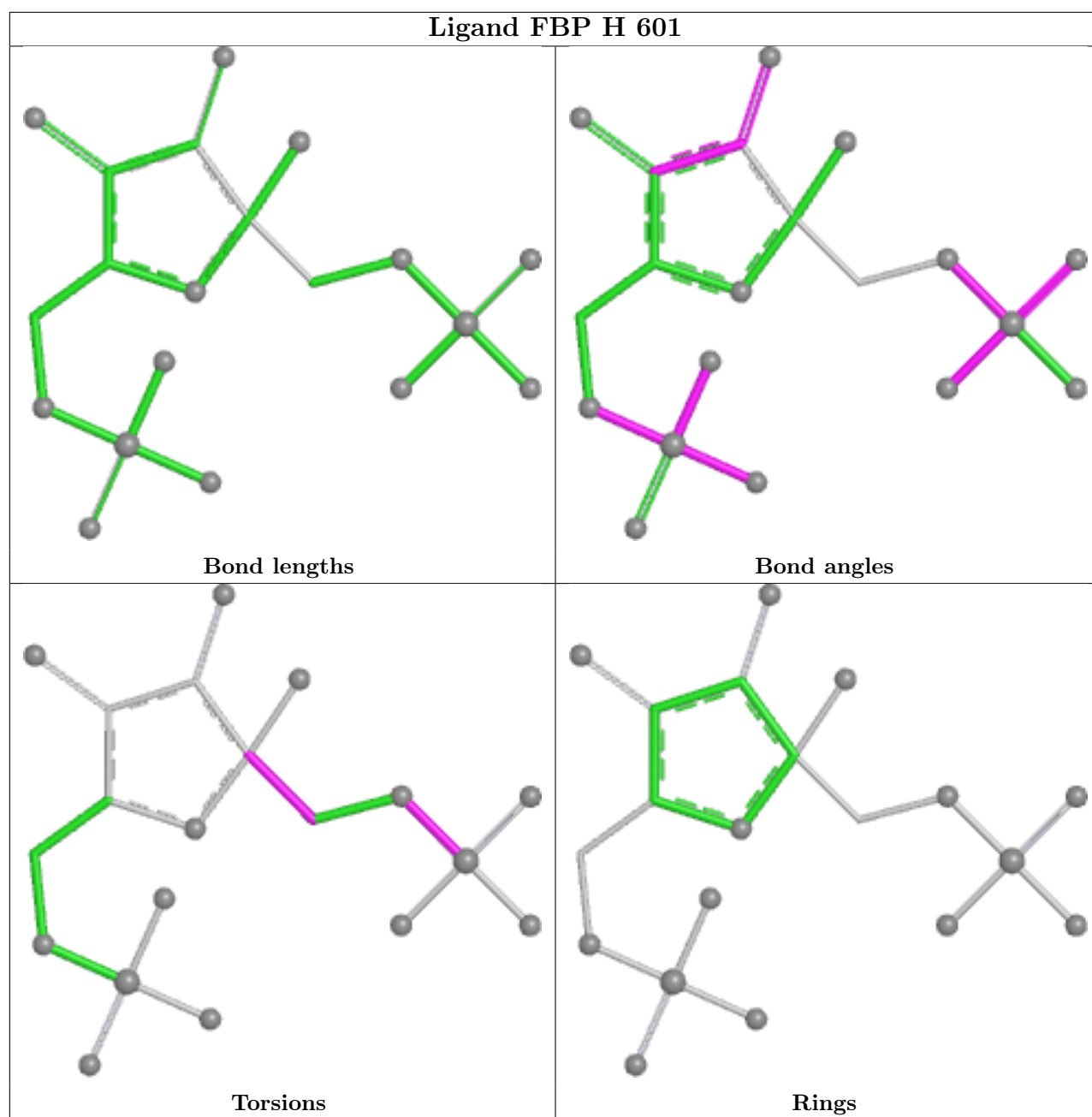
Ligand FBP E 601

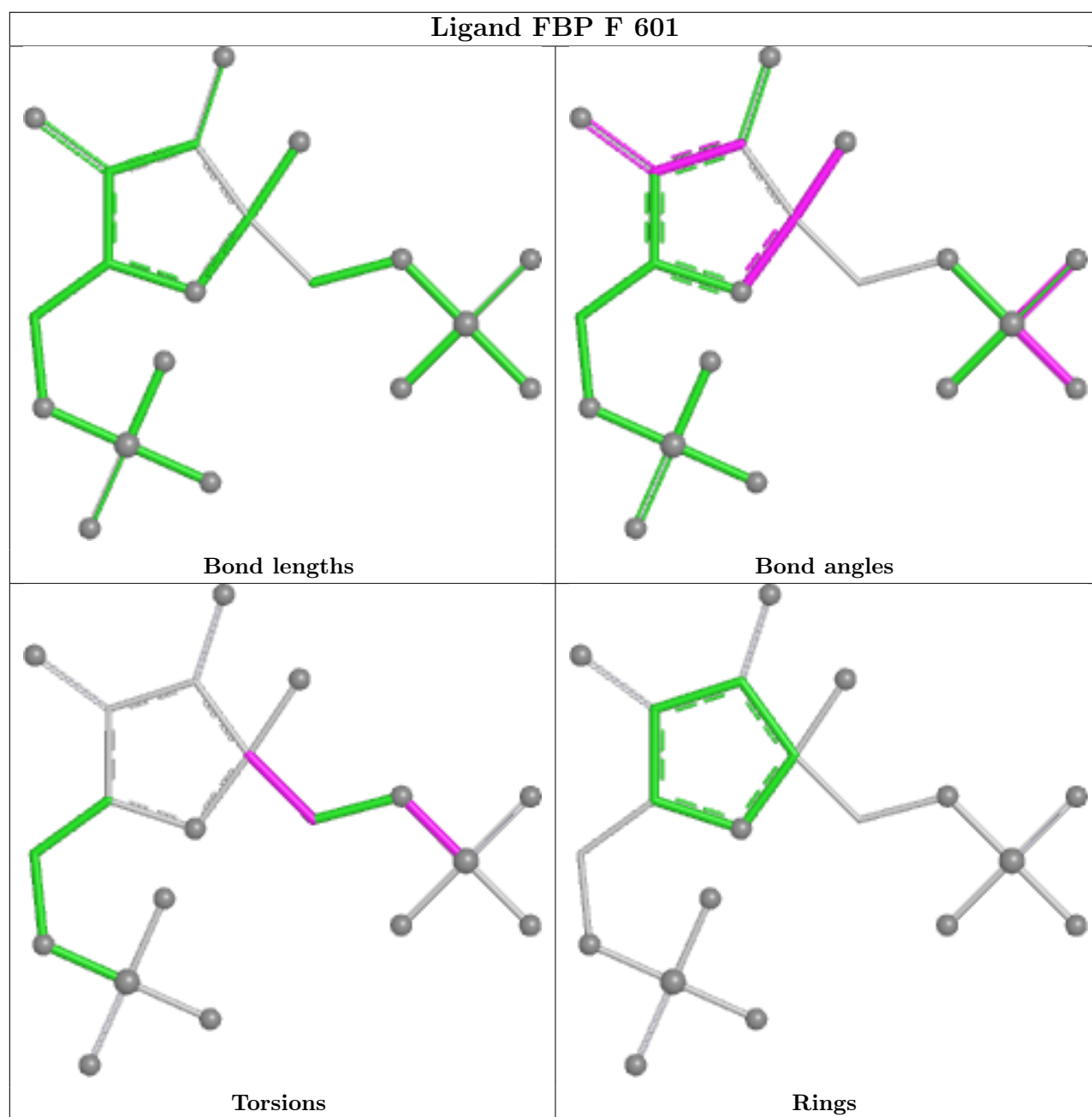












5.7 Other polymers [i](#)

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	501/521 (96%)	0.12	5 (0%)	79 79	23, 38, 63, 89	0
1	B	501/521 (96%)	0.15	3 (0%)	85 85	27, 41, 63, 95	0
1	C	501/521 (96%)	0.42	14 (2%)	55 54	28, 47, 77, 107	0
1	D	501/521 (96%)	0.18	5 (0%)	79 79	23, 41, 66, 97	0
1	E	499/521 (95%)	1.07	65 (13%)	7 6	33, 61, 87, 105	0
1	F	501/521 (96%)	0.62	34 (6%)	23 22	28, 48, 94, 132	0
1	G	500/521 (95%)	0.44	22 (4%)	39 38	28, 46, 80, 103	0
1	H	412/521 (79%)	0.59	14 (3%)	48 47	30, 51, 88, 112	0
All	All	3916/4168 (93%)	0.45	162 (4%)	41 40	23, 46, 81, 132	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	23	PHE	5.0
1	G	98	LEU	4.5
1	F	35	VAL	4.2
1	F	33	LEU	4.0
1	D	486	VAL	3.9
1	E	11	LEU	3.9
1	F	172	VAL	3.8
1	H	486	VAL	3.7
1	E	33	LEU	3.7
1	F	122	ILE	3.6
1	C	242	HIS	3.6
1	A	486	VAL	3.5
1	E	15	VAL	3.5
1	E	74	LEU	3.5
1	F	17	ILE	3.4
1	H	188	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	194	PRO	3.2
1	E	349	PRO	3.2
1	F	24	GLY	3.2
1	F	170	PHE	3.2
1	D	1	MET	3.2
1	E	94	ILE	3.2
1	F	1	MET	3.1
1	E	48	ALA	3.1
1	E	199	ALA	3.1
1	F	29	TRP	3.0
1	F	162	ALA	3.0
1	E	210	LEU	3.0
1	E	17	ILE	3.0
1	E	52	THR	3.0
1	E	317	ARG	2.9
1	E	35	VAL	2.9
1	G	193	ILE	2.9
1	E	78	ILE	2.9
1	H	27	GLY	2.9
1	G	181	ALA	2.9
1	E	72	VAL	2.8
1	E	486	VAL	2.8
1	F	28	TYR	2.8
1	H	1	MET	2.8
1	F	98	LEU	2.8
1	E	170	PHE	2.8
1	B	370	TYR	2.8
1	E	181	ALA	2.8
1	C	1	MET	2.8
1	E	179	ILE	2.8
1	E	353	VAL	2.7
1	G	103	ALA	2.7
1	B	161	VAL	2.7
1	F	114	ILE	2.7
1	E	462	ALA	2.7
1	E	270	ILE	2.7
1	F	486	VAL	2.7
1	G	165	ASP	2.7
1	C	24	GLY	2.7
1	E	41	ASN	2.6
1	F	11	LEU	2.6
1	E	276	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	124	SER	2.6
1	G	1	MET	2.5
1	G	101	GLY	2.5
1	E	51	ASN	2.5
1	H	95	ARG	2.5
1	F	103	ALA	2.5
1	E	99	PHE	2.5
1	H	29	TRP	2.5
1	F	129	ILE	2.5
1	H	8	VAL	2.5
1	H	194	PRO	2.5
1	E	87	LEU	2.5
1	G	137	LEU	2.5
1	E	28	TYR	2.5
1	D	455	THR	2.5
1	H	185	GLY	2.5
1	G	190	ASN	2.5
1	D	485	PRO	2.4
1	H	189	PRO	2.4
1	E	103	ALA	2.4
1	G	99	PHE	2.4
1	G	486	VAL	2.4
1	G	108	TYR	2.4
1	C	451	ALA	2.4
1	E	197	ALA	2.4
1	E	216	PHE	2.4
1	C	34	ASP	2.4
1	G	179	ILE	2.4
1	F	26	ASP	2.4
1	H	193	ILE	2.4
1	F	131	LEU	2.3
1	E	23	PHE	2.3
1	E	69	MET	2.3
1	E	85	PHE	2.3
1	E	195	PHE	2.3
1	C	94	ILE	2.3
1	E	214	ILE	2.3
1	F	128	VAL	2.3
1	F	174	VAL	2.3
1	E	316	PRO	2.3
1	F	117	ALA	2.3
1	G	166	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	27	GLY	2.3
1	E	339	LEU	2.3
1	H	24	GLY	2.3
1	G	455	THR	2.3
1	A	422	ASN	2.3
1	C	103	ALA	2.3
1	F	181	ALA	2.3
1	F	161	VAL	2.3
1	G	96	THR	2.3
1	C	21	LYS	2.3
1	E	451	ALA	2.3
1	E	433	LEU	2.3
1	E	348	TYR	2.3
1	F	99	PHE	2.2
1	A	179	ILE	2.2
1	E	234	ILE	2.2
1	E	116	VAL	2.2
1	H	490	VAL	2.2
1	B	1	MET	2.2
1	C	121	GLY	2.2
1	E	59	HIS	2.2
1	E	57	PHE	2.2
1	E	196	PRO	2.2
1	F	163	LYS	2.2
1	G	139	ILE	2.2
1	E	53	PHE	2.2
1	E	221	PHE	2.2
1	D	34	ASP	2.2
1	C	100	GLU	2.2
1	E	39	ALA	2.2
1	C	106	TYR	2.2
1	F	370	TYR	2.2
1	C	468	GLU	2.1
1	E	262	ILE	2.1
1	F	180	ILE	2.1
1	G	24	GLY	2.1
1	G	117	ALA	2.1
1	F	137	LEU	2.1
1	E	352	SER	2.1
1	E	142	ASP	2.1
1	E	19	GLY	2.1
1	E	145	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	243	VAL	2.1
1	E	95	ARG	2.1
1	E	166	ALA	2.1
1	F	37	ALA	2.1
1	E	261	ILE	2.1
1	F	119	LYS	2.1
1	G	119	LYS	2.1
1	G	451	ALA	2.1
1	E	192	LYS	2.1
1	C	486	VAL	2.1
1	E	500	VAL	2.1
1	E	68	ARG	2.0
1	H	242	HIS	2.0
1	F	116	VAL	2.0
1	A	1	MET	2.0
1	E	134	ALA	2.0
1	E	428	LEU	2.0
1	C	152	ASP	2.0
1	E	205	ASP	2.0
1	F	13	PRO	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(Å ²)	Q<0.9
8	PG4	F	605	13/13	0.83	0.14	46,54,61,62	0
7	PGE	G	605	10/10	0.84	0.14	53,56,60,62	0
7	PGE	D	605	10/10	0.86	0.14	49,59,61,62	0

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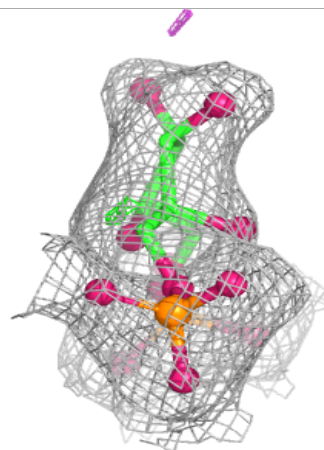
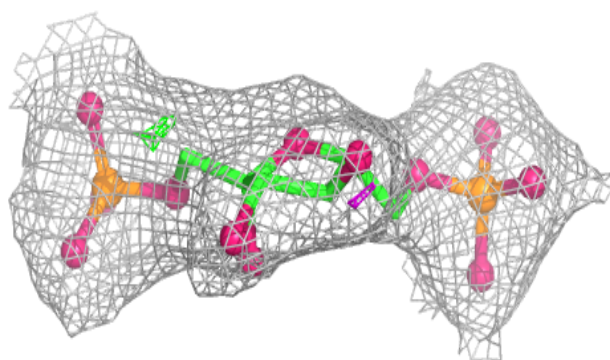
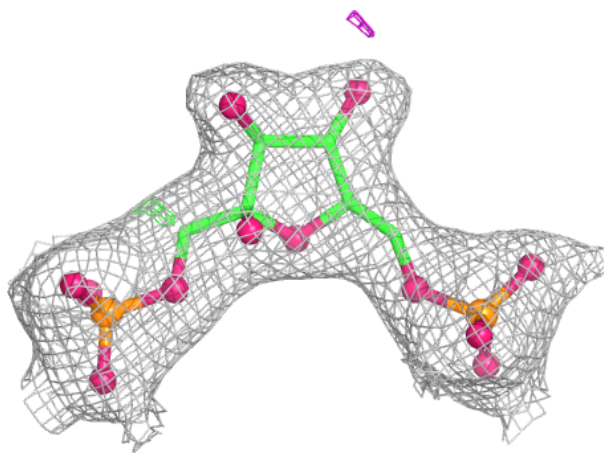
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OXL	H	603	6/6	0.88	0.10	57,69,73,74	0
4	OXL	G	603	6/6	0.90	0.09	38,49,60,61	0
7	PGE	C	605	10/10	0.91	0.11	49,57,65,67	0
4	OXL	C	603	6/6	0.91	0.08	42,45,54,57	0
5	K	C	604	1/1	0.91	0.15	71,71,71,71	0
7	PGE	B	605	10/10	0.91	0.10	42,50,53,55	0
4	OXL	B	603	6/6	0.92	0.08	37,44,47,49	0
4	OXL	D	603	6/6	0.92	0.08	39,40,51,55	0
6	PEG	H	605	7/7	0.93	0.08	44,50,56,63	0
6	PEG	A	605	7/7	0.93	0.10	43,48,54,58	0
4	OXL	A	603	6/6	0.94	0.10	38,45,55,60	0
4	OXL	F	603	6/6	0.94	0.09	42,56,66,66	0
2	FBP	G	601	20/20	0.95	0.07	43,50,59,65	0
2	FBP	H	601	20/20	0.95	0.08	37,48,53,55	0
5	K	D	604	1/1	0.95	0.11	65,65,65,65	0
2	FBP	C	601	20/20	0.95	0.07	42,54,59,60	0
2	FBP	D	601	20/20	0.95	0.08	39,50,60,62	0
2	FBP	E	601	20/20	0.96	0.06	37,52,58,67	0
5	K	H	604	1/1	0.96	0.17	74,74,74,74	0
2	FBP	F	601	20/20	0.96	0.06	41,51,57,58	0
3	MG	H	602	1/1	0.97	0.04	58,58,58,58	0
2	FBP	A	601	20/20	0.97	0.06	32,42,49,49	0
5	K	F	604	1/1	0.97	0.09	64,64,64,64	0
5	K	G	604	1/1	0.97	0.11	60,60,60,60	0
2	FBP	B	601	20/20	0.97	0.06	34,41,45,50	0
3	MG	F	602	1/1	0.97	0.04	51,51,51,51	0
3	MG	A	602	1/1	0.98	0.06	38,38,38,38	0
3	MG	G	602	1/1	0.98	0.03	50,50,50,50	0
5	K	A	604	1/1	0.98	0.11	50,50,50,50	0
3	MG	C	602	1/1	0.98	0.04	58,58,58,58	0
3	MG	D	602	1/1	0.98	0.06	40,40,40,40	0
3	MG	B	602	1/1	0.99	0.03	39,39,39,39	0
5	K	B	604	1/1	0.99	0.08	46,46,46,46	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.

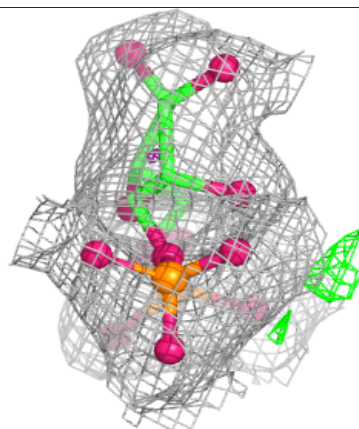
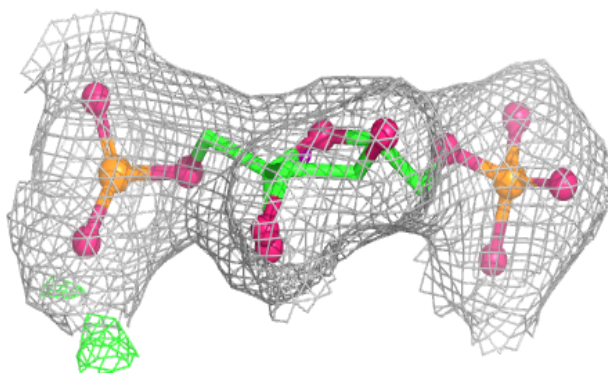
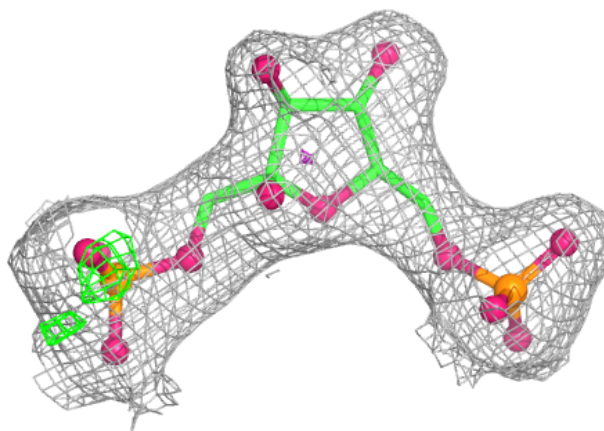
Electron density around FBP G 601:

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



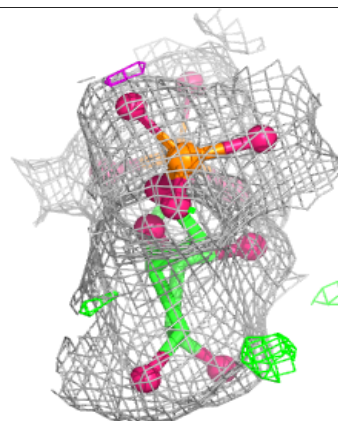
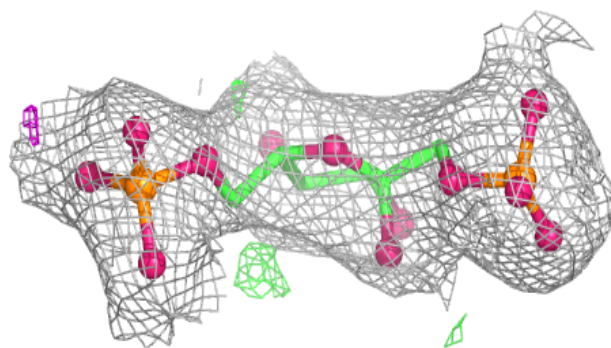
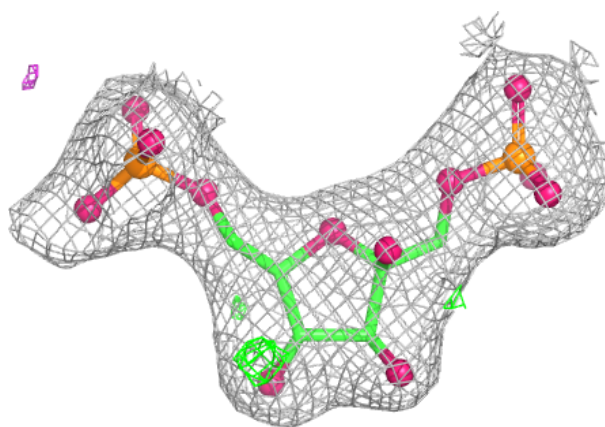
Electron density around FBP H 601:

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



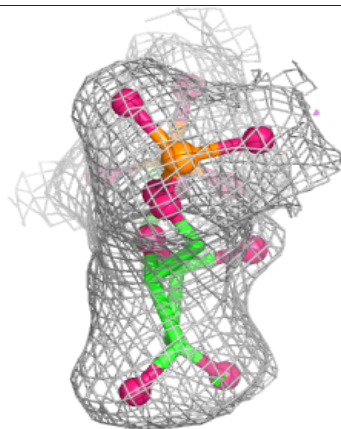
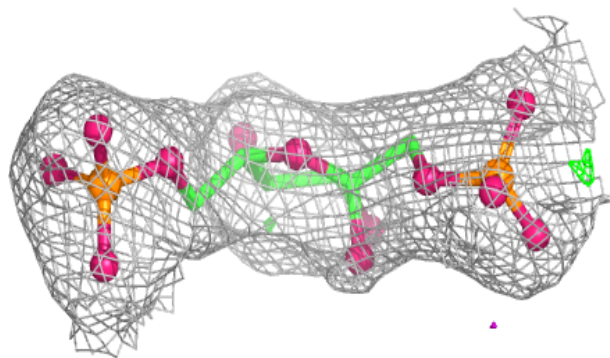
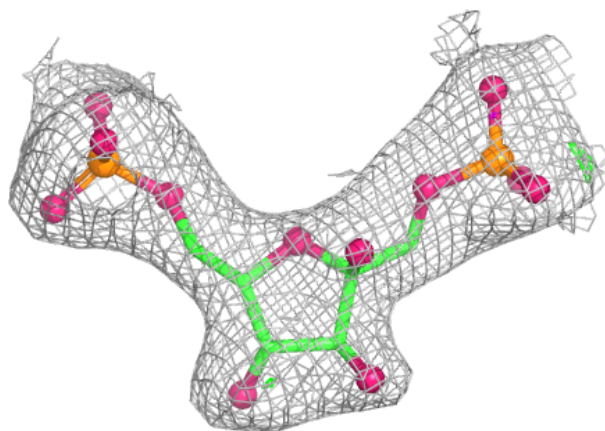
Electron density around FBP C 601:

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



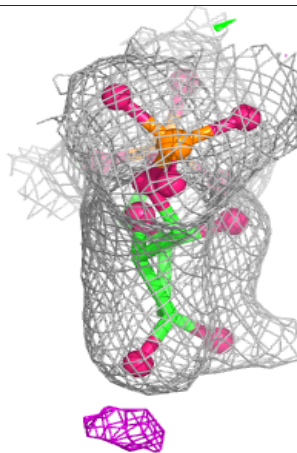
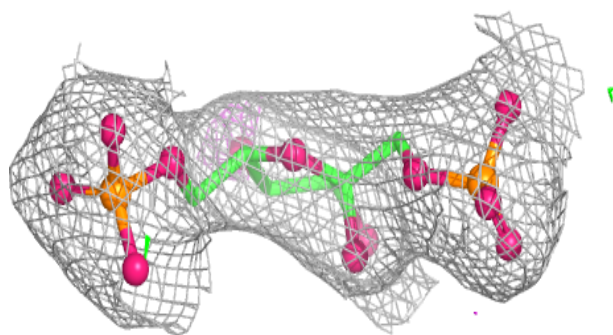
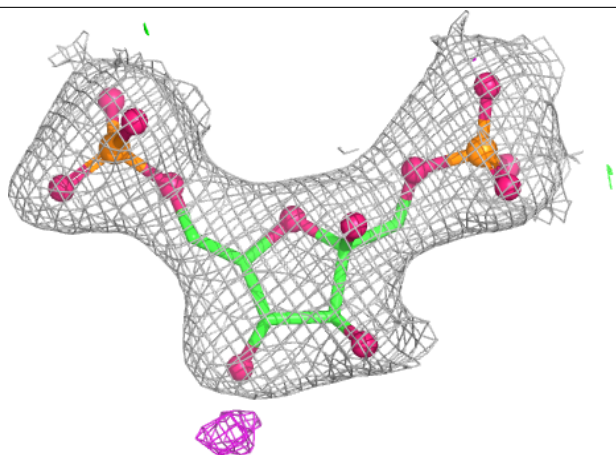
Electron density around FBP D 601:

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



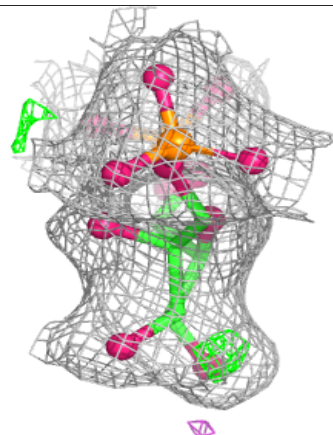
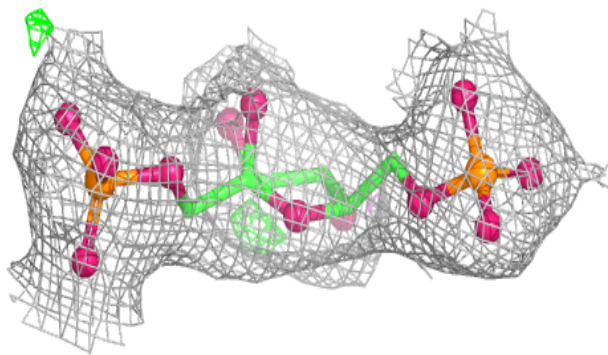
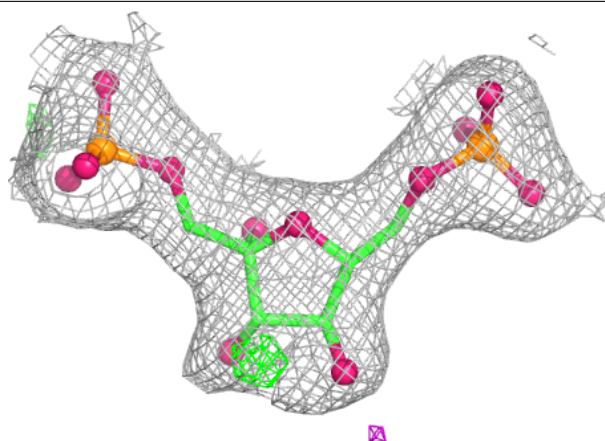
Electron density around FBP E 601:

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



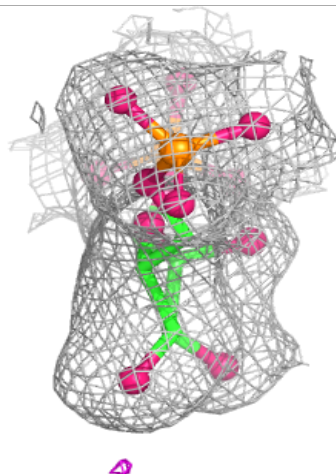
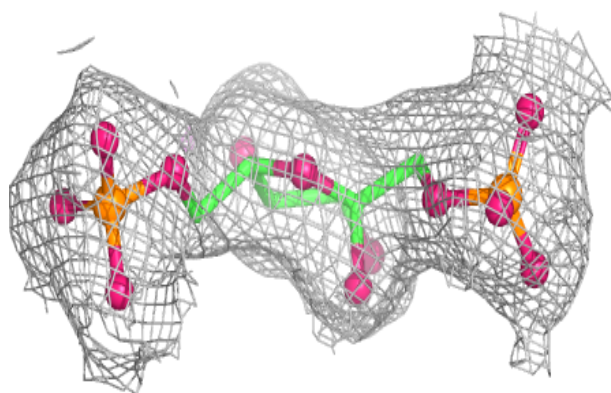
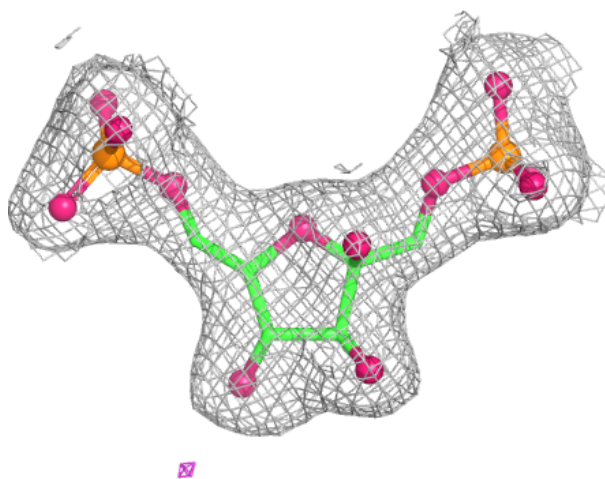
Electron density around FBP F 601:

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



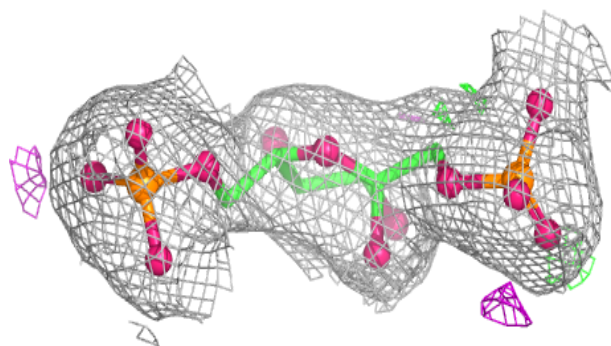
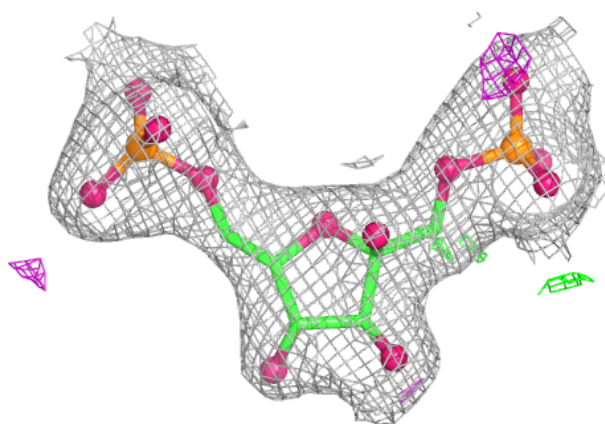
Electron density around FBP A 601:

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



Electron density around FBP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.