



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2025 – 05:18 pm BST

PDB ID : 9R3L / pdb_00009r3l
Title : Structure of liver pyruvate kinase in complex with fluorescent probe 4d
Authors : Bogucka, A.; Nilsson, O.; Grotli, M.; Hyvonen, M.
Deposited on : 2025-05-05
Resolution : 2.16 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

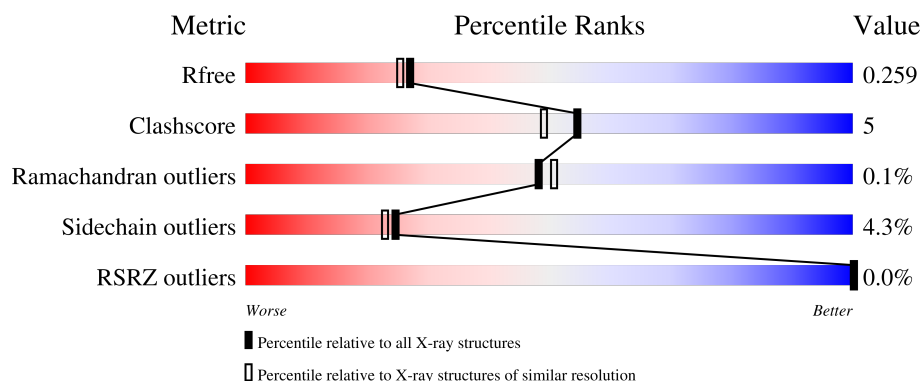
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	 83% 11% • 5%
1	B	447	 82% 13% • 5%
1	C	447	 80% 14% • 5%
1	D	447	 78% 16% • 5%
1	E	447	 83% 12% • •

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Mol	Chain	Length	Quality of chain
1	F	447	<div><div></div><div>81%</div><div>13%</div><div>• •</div></div>
1	G	447	<div><div></div><div>83%</div><div>11%</div><div>• 5%</div></div>
1	H	447	<div><div></div><div>81%</div><div>13%</div><div>• 5%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26951 atoms, of which 164 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 Isoform L-type of Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3231	2029	586	598	18			
1	B	426	Total	C	N	O	S	0	0	0
			3228	2026	586	598	18			
1	C	424	Total	C	N	O	S	0	1	0
			3225	2023	585	599	18			
1	D	424	Total	C	N	O	S	0	0	0
			3216	2018	584	596	18			
1	E	429	Total	C	N	O	S	0	0	0
			3253	2040	590	605	18			
1	F	433	Total	C	N	O	S	0	0	0
			3282	2059	595	610	18			
1	G	423	Total	C	N	O	S	0	0	0
			3209	2014	583	594	18			
1	H	423	Total	C	N	O	S	0	0	0
			3209	2014	583	594	18			

There are 832 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	12	ASP	SER	conflict	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	LYS	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ASP	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	ALA	deletion	UNP P30613
A	?	-	PHE	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	ALA	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	TRP	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ASP	deletion	UNP P30613
A	?	-	TYR	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	TYR	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	ASP	deletion	UNP P30613
A	?	-	ASP	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	LYS	deletion	UNP P30613
A	?	-	ILE	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	PRO	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	THR	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	GLU	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	SER	deletion	UNP P30613
A	?	-	ARG	deletion	UNP P30613
A	?	-	LYS	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	VAL	deletion	UNP P30613
A	?	-	ASN	deletion	UNP P30613
A	?	-	LEU	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P30613
A	?	-	GLY	deletion	UNP P30613
A	?	-	ALA	deletion	UNP P30613
A	?	-	GLN	deletion	UNP P30613
A	130	GLY	VAL	linker	UNP P30613
A	229	SER	ASP	linker	UNP P30613
A	230	GLY	LEU	linker	UNP P30613
B	-1	GLY	-	expression tag	UNP P30613
B	0	SER	-	expression tag	UNP P30613
B	12	ASP	SER	conflict	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	LYS	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	ALA	deletion	UNP P30613
B	?	-	PHE	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	ALA	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	TRP	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	TYR	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	TYR	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	ASP	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	LYS	deletion	UNP P30613
B	?	-	ILE	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	THR	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	GLU	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	SER	deletion	UNP P30613
B	?	-	ARG	deletion	UNP P30613
B	?	-	LYS	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	VAL	deletion	UNP P30613
B	?	-	ASN	deletion	UNP P30613
B	?	-	LEU	deletion	UNP P30613
B	?	-	PRO	deletion	UNP P30613
B	?	-	GLY	deletion	UNP P30613
B	?	-	ALA	deletion	UNP P30613
B	?	-	GLN	deletion	UNP P30613
B	130	GLY	VAL	linker	UNP P30613
B	229	SER	ASP	linker	UNP P30613
B	230	GLY	LEU	linker	UNP P30613
C	-1	GLY	-	expression tag	UNP P30613
C	0	SER	-	expression tag	UNP P30613
C	12	ASP	SER	conflict	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LYS	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	SER	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	PHE	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	ALA	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	TRP	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	TYR	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	TYR	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	ASP	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	SER	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	LYS	deletion	UNP P30613
C	?	-	ILE	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	THR	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	GLU	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	SER	deletion	UNP P30613
C	?	-	ARG	deletion	UNP P30613
C	?	-	LYS	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613
C	?	-	VAL	deletion	UNP P30613
C	?	-	ASN	deletion	UNP P30613
C	?	-	LEU	deletion	UNP P30613
C	?	-	PRO	deletion	UNP P30613
C	?	-	GLY	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP P30613
C	?	-	GLN	deletion	UNP P30613
C	130	GLY	VAL	linker	UNP P30613
C	229	SER	ASP	linker	UNP P30613
C	230	GLY	LEU	linker	UNP P30613
D	-1	GLY	-	expression tag	UNP P30613
D	0	SER	-	expression tag	UNP P30613
D	12	ASP	SER	conflict	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	LYS	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	ASP	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	ALA	deletion	UNP P30613
D	?	-	PHE	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	ALA	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	TRP	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	ASP	deletion	UNP P30613
D	?	-	TYR	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	TYR	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	ASP	deletion	UNP P30613
D	?	-	ASP	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	LYS	deletion	UNP P30613
D	?	-	ILE	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP P30613
D	?	-	THR	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	GLU	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	SER	deletion	UNP P30613
D	?	-	ARG	deletion	UNP P30613
D	?	-	LYS	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	VAL	deletion	UNP P30613
D	?	-	ASN	deletion	UNP P30613
D	?	-	LEU	deletion	UNP P30613
D	?	-	PRO	deletion	UNP P30613
D	?	-	GLY	deletion	UNP P30613
D	?	-	ALA	deletion	UNP P30613
D	?	-	GLN	deletion	UNP P30613
D	130	GLY	VAL	linker	UNP P30613
D	229	SER	ASP	linker	UNP P30613
D	230	GLY	LEU	linker	UNP P30613
E	-1	GLY	-	expression tag	UNP P30613
E	0	SER	-	expression tag	UNP P30613
E	12	ASP	SER	conflict	UNP P30613
E	?	-	GLU	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	ARG	deletion	UNP P30613
E	?	-	THR	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	GLN	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	?	-	GLU	deletion	UNP P30613
E	?	-	SER	deletion	UNP P30613
E	?	-	GLU	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	VAL	deletion	UNP P30613
E	?	-	GLU	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	LYS	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	SER	deletion	UNP P30613
E	?	-	GLN	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	THR	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	ASP	deletion	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	?	-	ALA	deletion	UNP P30613
E	?	-	PHE	deletion	UNP P30613
E	?	-	ARG	deletion	UNP P30613
E	?	-	THR	deletion	UNP P30613
E	?	-	ARG	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	ASN	deletion	UNP P30613
E	?	-	ALA	deletion	UNP P30613
E	?	-	ASN	deletion	UNP P30613
E	?	-	THR	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	TRP	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	ASP	deletion	UNP P30613
E	?	-	TYR	deletion	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	?	-	ASN	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	ARG	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	ARG	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ILE	deletion	UNP P30613
E	?	-	TYR	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	ASP	deletion	UNP P30613
E	?	-	ASP	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	SER	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	GLN	deletion	UNP P30613
E	?	-	LYS	deletion	UNP P30613
E	?	-	ILE	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	?	-	GLU	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	THR	deletion	UNP P30613
E	?	-	GLN	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	GLU	deletion	UNP P30613
E	?	-	ASN	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	SER	deletion	UNP P30613
E	?	-	ARG	deletion	UNP P30613
E	?	-	LYS	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	VAL	deletion	UNP P30613
E	?	-	ASN	deletion	UNP P30613
E	?	-	LEU	deletion	UNP P30613
E	?	-	PRO	deletion	UNP P30613
E	?	-	GLY	deletion	UNP P30613
E	?	-	ALA	deletion	UNP P30613
E	?	-	GLN	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
E	130	GLY	VAL	linker	UNP P30613
E	229	SER	ASP	linker	UNP P30613
E	230	GLY	LEU	linker	UNP P30613
F	-1	GLY	-	expression tag	UNP P30613
F	0	SER	-	expression tag	UNP P30613
F	12	ASP	SER	conflict	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	GLN	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	SER	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	LYS	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	SER	deletion	UNP P30613
F	?	-	GLN	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	ASP	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	ALA	deletion	UNP P30613
F	?	-	PHE	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	TRP	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	ASP	deletion	UNP P30613
F	?	-	TYR	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	TYR	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	ASP	deletion	UNP P30613
F	?	-	ASP	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	SER	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	GLN	deletion	UNP P30613
F	?	-	LYS	deletion	UNP P30613
F	?	-	ILE	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	THR	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	GLU	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	SER	deletion	UNP P30613
F	?	-	ARG	deletion	UNP P30613
F	?	-	LYS	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	VAL	deletion	UNP P30613
F	?	-	ASN	deletion	UNP P30613
F	?	-	LEU	deletion	UNP P30613
F	?	-	PRO	deletion	UNP P30613
F	?	-	GLY	deletion	UNP P30613
F	?	-	ALA	deletion	UNP P30613
F	?	-	GLN	deletion	UNP P30613
F	130	GLY	VAL	linker	UNP P30613
F	229	SER	ASP	linker	UNP P30613
F	230	GLY	LEU	linker	UNP P30613
G	-1	GLY	-	expression tag	UNP P30613
G	0	SER	-	expression tag	UNP P30613
G	12	ASP	SER	conflict	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	THR	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	SER	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LEU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	LYS	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	SER	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	THR	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	ASP	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	ALA	deletion	UNP P30613
G	?	-	PHE	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	THR	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	ASN	deletion	UNP P30613
G	?	-	ALA	deletion	UNP P30613
G	?	-	ASN	deletion	UNP P30613
G	?	-	THR	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	TRP	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	ASP	deletion	UNP P30613
G	?	-	TYR	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	ASN	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	TYR	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ILE	deletion	UNP P30613
G	?	-	ASP	deletion	UNP P30613
G	?	-	ASP	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	SER	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	?	-	LYS	deletion	UNP P30613
G	?	-	ILE	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	THR	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	GLU	deletion	UNP P30613
G	?	-	ASN	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	SER	deletion	UNP P30613
G	?	-	ARG	deletion	UNP P30613
G	?	-	LYS	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	VAL	deletion	UNP P30613
G	?	-	ASN	deletion	UNP P30613
G	?	-	LEU	deletion	UNP P30613
G	?	-	PRO	deletion	UNP P30613
G	?	-	GLY	deletion	UNP P30613
G	?	-	ALA	deletion	UNP P30613
G	?	-	GLN	deletion	UNP P30613
G	130	GLY	VAL	linker	UNP P30613
G	229	SER	ASP	linker	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
G	230	GLY	LEU	linker	UNP P30613
H	-1	GLY	-	expression tag	UNP P30613
H	0	SER	-	expression tag	UNP P30613
H	12	ASP	SER	conflict	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LYS	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ALA	deletion	UNP P30613
H	?	-	PHE	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	ALA	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613

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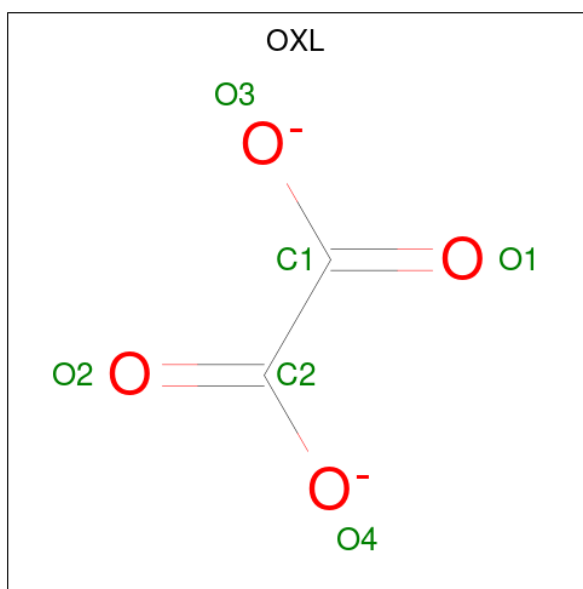
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	THR	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	TRP	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	TYR	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	TYR	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	ASP	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	?	-	LYS	deletion	UNP P30613
H	?	-	ILE	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	GLU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	THR	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	SER	deletion	UNP P30613
H	?	-	ARG	deletion	UNP P30613
H	?	-	LYS	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	VAL	deletion	UNP P30613
H	?	-	ASN	deletion	UNP P30613
H	?	-	LEU	deletion	UNP P30613
H	?	-	PRO	deletion	UNP P30613
H	?	-	GLY	deletion	UNP P30613
H	?	-	ALA	deletion	UNP P30613
H	?	-	GLN	deletion	UNP P30613
H	130	GLY	VAL	linker	UNP P30613
H	229	SER	ASP	linker	UNP P30613
H	230	GLY	LEU	linker	UNP P30613

- Molecule 2 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



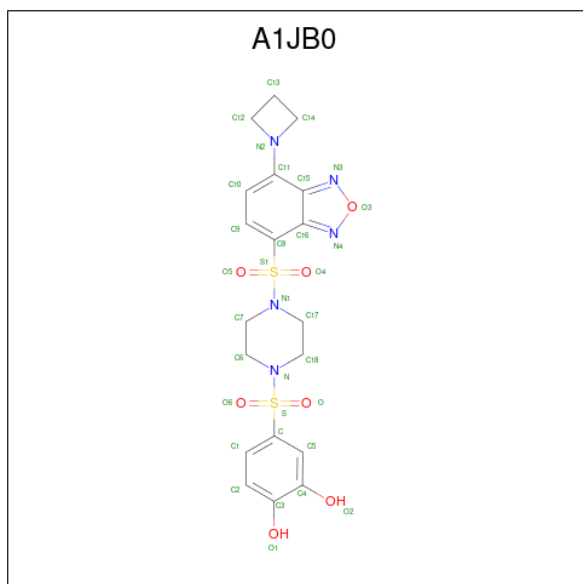
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		

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

- Molecule 3 is 4-[4-[[7-(azetidin-1-yl)-2,1,3-benzoxadiazol-4-yl]sulfonyl]piperazin-1-yl]sulfonylbenzene-1,2-diol (CCD ID: A1JB0) (formula: C₁₉H₂₁N₅O₇S₂) (labeled as "Ligand of Interest" by depositor).



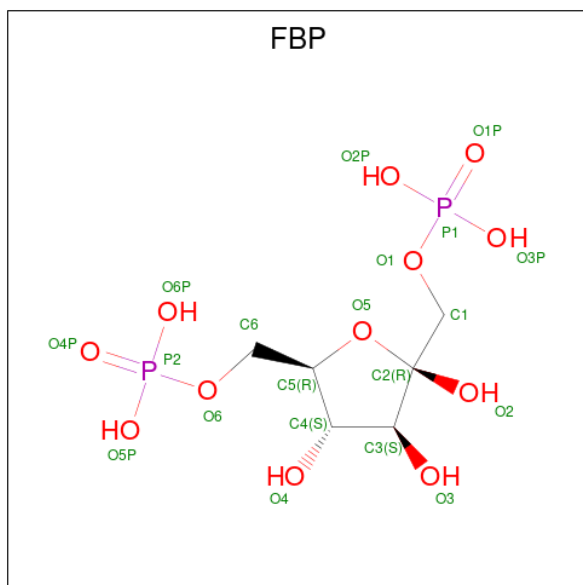
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	21	0
			54	19	21	5	7	2		
3	F	1	Total	C	H	N	O	S	21	0
			54	19	21	5	7	2		
3	G	1	Total	C	H	N	O	S	21	0
			54	19	21	5	7	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	H	N	O	21	0
			54	19	21	5	7		

- Molecule 4 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
4	A	1	Total	C	H	O	P	10	0
			30	6	10	12	2		
4	B	1	Total	C	H	O	P	10	0
			30	6	10	12	2		
4	C	1	Total	C	H	O	P	10	0
			30	6	10	12	2		
4	D	1	Total	C	H	O	P	10	0
			30	6	10	12	2		
4	E	1	Total	C	H	O	P	10	0
			30	6	10	12	2		
4	F	1	Total	C	H	O	P	10	0
			30	6	10	12	2		
4	G	1	Total	C	H	O	P	10	0
			30	6	10	12	2		
4	H	1	Total	C	H	O	P	10	0
			30	6	10	12	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	B	1	Total Mg 1 1	0	0
5	C	2	Total Mg 2 2	0	0
5	E	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	2	Total K 2 2	0	0
6	F	1	Total K 1 1	0	0
6	G	1	Total K 1 1	0	0

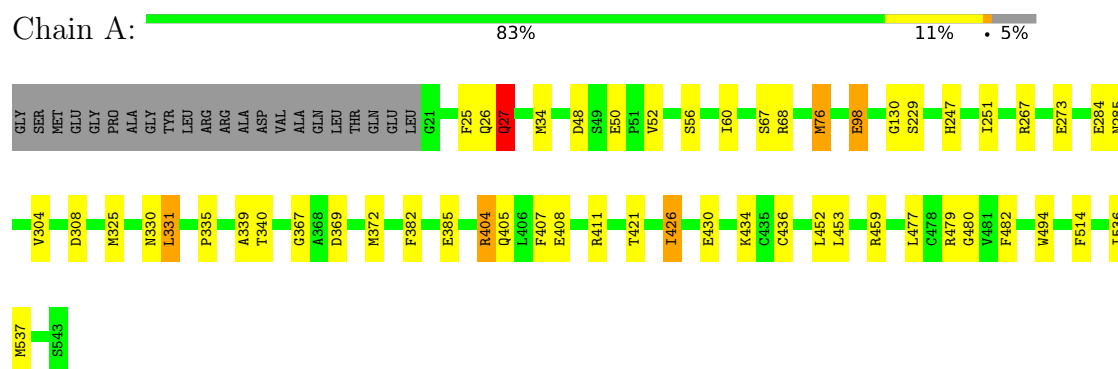
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	121	Total O 121 121	0	0
7	B	113	Total O 113 113	0	0
7	C	116	Total O 116 116	0	0
7	D	101	Total O 101 101	0	0
7	E	37	Total O 37 37	0	0
7	F	36	Total O 36 36	0	0
7	G	25	Total O 25 25	0	0
7	H	33	Total O 33 33	0	0

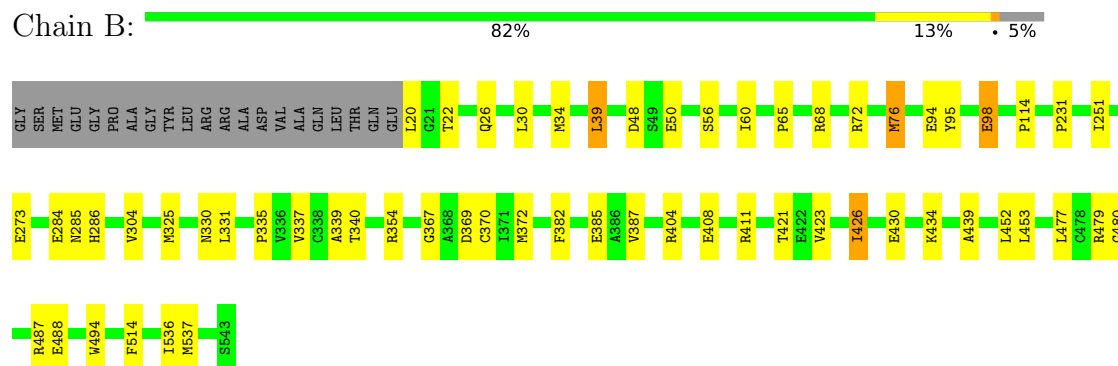
3 Residue-property plots

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

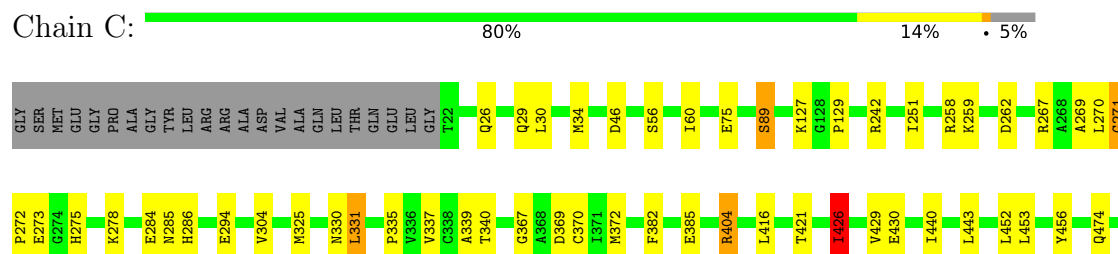
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

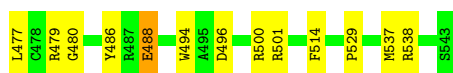


- Molecule 1: Isoform L-type of Pyruvate kinase PKLR



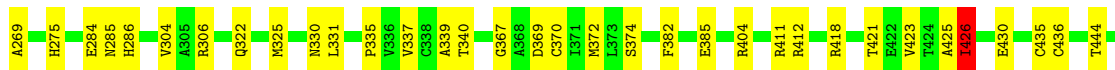
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR





- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain D: 78% 16% 5%



- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain E: 83% 12% 5%



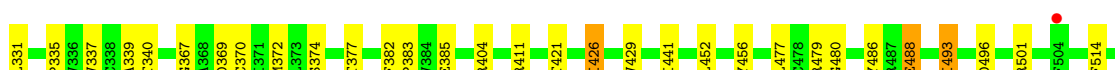
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain F: 81% 13% 6%



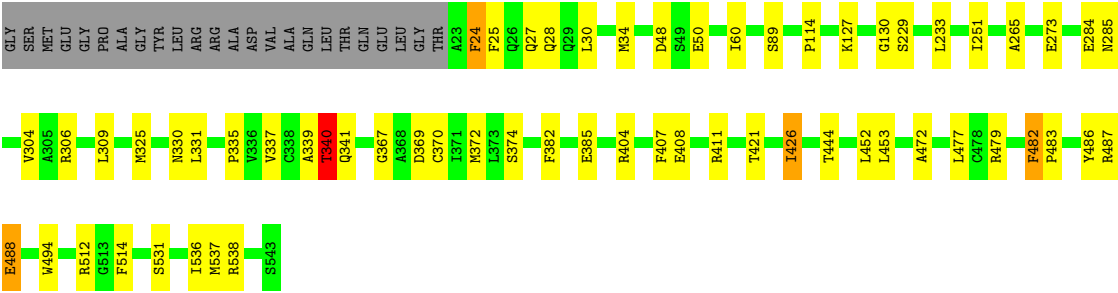
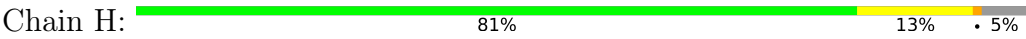
- Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain G: 83% 11% 6%





● Molecule 1: Isoform L-type of Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.88Å 111.31Å 118.98Å 103.60° 104.13° 118.12°	Depositor
Resolution (Å)	105.26 – 2.16 105.26 – 2.16	Depositor EDS
% Data completeness (in resolution range)	40.6 (105.26-2.16) 40.6 (105.26-2.16)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.239 , 0.273 0.229 , 0.259	Depositor DCC
R_{free} test set	4943 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.126 for k,h,-h-k-l 0.000 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26951	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: K, FBP, A1JB0, OXL, MG

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	0.78	1/3287 (0.0%)	1.13	11/4446 (0.2%)
1	B	0.77	1/3283 (0.0%)	1.13	9/4441 (0.2%)
1	C	0.79	0/3280	1.15	12/4437 (0.3%)
1	D	0.78	2/3271 (0.1%)	1.17	13/4425 (0.3%)
1	E	0.64	0/3308	1.06	6/4475 (0.1%)
1	F	0.67	1/3337 (0.0%)	1.06	6/4515 (0.1%)
1	G	0.64	0/3264	1.08	5/4415 (0.1%)
1	H	0.66	0/3264	1.06	9/4415 (0.2%)
All	All	0.72	5/26294 (0.0%)	1.11	71/35569 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	SD-CE	-10.50	1.53	1.79
1	B	76	MET	SD-CE	-7.03	1.61	1.79
1	F	475	VAL	CA-C	5.27	1.58	1.52
1	D	425	ALA	C-N	5.15	1.40	1.33
1	D	537	MET	SD-CE	-5.06	1.66	1.79

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	PHE	CA-CB-CG	7.76	121.56	113.80
1	B	339	ALA	N-CA-C	7.75	123.24	112.93
1	A	340	THR	CA-C-N	7.63	133.30	122.08
1	A	340	THR	C-N-CA	7.63	133.30	122.08
1	E	339	ALA	N-CA-C	7.45	122.84	112.93
1	F	339	ALA	N-CA-C	7.41	122.78	112.93
1	C	339	ALA	N-CA-C	7.35	122.70	112.93
1	G	339	ALA	N-CA-C	7.27	122.60	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	ALA	N-CA-C	7.01	122.26	112.93
1	G	257	VAL	N-CA-CB	6.95	118.10	110.53
1	A	514	PHE	CA-CB-CG	6.86	120.66	113.80
1	H	339	ALA	N-CA-C	6.83	122.01	112.93
1	C	426	ILE	N-CA-CB	6.80	119.78	110.54
1	B	426	ILE	N-CA-CB	6.73	119.70	110.54
1	D	426	ILE	N-CA-CB	6.66	119.60	110.54
1	A	426	ILE	N-CA-CB	6.58	119.49	110.54
1	H	426	ILE	N-CA-CB	6.51	119.40	110.54
1	E	426	ILE	N-CA-CB	6.47	119.34	110.54
1	H	482	PHE	CA-CB-CG	-6.45	107.35	113.80
1	E	514	PHE	CA-CB-CG	6.44	120.24	113.80
1	G	426	ILE	N-CA-CB	6.37	119.20	110.54
1	F	426	ILE	N-CA-CB	6.24	119.03	110.54
1	A	27	GLN	CA-C-N	6.21	130.95	122.07
1	A	27	GLN	C-N-CA	6.21	130.95	122.07
1	E	340	THR	N-CA-C	6.02	119.28	109.59
1	B	514	PHE	CA-CB-CG	6.01	119.81	113.80
1	G	514	PHE	CA-CB-CG	6.00	119.80	113.80
1	F	340	THR	N-CA-C	5.84	118.99	109.59
1	C	440	ILE	N-CA-CB	5.83	119.02	111.67
1	A	339	ALA	CA-C-N	5.81	132.63	121.54
1	A	339	ALA	C-N-CA	5.81	132.63	121.54
1	C	488	GLU	N-CA-C	5.77	118.04	110.08
1	G	340	THR	N-CA-C	5.73	118.81	109.59
1	D	482	PHE	CA-CB-CG	-5.66	108.14	113.80
1	C	453	LEU	CA-C-N	5.65	127.85	120.28
1	C	453	LEU	C-N-CA	5.65	127.85	120.28
1	B	439	ALA	CA-C-N	5.63	130.68	123.13
1	B	439	ALA	C-N-CA	5.63	130.68	123.13
1	B	340	THR	N-CA-C	5.56	118.54	109.59
1	D	340	THR	N-CA-C	5.54	118.51	109.59
1	C	270	LEU	CA-C-N	5.52	130.54	121.87
1	C	270	LEU	C-N-CA	5.52	130.54	121.87
1	E	453	LEU	CA-C-N	5.49	127.64	120.28
1	E	453	LEU	C-N-CA	5.49	127.64	120.28
1	B	453	LEU	CA-C-N	5.48	127.63	120.28
1	B	453	LEU	C-N-CA	5.48	127.63	120.28
1	F	514	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	482	PHE	CA-CB-CG	-5.39	108.41	113.80
1	H	453	LEU	CA-C-N	5.38	127.48	120.28
1	H	453	LEU	C-N-CA	5.38	127.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	514	PHE	CA-CB-CG	5.33	119.13	113.80
1	C	340	THR	N-CA-C	5.32	118.16	109.59
1	A	453	LEU	CA-C-N	5.31	127.39	120.28
1	A	453	LEU	C-N-CA	5.31	127.39	120.28
1	B	488	GLU	N-CA-C	5.28	115.67	109.60
1	D	507	GLU	CA-C-N	5.26	127.28	120.44
1	D	507	GLU	C-N-CA	5.26	127.28	120.44
1	D	504	PHE	CA-C-N	5.26	125.82	119.98
1	D	504	PHE	C-N-CA	5.26	125.82	119.98
1	D	514	PHE	CA-CB-CG	5.19	118.99	113.80
1	D	453	LEU	CA-C-N	5.15	127.69	120.28
1	D	453	LEU	C-N-CA	5.15	127.69	120.28
1	H	340	THR	N-CA-C	5.15	118.14	109.95
1	H	340	THR	CA-C-N	5.14	129.63	122.08
1	H	340	THR	C-N-CA	5.14	129.63	122.08
1	D	515	LEU	CA-C-N	5.14	130.66	122.59
1	D	515	LEU	C-N-CA	5.14	130.66	122.59
1	F	453	LEU	CA-C-N	5.09	127.09	120.28
1	F	453	LEU	C-N-CA	5.09	127.09	120.28
1	C	496	ASP	CA-C-N	5.03	127.02	120.28
1	C	496	ASP	C-N-CA	5.03	127.02	120.28

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	3231	0	3274	30	0
1	B	3228	0	3277	36	0
1	C	3225	0	3268	33	0
1	D	3216	0	3263	41	0
1	E	3253	0	3298	30	0
1	F	3282	0	3330	48	0
1	G	3209	0	3255	27	0
1	H	3209	0	3256	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	1	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
2	E	6	0	0	0	0
2	F	6	0	0	1	0
2	G	6	0	0	0	0
2	H	6	0	0	0	0
3	A	33	21	0	1	0
3	F	33	21	0	3	0
3	G	33	21	0	1	0
3	H	33	21	0	1	0
4	A	20	10	10	2	0
4	B	20	10	10	1	0
4	C	20	10	10	1	0
4	D	20	10	10	6	0
4	E	20	10	10	3	0
4	F	20	10	10	5	0
4	G	20	10	10	1	0
4	H	20	10	10	3	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	2	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
6	C	2	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
7	A	121	0	0	2	0
7	B	113	0	0	0	0
7	C	116	0	0	1	0
7	D	101	0	0	2	0
7	E	37	0	0	1	0
7	F	36	0	0	1	0
7	G	25	0	0	0	0
7	H	33	0	0	0	0
All	All	26787	164	26301	247	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 (247) 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:H:89:SER:HA	1:H:127:LYS:HD2	1.18	1.16
1:A:60:ILE:HB	1:A:372:MET:HG3	1.42	1.00
1:A:405:GLN:HE22	1:E:405:GLN:HE22	1.18	0.85
1:D:494:TRP:HH2	4:D:602:FBP:H11	1.40	0.85
1:A:68:ARG:NH2	1:A:98:GLU:HB3	1.94	0.82
1:F:411:ARG:HH21	1:H:411:ARG:NH2	1.83	0.77
1:B:494:TRP:HZ3	4:B:602:FBP:O1P	1.68	0.76
1:H:482:PHE:HE2	1:H:512:ARG:NH1	1.84	0.75
1:F:411:ARG:NH2	1:H:411:ARG:HH21	1.85	0.75
1:H:482:PHE:HE2	1:H:512:ARG:HH12	1.34	0.75
1:A:68:ARG:HH22	1:A:98:GLU:HB3	1.50	0.74
1:C:29:GLN:HE22	1:C:46:ASP:H	1.34	0.74
1:F:28:GLN:HG2	1:F:52:VAL:H	1.50	0.74
1:F:411:ARG:NH2	1:H:411:ARG:NH2	2.37	0.72
1:H:89:SER:CA	1:H:127:LYS:HD2	2.12	0.68
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.77	0.66
1:E:411:ARG:NH2	1:G:411:ARG:HH21	1.96	0.63
1:E:67:SER:HB2	1:E:76:MET:HE1	1.79	0.63
1:E:411:ARG:HH21	1:G:411:ARG:NH2	1.96	0.63
1:B:354:ARG:HG2	1:F:341:GLN:NE2	2.14	0.62
1:B:354:ARG:HG2	1:F:341:GLN:HE21	1.65	0.62
1:E:411:ARG:NH2	1:G:411:ARG:NH2	2.48	0.61
1:H:233:LEU:HD23	1:H:233:LEU:H	1.64	0.61
1:G:501:ARG:NH1	4:G:4003:FBP:O2P	2.29	0.60
1:D:286:HIS:HE1	1:H:48:ASP:OD1	1.85	0.59
1:A:308:ASP:OD2	2:A:601:OXL:O2	2.20	0.59
1:H:482:PHE:CE2	1:H:512:ARG:NH1	2.69	0.59
1:D:523:VAL:HG21	1:D:540:LEU:HD12	1.85	0.58
1:A:48:ASP:OD1	1:E:286:HIS:HE1	1.86	0.58
1:C:242:ARG:HH22	1:C:271:GLY:HA3	1.68	0.58
1:F:17:THR:HG22	1:F:25:PHE:CD2	2.38	0.58
1:E:28:GLN:HG2	1:E:52:VAL:H	1.66	0.58
1:H:472:ALA:O	1:H:483:PRO:HG3	2.04	0.58
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.86	0.58
1:G:56:SER:HB2	1:G:480:GLY:HA2	1.86	0.58
1:D:494:TRP:CH2	4:D:602:FBP:H11	2.30	0.57
1:F:67:SER:HB2	1:F:76:MET:HE1	1.87	0.57
1:B:434:LYS:HG2	1:D:426:ILE:HD11	1.87	0.57
1:F:494:TRP:HH2	4:F:603:FBP:H62	1.69	0.57
1:G:337:VAL:HG22	1:G:370:CYS:HB2	1.86	0.57
1:F:337:VAL:HG22	1:F:370:CYS:HB2	1.87	0.57
1:A:331:LEU:HG	1:E:39:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:OD1	1:F:286:HIS:HE1	1.88	0.57
1:D:251:ILE:HG12	1:D:477:LEU:HD11	1.87	0.56
1:E:337:VAL:HG22	1:E:370:CYS:HB2	1.87	0.56
1:C:286:HIS:HE1	1:G:48:ASP:OD1	1.88	0.56
1:B:354:ARG:H	1:F:341:GLN:NE2	2.03	0.56
1:H:251:ILE:HG12	1:H:477:LEU:HD11	1.88	0.56
1:E:256:PHE:O	1:E:258:ARG:HD2	2.06	0.56
1:F:56:SER:HB2	1:F:480:GLY:HA2	1.87	0.55
1:G:535:ASN:ND2	1:G:536:ILE:HG13	2.22	0.55
1:B:39:LEU:HD11	1:F:331:LEU:HG	1.89	0.55
1:B:286:HIS:HE1	1:F:48:ASP:OD1	1.88	0.55
1:H:337:VAL:HG22	1:H:370:CYS:HB2	1.88	0.55
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.89	0.55
3:A:602:A1JB0:C13	7:A:813:HOH:O	2.55	0.54
1:B:411:ARG:HH21	1:D:411:ARG:NH2	2.05	0.54
1:C:486:TYR:CZ	1:C:488:GLU:HB2	2.43	0.54
1:C:272:PRO:HD2	1:C:273:GLU:OE2	2.08	0.54
1:F:404:ARG:HG2	7:F:733:HOH:O	2.08	0.54
1:A:494:TRP:HZ3	4:A:603:FBP:O5P	1.91	0.53
1:D:337:VAL:HG22	1:D:370:CYS:HB2	1.90	0.53
1:F:28:GLN:HG3	1:F:52:VAL:HG22	1.89	0.53
1:F:475:VAL:CG1	1:F:483:PRO:HB3	2.38	0.53
1:B:411:ARG:NH2	1:D:411:ARG:HH21	2.05	0.53
1:D:275:HIS:HB2	7:D:745:HOH:O	2.08	0.53
1:E:530:GLY:O	4:E:602:FBP:O4	2.24	0.53
1:C:269:ALA:C	1:C:271:GLY:H	2.17	0.52
1:C:331:LEU:HG	1:G:39:LEU:HD21	1.90	0.52
1:H:494:TRP:HH2	4:H:603:FBP:H11	1.73	0.52
1:F:251:ILE:HG12	1:F:477:LEU:HD11	1.92	0.52
1:D:42:LEU:HD12	3:H:601:A1JB0:C12	2.40	0.52
1:D:501:ARG:NH1	4:D:602:FBP:O3P	2.38	0.52
1:E:56:SER:HB2	1:E:480:GLY:HA2	1.90	0.52
1:H:382:PHE:HB3	1:H:385:GLU:HB2	1.92	0.51
1:G:251:ILE:HG12	1:G:477:LEU:HD11	1.92	0.51
1:B:411:ARG:NH2	1:D:411:ARG:NH2	2.58	0.51
1:F:14:ALA:HB1	1:F:17:THR:HG23	1.92	0.51
1:B:60:ILE:HB	1:B:372:MET:HG3	1.93	0.51
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.93	0.51
1:B:94:GLU:O	1:B:98:GLU:HG3	2.10	0.51
1:B:430:GLU:OE2	1:D:430:GLU:OE2	2.29	0.51
1:D:28:GLN:HB3	1:D:52:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:LYS:NZ	1:F:236:GLN:HG2	2.26	0.51
1:C:56:SER:HB2	1:C:480:GLY:CA	2.41	0.51
1:F:16:LEU:HD22	1:F:20:LEU:HD22	1.93	0.50
1:E:251:ILE:HG12	1:E:477:LEU:HD11	1.93	0.50
1:F:494:TRP:CH2	4:F:603:FBP:H62	2.46	0.50
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.92	0.50
1:D:330:ASN:HD21	1:D:367:GLY:HA3	1.77	0.50
1:F:531:SER:HB2	4:F:603:FBP:O1P	2.11	0.50
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.94	0.50
1:B:423:VAL:HG21	1:D:435:CYS:HB3	1.94	0.49
1:F:284:GLU:OE2	2:F:601:OXL:O3	2.30	0.49
1:B:39:LEU:HD23	3:F:602:A1JB0:C12	2.42	0.49
1:H:24:PHE:HD1	1:H:30:LEU:HD13	1.78	0.49
1:C:382:PHE:HB3	1:C:385:GLU:HB2	1.93	0.49
1:E:382:PHE:HB3	1:E:385:GLU:HB2	1.94	0.49
1:G:382:PHE:HB3	1:G:385:GLU:HB2	1.94	0.49
1:F:382:PHE:HB3	1:F:385:GLU:HB2	1.92	0.49
1:C:251:ILE:HG12	1:C:477:LEU:HD11	1.95	0.49
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.93	0.49
1:G:60:ILE:HB	1:G:372:MET:HG3	1.95	0.49
1:A:404:ARG:HH22	1:A:459:ARG:HH22	1.61	0.49
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.95	0.49
1:G:330:ASN:HD21	1:G:367:GLY:HA3	1.77	0.49
1:A:405:GLN:NE2	1:E:405:GLN:HE22	1.97	0.48
1:B:330:ASN:HD21	1:B:367:GLY:HA3	1.76	0.48
1:F:475:VAL:HG12	1:F:483:PRO:HB3	1.95	0.48
1:C:330:ASN:HD21	1:C:367:GLY:HA3	1.78	0.48
1:H:340:THR:HG22	1:H:341:GLN:HG3	1.96	0.48
1:H:306:ARG:HA	1:H:309:LEU:HB3	1.96	0.48
1:A:25[B]:PHE:CD1	1:A:27:GLN:HG3	2.49	0.48
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.94	0.48
1:F:538:ARG:HG2	1:H:536:ILE:HG12	1.96	0.48
7:C:814:HOH:O	1:G:39:LEU:HD22	2.13	0.48
1:B:30:LEU:O	1:B:34:MET:HG2	2.13	0.47
1:E:304:VAL:HG22	1:E:325:MET:HE3	1.96	0.47
1:F:60:ILE:HB	1:F:372:MET:HG3	1.96	0.47
1:A:407:PHE:CZ	1:A:411:ARG:HD2	2.50	0.47
1:B:382:PHE:HB3	1:B:385:GLU:HB2	1.95	0.47
1:D:67:SER:HB2	1:D:76:MET:HE1	1.97	0.47
1:B:72:ARG:HG3	1:B:76:MET:HE2	1.97	0.47
1:G:257:VAL:HG11	1:G:281:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:ASN:HD21	1:E:367:GLY:HA3	1.79	0.47
1:F:330:ASN:HD21	1:F:367:GLY:HA3	1.77	0.47
1:D:60:ILE:HB	1:D:372:MET:HG3	1.96	0.47
1:H:330:ASN:HD21	1:H:367:GLY:HA3	1.78	0.47
1:C:501:ARG:NH1	4:C:602:FBP:O6P	2.35	0.47
1:B:251:ILE:HG12	1:B:477:LEU:HD11	1.97	0.46
1:D:494:TRP:HH2	4:D:602:FBP:C1	2.18	0.46
1:H:60:ILE:HB	1:H:372:MET:HG3	1.97	0.46
1:A:494:TRP:HH2	4:A:603:FBP:O6	1.97	0.46
1:B:68:ARG:NH2	1:B:95:TYR:O	2.48	0.46
1:B:76:MET:HG2	1:B:387:VAL:HG21	1.96	0.46
1:C:259:LYS:O	1:C:262:ASP:HB2	2.15	0.46
1:E:530:GLY:C	4:E:602:FBP:HO4	2.22	0.46
1:C:30:LEU:O	1:C:34:MET:HG2	2.15	0.46
1:F:333:GLY:HA3	1:F:455:ARG:HD2	1.97	0.46
1:H:233:LEU:HD22	1:H:265:ALA:HB1	1.97	0.46
1:H:89:SER:HA	1:H:127:LYS:CD	2.13	0.46
1:A:251:ILE:HG12	1:A:477:LEU:HD11	1.97	0.46
1:C:304:VAL:HG22	1:C:325:MET:HE3	1.98	0.46
1:D:233:LEU:HD22	1:D:237:ASP:HB3	1.97	0.46
1:D:423:VAL:O	1:D:426:ILE:HD12	2.16	0.46
1:F:501:ARG:NH1	4:F:603:FBP:O6P	2.41	0.46
1:A:330:ASN:HD21	1:A:367:GLY:HA3	1.80	0.45
1:C:278:LYS:HG2	1:C:474:GLN:NE2	2.31	0.45
1:D:241:LEU:HD13	1:D:269:ALA:HB3	1.97	0.45
1:C:60:ILE:HB	1:C:372:MET:HG3	1.97	0.45
1:C:494:TRP:CD1	1:C:529:PRO:HG3	2.52	0.45
1:D:486:TYR:CZ	1:D:488:GLU:HB2	2.52	0.45
1:H:421:THR:HG22	1:H:452:LEU:HD12	1.99	0.45
1:A:304:VAL:HG22	1:A:325:MET:HE3	1.98	0.45
1:E:60:ILE:HB	1:E:372:MET:HG3	1.97	0.45
1:A:247:HIS:HD2	7:A:794:HOH:O	1.99	0.45
1:D:304:VAL:HG22	1:D:325:MET:HE3	1.99	0.45
1:D:421:THR:HG22	1:D:452:LEU:HD12	1.98	0.45
1:H:304:VAL:HG22	1:H:325:MET:HE3	1.97	0.45
1:D:531:SER:HA	4:D:602:FBP:H5	1.98	0.45
1:F:330:ASN:HD22	3:F:602:A1JB0:C13	2.30	0.45
1:A:411:ARG:NH1	1:C:404:ARG:HH21	2.15	0.44
1:E:18:GLN:HA	7:E:736:HOH:O	2.17	0.44
1:F:304:VAL:HG22	1:F:325:MET:HE3	1.98	0.44
1:A:404:ARG:NH2	1:A:459:ARG:HH22	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:PRO:HB3	1:D:477:LEU:O	2.17	0.44
1:E:526:GLY:HA3	4:E:602:FBP:O3	2.16	0.44
1:D:267:ARG:HD2	1:D:275:HIS:HD2	1.83	0.44
1:G:421:THR:HG22	1:G:452:LEU:HD12	2.00	0.44
1:C:267:ARG:HD2	1:C:275:HIS:HD2	1.83	0.44
1:F:486:TYR:CZ	1:F:488:GLU:HB2	2.53	0.44
1:E:306:ARG:HH11	1:E:322:GLN:HE22	1.66	0.44
1:E:335:PRO:HB3	1:E:477:LEU:O	2.17	0.44
1:H:486:TYR:CZ	1:H:488:GLU:HB2	2.53	0.44
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.99	0.43
1:F:127:LYS:NZ	1:F:236:GLN:CG	2.81	0.43
1:G:304:VAL:HG22	1:G:325:MET:HE3	1.98	0.43
1:H:369:ASP:HA	1:H:479:ARG:HB2	2.01	0.43
1:A:536:ILE:HG12	1:C:538:ARG:HG2	2.00	0.43
1:D:444:THR:HA	4:D:602:FBP:H61	1.99	0.43
1:E:114:PRO:HB3	1:E:487:ARG:HE	1.83	0.43
1:E:421:THR:HG22	1:E:452:LEU:HD12	1.99	0.43
1:A:335:PRO:HB3	1:A:477:LEU:O	2.17	0.43
1:A:430:GLU:OE2	1:C:430:GLU:OE2	2.35	0.43
1:B:39:LEU:HD23	3:F:602:A1JB0:C13	2.49	0.43
1:F:421:THR:HG22	1:F:452:LEU:HD12	1.99	0.43
1:B:354:ARG:H	1:F:341:GLN:HE21	1.67	0.43
1:F:114:PRO:HB3	1:F:487:ARG:HE	1.84	0.43
1:F:335:PRO:HB3	1:F:477:LEU:O	2.18	0.43
1:H:233:LEU:H	1:H:233:LEU:CD2	2.31	0.43
1:B:68:ARG:NH1	1:B:98:GLU:OE2	2.35	0.43
1:C:335:PRO:HB3	1:C:477:LEU:O	2.19	0.43
1:C:369:ASP:HA	1:C:479:ARG:HB2	2.01	0.43
1:F:127:LYS:HZ1	1:F:236:GLN:HG2	1.83	0.43
1:H:130:GLY:HA2	1:H:229:SER:HA	1.70	0.43
1:B:304:VAL:HG22	1:B:325:MET:HE3	2.00	0.43
1:B:536:ILE:HG12	1:D:538:ARG:HG2	2.01	0.43
1:F:536:ILE:HG12	1:H:538:ARG:HG2	2.01	0.43
1:G:257:VAL:CG1	1:G:281:SER:HB3	2.49	0.43
1:G:493:ILE:CG2	1:G:496:ASP:OD2	2.66	0.43
1:A:369:ASP:HA	1:A:479:ARG:HB2	2.01	0.43
1:B:335:PRO:HB3	1:B:477:LEU:O	2.19	0.43
1:G:369:ASP:HA	1:G:479:ARG:HB2	2.01	0.43
1:F:462:VAL:HG12	1:F:481:VAL:HG13	2.01	0.42
1:A:434:LYS:CE	1:C:426:ILE:HD11	2.49	0.42
1:F:67:SER:HB2	1:F:76:MET:CE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:ASP:HA	1:F:479:ARG:HB2	2.01	0.42
1:F:530:GLY:O	4:F:603:FBP:O2	2.35	0.42
1:D:412:ARG:HD3	7:D:794:HOH:O	2.19	0.42
1:B:423:VAL:CG2	1:D:435:CYS:HB3	2.49	0.42
1:H:372:MET:HE3	1:H:374:SER:HB3	2.02	0.42
1:D:73:LEU:HD23	1:D:76:MET:CE	2.49	0.42
1:H:30:LEU:O	1:H:34:MET:HG2	2.19	0.42
1:D:426:ILE:HG23	1:D:456:TYR:CE1	2.55	0.42
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.20	0.42
1:G:335:PRO:HB3	1:G:477:LEU:O	2.19	0.42
1:E:486:TYR:CZ	1:E:488:GLU:HB2	2.55	0.42
1:G:257:VAL:HG11	1:G:281:SER:CB	2.50	0.42
1:A:436:CYS:SG	1:C:416:LEU:HD13	2.61	0.41
1:D:369:ASP:HA	1:D:479:ARG:HB2	2.02	0.41
1:G:39:LEU:HD13	3:G:4001:A1JB0:C13	2.50	0.41
1:G:372:MET:HE3	1:G:374:SER:HB3	2.02	0.41
1:B:421:THR:HG22	1:B:452:LEU:HD12	2.02	0.41
1:B:114:PRO:HB3	1:B:487:ARG:HE	1.85	0.41
1:G:377:THR:HA	1:G:383:PRO:HB3	2.02	0.41
1:H:444:THR:OG1	4:H:603:FBP:O5P	2.34	0.41
1:H:531:SER:HB2	4:H:603:FBP:O4P	2.20	0.41
1:C:129:PRO:HG2	1:C:258:ARG:NH2	2.36	0.41
1:D:372:MET:HE3	1:D:374:SER:HB3	2.02	0.41
1:E:30:LEU:O	1:E:34:MET:HG2	2.20	0.41
1:E:369:ASP:HA	1:E:479:ARG:HB2	2.03	0.41
1:F:429:VAL:HG21	1:F:456:TYR:HB2	2.03	0.41
1:A:67:SER:HB2	1:A:76:MET:HE1	2.02	0.41
1:B:65:PRO:HG3	1:C:500:ARG:HG3	2.03	0.41
1:H:335:PRO:HB3	1:H:477:LEU:O	2.20	0.41
1:D:306:ARG:HH11	1:D:322:GLN:HE22	1.69	0.40
1:E:407:PHE:CZ	1:E:411:ARG:HD3	2.56	0.40
1:H:407:PHE:CZ	1:H:411:ARG:HD3	2.55	0.40
1:C:89:SER:HA	1:C:127:LYS:HG3	2.02	0.40
1:E:372:MET:HE3	1:E:374:SER:HB3	2.03	0.40
1:B:369:ASP:HA	1:B:479:ARG:HB2	2.03	0.40
1:C:429:VAL:HG21	1:C:456:TYR:HB2	2.02	0.40
1:H:114:PRO:HB3	1:H:487:ARG:HE	1.86	0.40
1:A:267:ARG:HA	1:A:267:ARG:HD3	1.96	0.40
1:F:407:PHE:CZ	1:F:411:ARG:HD3	2.56	0.40
1:G:429:VAL:HG21	1:G:456:TYR:HB2	2.03	0.40
1:G:486:TYR:CZ	1:G:488:GLU:HG2	2.56	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	424/447 (95%)	412 (97%)	11 (3%)	1 (0%)	44	44
1	B	424/447 (95%)	418 (99%)	5 (1%)	1 (0%)	44	44
1	C	423/447 (95%)	415 (98%)	7 (2%)	1 (0%)	44	44
1	D	422/447 (94%)	417 (99%)	3 (1%)	2 (0%)	25	20
1	E	427/447 (96%)	422 (99%)	5 (1%)	0	100	100
1	F	431/447 (96%)	425 (99%)	6 (1%)	0	100	100
1	G	421/447 (94%)	414 (98%)	7 (2%)	0	100	100
1	H	421/447 (94%)	409 (97%)	12 (3%)	0	100	100
All	All	3393/3576 (95%)	3332 (98%)	56 (2%)	5 (0%)	48	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	PRO
1	A	130	GLY
1	C	271	GLY
1	D	130	GLY
1	D	535	ASN

5.3.2 Protein sidechains [i](#)

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	337/352 (96%)	322 (96%)	15 (4%)	23	21
1	B	337/352 (96%)	323 (96%)	14 (4%)	25	24
1	C	337/352 (96%)	326 (97%)	11 (3%)	33	33
1	D	336/352 (96%)	321 (96%)	15 (4%)	23	21
1	E	340/352 (97%)	328 (96%)	12 (4%)	31	30
1	F	343/352 (97%)	326 (95%)	17 (5%)	20	17
1	G	335/352 (95%)	318 (95%)	17 (5%)	20	16
1	H	335/352 (95%)	320 (96%)	15 (4%)	23	21
All	All	2700/2816 (96%)	2584 (96%)	116 (4%)	25	23

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	34	MET
1	A	50	GLU
1	A	52	VAL
1	A	98	GLU
1	A	229	SER
1	A	273	GLU
1	A	284	GLU
1	A	285	ASN
1	A	331	LEU
1	A	404	ARG
1	A	408	GLU
1	A	426	ILE
1	A	537	MET
1	B	20	LEU
1	B	22	THR
1	B	26	GLN
1	B	39	LEU
1	B	50	GLU
1	B	98	GLU
1	B	273	GLU
1	B	284	GLU
1	B	285	ASN
1	B	331	LEU
1	B	404	ARG
1	B	408	GLU

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Mol	Chain	Res	Type
1	B	426	ILE
1	B	537	MET
1	C	26	GLN
1	C	75	GLU
1	C	89	SER
1	C	284	GLU
1	C	285	ASN
1	C	294	GLU
1	C	331	LEU
1	C	404	ARG
1	C	426	ILE
1	C	443	LEU
1	C	537	MET
1	D	34	MET
1	D	50	GLU
1	D	75	GLU
1	D	116	SER
1	D	284	GLU
1	D	285	ASN
1	D	331	LEU
1	D	404	ARG
1	D	418	ARG
1	D	426	ILE
1	D	436	CYS
1	D	455	ARG
1	D	478	CYS
1	D	515	LEU
1	D	537	MET
1	E	17	THR
1	E	18	GLN
1	E	118	ARG
1	E	258	ARG
1	E	284	GLU
1	E	285	ASN
1	E	331	LEU
1	E	404	ARG
1	E	408	GLU
1	E	426	ILE
1	E	500	ARG
1	E	537	MET
1	F	15	GLN
1	F	16	LEU

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Mol	Chain	Res	Type
1	F	28	GLN
1	F	34	MET
1	F	44	LEU
1	F	49	SER
1	F	52	VAL
1	F	235	GLU
1	F	273	GLU
1	F	284	GLU
1	F	285	ASN
1	F	331	LEU
1	F	404	ARG
1	F	408	GLU
1	F	426	ILE
1	F	475	VAL
1	F	488	GLU
1	G	25	PHE
1	G	28	GLN
1	G	34	MET
1	G	50	GLU
1	G	71	GLU
1	G	257	VAL
1	G	284	GLU
1	G	285	ASN
1	G	311	ILE
1	G	331	LEU
1	G	404	ARG
1	G	426	ILE
1	G	441	ILE
1	G	488	GLU
1	G	493	ILE
1	G	535	ASN
1	G	537	MET
1	H	24	PHE
1	H	25	PHE
1	H	27	GLN
1	H	28	GLN
1	H	50	GLU
1	H	273	GLU
1	H	284	GLU
1	H	285	ASN
1	H	331	LEU
1	H	340	THR

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Mol	Chain	Res	Type
1	H	404	ARG
1	H	408	GLU
1	H	426	ILE
1	H	488	GLU
1	H	537	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	90	HIS
1	A	247	HIS
1	A	286	HIS
1	A	330	ASN
1	A	381	ASN
1	A	390	GLN
1	A	405	GLN
1	A	503	GLN
1	B	90	HIS
1	B	286	HIS
1	B	330	ASN
1	B	390	GLN
1	B	503	GLN
1	C	29	GLN
1	C	90	HIS
1	C	275	HIS
1	C	286	HIS
1	C	330	ASN
1	C	381	ASN
1	C	390	GLN
1	C	474	GLN
1	D	26	GLN
1	D	28	GLN
1	D	275	HIS
1	D	286	HIS
1	D	322	GLN
1	D	330	ASN
1	D	390	GLN
1	D	503	GLN
1	E	18	GLN
1	E	286	HIS
1	E	322	GLN

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Mol	Chain	Res	Type
1	E	330	ASN
1	F	286	HIS
1	F	330	ASN
1	F	341	GLN
1	F	390	GLN
1	F	503	GLN
1	G	87	ASN
1	G	90	HIS
1	G	330	ASN
1	G	390	GLN
1	G	503	GLN
1	G	535	ASN
1	H	26	GLN
1	H	90	HIS
1	H	286	HIS
1	H	330	ASN
1	H	381	ASN
1	H	390	GLN
1	H	503	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 12 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	OXL	A	601	5	5,5,5	1.89	2 (40%)	6,6,6	1.12	1 (16%)
2	OXL	G	4002	5	5,5,5	1.85	2 (40%)	6,6,6	1.35	1 (16%)
3	A1JB0	H	601	-	33,37,37	0.73	1 (3%)	43,57,57	0.52	0
2	OXL	F	601	5	5,5,5	2.03	2 (40%)	6,6,6	1.31	1 (16%)
3	A1JB0	F	602	-	33,37,37	0.67	1 (3%)	43,57,57	0.53	0
4	FBP	B	602	-	18,20,20	0.64	0	23,32,32	1.23	3 (13%)
2	OXL	H	602	5	5,5,5	1.97	2 (40%)	6,6,6	1.11	1 (16%)
2	OXL	C	601	5	5,5,5	1.87	2 (40%)	6,6,6	1.11	1 (16%)
4	FBP	A	603	-	18,20,20	0.84	1 (5%)	23,32,32	1.70	5 (21%)
2	OXL	D	601	5	5,5,5	2.12	2 (40%)	6,6,6	1.08	0
4	FBP	H	603	-	18,20,20	0.56	0	23,32,32	1.09	2 (8%)
3	A1JB0	G	4001	-	33,37,37	0.62	1 (3%)	43,57,57	0.58	0
2	OXL	B	601	5	5,5,5	2.01	2 (40%)	6,6,6	1.08	0
4	FBP	F	603	-	18,20,20	0.49	0	23,32,32	1.12	3 (13%)
4	FBP	C	602	-	18,20,20	0.39	0	23,32,32	1.13	1 (4%)
4	FBP	E	602	-	18,20,20	0.62	0	23,32,32	1.19	2 (8%)
3	A1JB0	A	602	-	33,37,37	0.60	1 (3%)	43,57,57	0.56	0
4	FBP	G	4003	-	18,20,20	0.51	0	23,32,32	0.76	1 (4%)
4	FBP	D	602	-	18,20,20	1.46	3 (16%)	23,32,32	1.68	4 (17%)
2	OXL	E	601	5	5,5,5	1.96	2 (40%)	6,6,6	1.22	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	OXL	A	601	5	-	0/4/4/4	-
2	OXL	G	4002	5	-	0/4/4/4	-
3	A1JB0	H	601	-	-	3/28/44/44	0/5/5/5
2	OXL	F	601	5	-	0/4/4/4	-
3	A1JB0	F	602	-	-	14/28/44/44	0/5/5/5
4	FBP	B	602	-	-	6/13/32/32	0/1/1/1
2	OXL	H	602	5	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OXL	C	601	5	-	0/4/4/4	-
4	FBP	A	603	-	-	7/13/32/32	0/1/1/1
2	OXL	D	601	5	-	0/4/4/4	-
4	FBP	H	603	-	-	4/13/32/32	0/1/1/1
3	A1JB0	G	4001	-	-	2/28/44/44	0/5/5/5
2	OXL	B	601	5	-	0/4/4/4	-
4	FBP	F	603	-	-	5/13/32/32	0/1/1/1
4	FBP	C	602	-	-	3/13/32/32	0/1/1/1
4	FBP	E	602	-	-	9/13/32/32	0/1/1/1
3	A1JB0	A	602	-	-	13/28/44/44	0/5/5/5
4	FBP	G	4003	-	-	5/13/32/32	0/1/1/1
4	FBP	D	602	-	-	11/13/32/32	0/1/1/1
2	OXL	E	601	5	-	0/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	FBP	P1-O1P	-3.95	1.37	1.50
2	F	601	OXL	O2-C2	3.68	1.32	1.22
2	B	601	OXL	O2-C2	3.59	1.32	1.22
2	D	601	OXL	O2-C2	3.57	1.32	1.22
2	H	602	OXL	O2-C2	3.36	1.31	1.22
2	A	601	OXL	O2-C2	3.23	1.31	1.22
2	C	601	OXL	O2-C2	3.20	1.31	1.22
2	E	601	OXL	O2-C2	3.14	1.31	1.22
2	G	4002	OXL	O2-C2	3.06	1.30	1.22
3	H	601	A1JB0	C8-C16	-2.91	1.40	1.42
3	F	602	A1JB0	C8-C16	-2.89	1.40	1.42
4	D	602	FBP	P2-O6	-2.77	1.51	1.60
2	E	601	OXL	O4-C2	-2.76	1.22	1.30
2	C	601	OXL	O4-C2	-2.66	1.22	1.30
2	G	4002	OXL	O4-C2	-2.59	1.23	1.30
2	A	601	OXL	O4-C2	-2.58	1.23	1.30
2	B	601	OXL	O4-C2	-2.58	1.23	1.30
2	H	602	OXL	O4-C2	-2.56	1.23	1.30
2	D	601	OXL	O4-C2	-2.53	1.23	1.30
3	A	602	A1JB0	C8-C16	-2.49	1.41	1.42
4	D	602	FBP	P2-O4P	-2.48	1.42	1.50
2	F	601	OXL	O4-C2	-2.24	1.24	1.30
4	A	603	FBP	P2-O6	-2.16	1.53	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4001	A1JB0	C8-C16	-2.02	1.41	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	FBP	P1-O1-C1	4.95	131.94	118.30
4	A	603	FBP	O6-P2-O4P	4.20	118.25	106.47
4	C	602	FBP	P1-O1-C1	4.14	129.69	118.30
4	B	602	FBP	O6-P2-O4P	3.92	117.47	106.47
4	H	603	FBP	O6-P2-O4P	3.80	117.14	106.47
4	A	603	FBP	P1-O1-C1	3.72	128.54	118.30
4	E	602	FBP	P2-O6-C6	3.68	128.44	118.30
4	A	603	FBP	O1-P1-O1P	3.49	116.26	106.47
4	F	603	FBP	O1-P1-O1P	3.36	115.91	106.47
4	D	602	FBP	P2-O6-C6	3.34	127.48	118.30
4	D	602	FBP	O1-P1-O1P	3.27	115.66	106.47
4	E	602	FBP	P1-O1-C1	2.93	126.37	118.30
4	F	603	FBP	P1-O1-C1	2.78	125.96	118.30
2	G	4002	OXL	O4-C2-C1	2.77	121.40	113.16
4	B	602	FBP	P1-O1-C1	2.72	125.80	118.30
2	F	601	OXL	O4-C2-C1	2.67	121.09	113.16
4	D	602	FBP	O6P-P2-O6	-2.45	100.21	106.73
4	F	603	FBP	P2-O6-C6	2.44	125.01	118.30
2	E	601	OXL	O4-C2-C1	2.29	119.97	113.16
4	G	4003	FBP	O6-P2-O4P	2.29	112.89	106.47
4	H	603	FBP	P1-O1-C1	2.27	124.54	118.30
4	B	602	FBP	O1-P1-O1P	2.23	112.74	106.47
2	H	602	OXL	O4-C2-C1	2.23	119.79	113.16
4	A	603	FBP	O5P-P2-O6	-2.23	100.81	106.73
2	A	601	OXL	O4-C2-C1	2.22	119.77	113.16
2	C	601	OXL	O4-C2-C1	2.18	119.64	113.16
4	A	603	FBP	P2-O6-C6	2.13	124.16	118.30

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	A1JB0	C16-C8-S1-O4
3	H	601	A1JB0	C15-C11-N2-C12
3	H	601	A1JB0	C10-C11-N2-C12
4	A	603	FBP	C1-O1-P1-O1P
4	A	603	FBP	C1-O1-P1-O3P

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Mol	Chain	Res	Type	Atoms
4	A	603	FBP	O1-C1-C2-O2
4	A	603	FBP	O1-C1-C2-C3
4	A	603	FBP	O1-C1-C2-O5
4	A	603	FBP	C4-C5-C6-O6
4	B	602	FBP	C1-O1-P1-O1P
4	B	602	FBP	C1-O1-P1-O2P
4	B	602	FBP	O1-C1-C2-C3
4	B	602	FBP	O1-C1-C2-O5
4	B	602	FBP	C4-C5-C6-O6
4	C	602	FBP	O1-C1-C2-O2
4	C	602	FBP	O1-C1-C2-C3
4	C	602	FBP	O1-C1-C2-O5
4	D	602	FBP	C1-O1-P1-O1P
4	D	602	FBP	C1-O1-P1-O2P
4	D	602	FBP	O1-C1-C2-O2
4	D	602	FBP	O1-C1-C2-C3
4	D	602	FBP	O1-C1-C2-O5
4	D	602	FBP	C6-O6-P2-O5P
4	D	602	FBP	C6-O6-P2-O6P
4	E	602	FBP	O1-C1-C2-O2
4	E	602	FBP	O1-C1-C2-C3
4	E	602	FBP	O1-C1-C2-O5
4	E	602	FBP	C6-O6-P2-O4P
4	E	602	FBP	C6-O6-P2-O5P
4	E	602	FBP	C6-O6-P2-O6P
4	G	4003	FBP	O1-C1-C2-O2
4	G	4003	FBP	O1-C1-C2-C3
4	G	4003	FBP	O1-C1-C2-O5
4	G	4003	FBP	C4-C5-C6-O6
4	H	603	FBP	C1-O1-P1-O1P
4	H	603	FBP	C1-O1-P1-O2P
4	H	603	FBP	C1-O1-P1-O3P
3	A	602	A1JB0	C17-N1-S1-O4
3	F	602	A1JB0	C17-N1-S1-O5
3	A	602	A1JB0	C17-N1-S1-C8
3	A	602	A1JB0	C6-N-S-O6
3	F	602	A1JB0	C17-N1-S1-C8
3	A	602	A1JB0	C17-N1-S1-O5
3	F	602	A1JB0	C6-N-S-O6
3	F	602	A1JB0	C18-N-S-O6
3	F	602	A1JB0	C6-N-S-O
3	A	602	A1JB0	C6-N-S-C

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Mol	Chain	Res	Type	Atoms
3	F	602	A1JB0	C17-N1-S1-O4
3	F	602	A1JB0	C18-N-S-O
3	F	602	A1JB0	C6-N-S-C
3	F	602	A1JB0	C18-N-S-C
4	D	602	FBP	C4-C5-C6-O6
4	D	602	FBP	O5-C5-C6-O6
3	A	602	A1JB0	C7-N1-S1-O5
3	A	602	A1JB0	C6-N-S-O
3	A	602	A1JB0	C7-N1-S1-O4
4	A	603	FBP	O5-C5-C6-O6
4	B	602	FBP	O5-C5-C6-O6
4	G	4003	FBP	O5-C5-C6-O6
3	A	602	A1JB0	C7-N1-S1-C8
3	F	602	A1JB0	C7-N1-S1-O4
3	F	602	A1JB0	C7-N1-S1-O5
3	A	602	A1JB0	C18-N-S-O
4	D	602	FBP	C6-O6-P2-O4P
3	A	602	A1JB0	C18-N-S-O6
4	F	603	FBP	C5-C6-O6-P2
3	A	602	A1JB0	C16-C8-S1-O5
3	G	4001	A1JB0	C16-C8-S1-O5
3	H	601	A1JB0	C10-C11-N2-C14
4	F	603	FBP	C6-O6-P2-O5P
4	F	603	FBP	C6-O6-P2-O6P
3	F	602	A1JB0	C7-N1-S1-C8
4	D	602	FBP	C2-C1-O1-P1
4	E	602	FBP	C1-O1-P1-O1P
4	F	603	FBP	C6-O6-P2-O4P
3	A	602	A1JB0	C18-N-S-C
3	F	602	A1JB0	C16-C8-S1-O5
3	G	4001	A1JB0	C15-C11-N2-C12
4	F	603	FBP	O1-C1-C2-C3
4	H	603	FBP	O1-C1-C2-C3
4	E	602	FBP	C1-O1-P1-O2P
4	E	602	FBP	O5-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 30 short contacts:

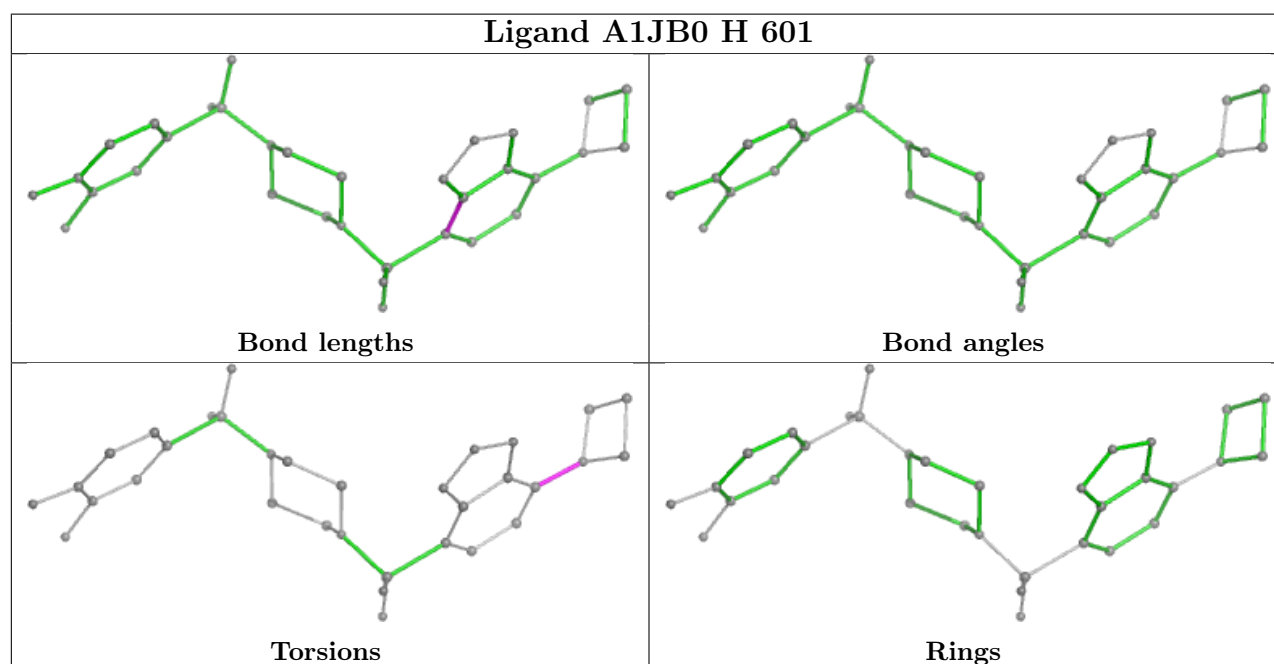
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	OXL	1	0
3	H	601	A1JB0	1	0

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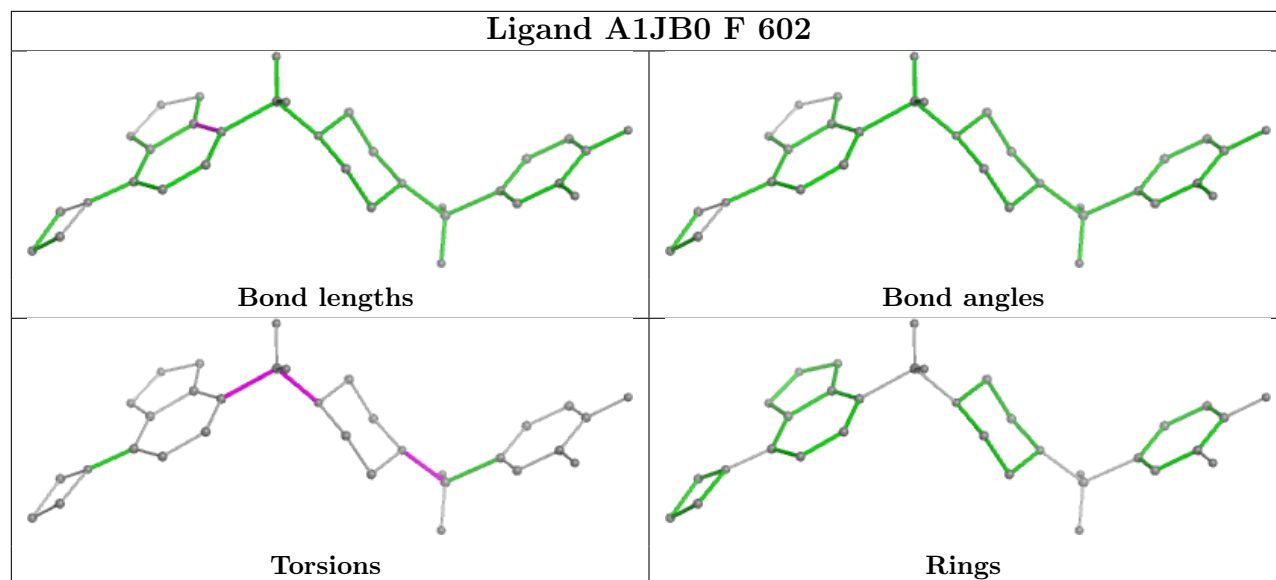
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	OXL	1	0
3	F	602	A1JB0	3	0
4	B	602	FBP	1	0
4	A	603	FBP	2	0
4	H	603	FBP	3	0
3	G	4001	A1JB0	1	0
4	F	603	FBP	5	0
4	C	602	FBP	1	0
4	E	602	FBP	3	0
3	A	602	A1JB0	1	0
4	G	4003	FBP	1	0
4	D	602	FBP	6	0

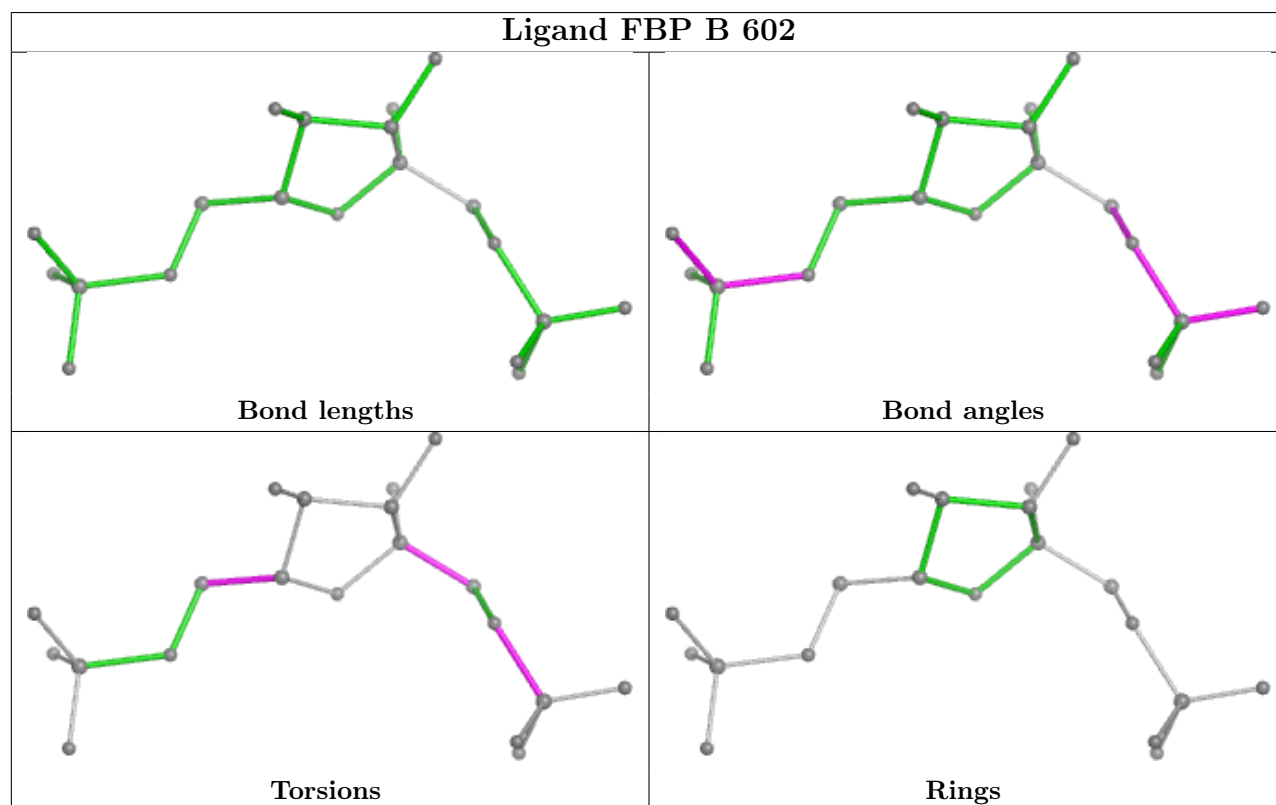
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

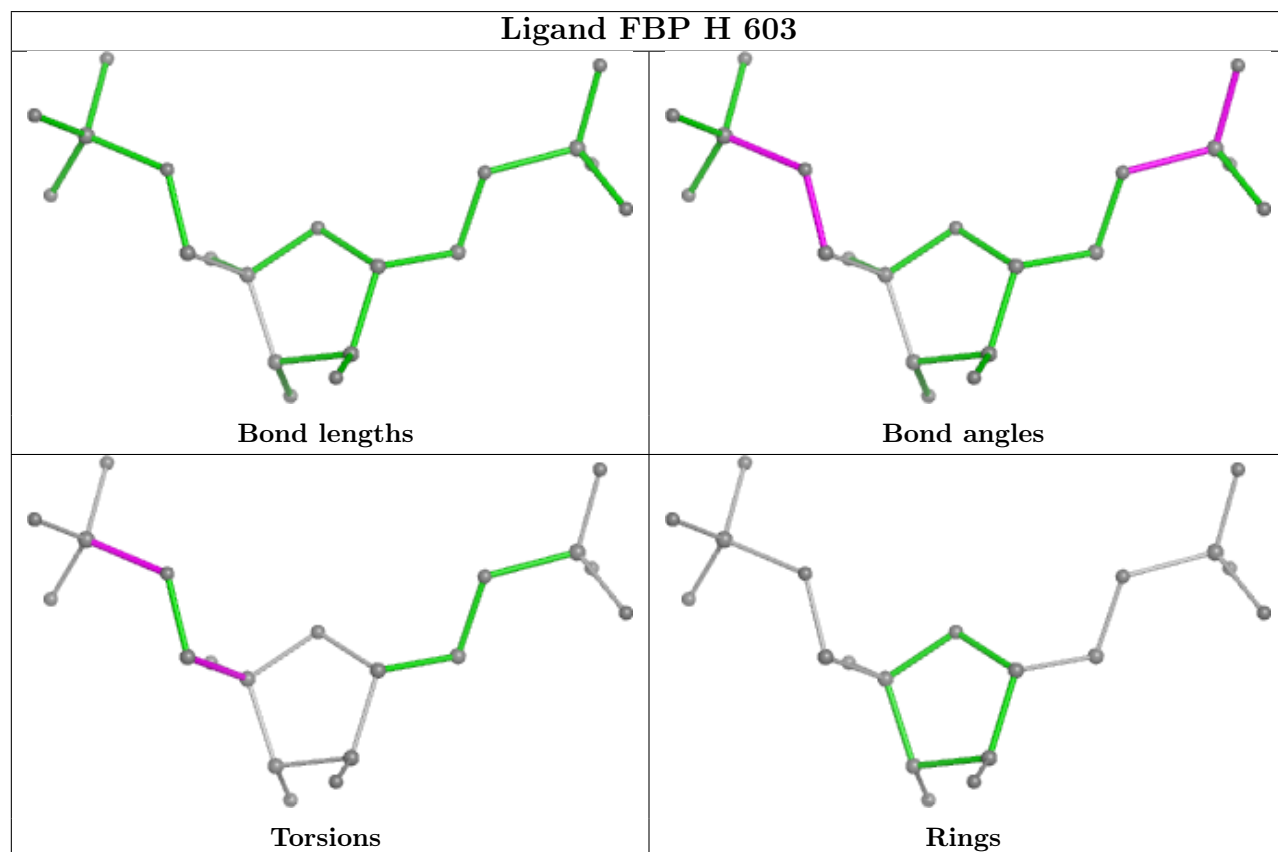
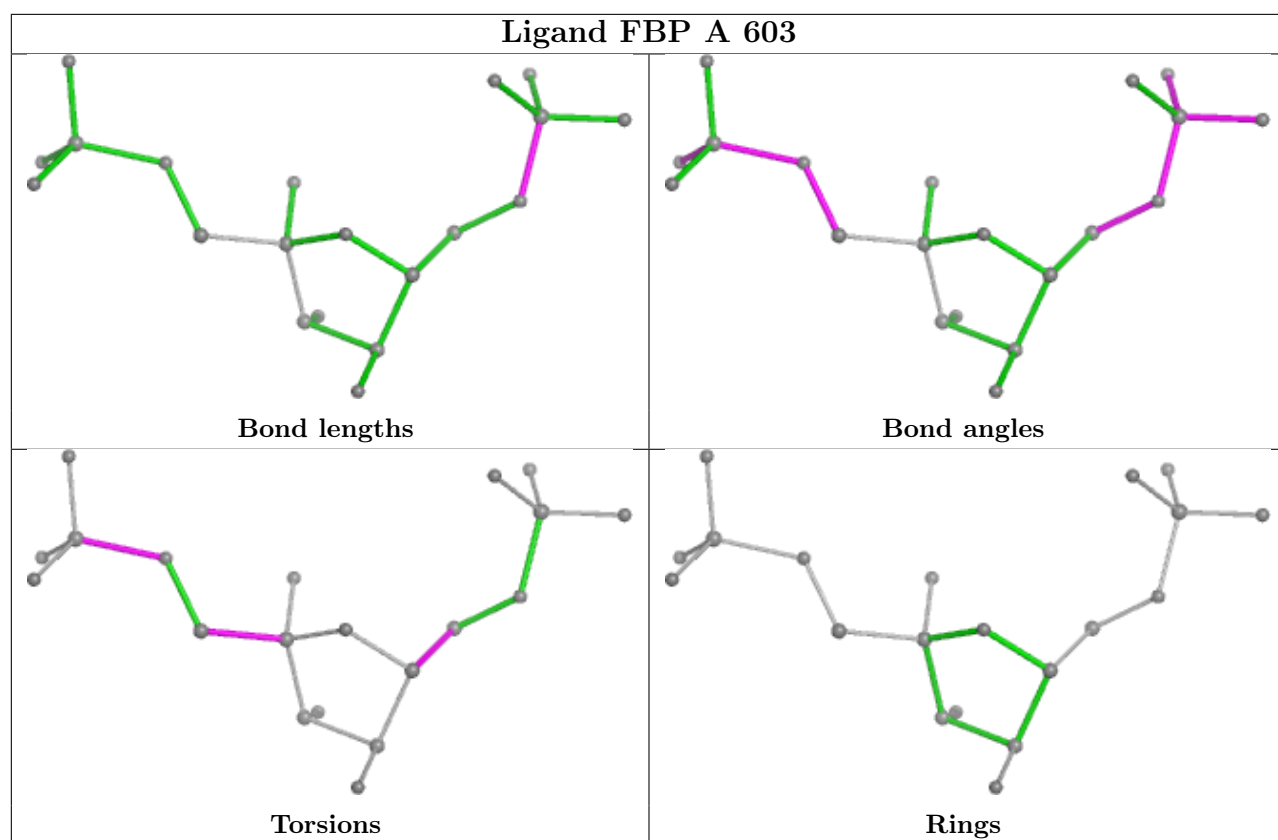


Ligand A1JB0 F 602

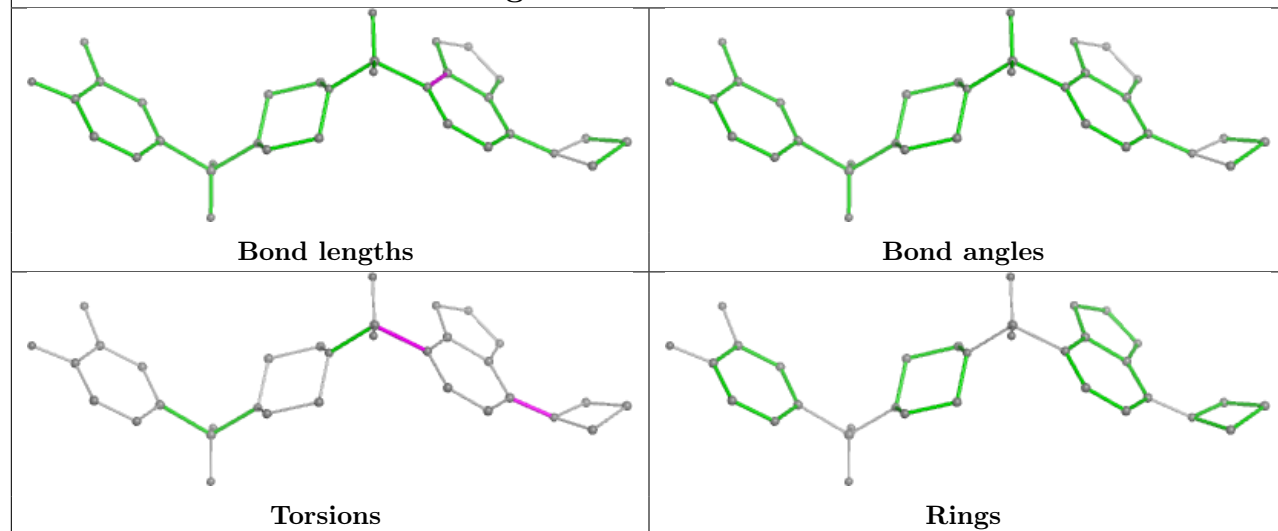


Ligand FBP B 602

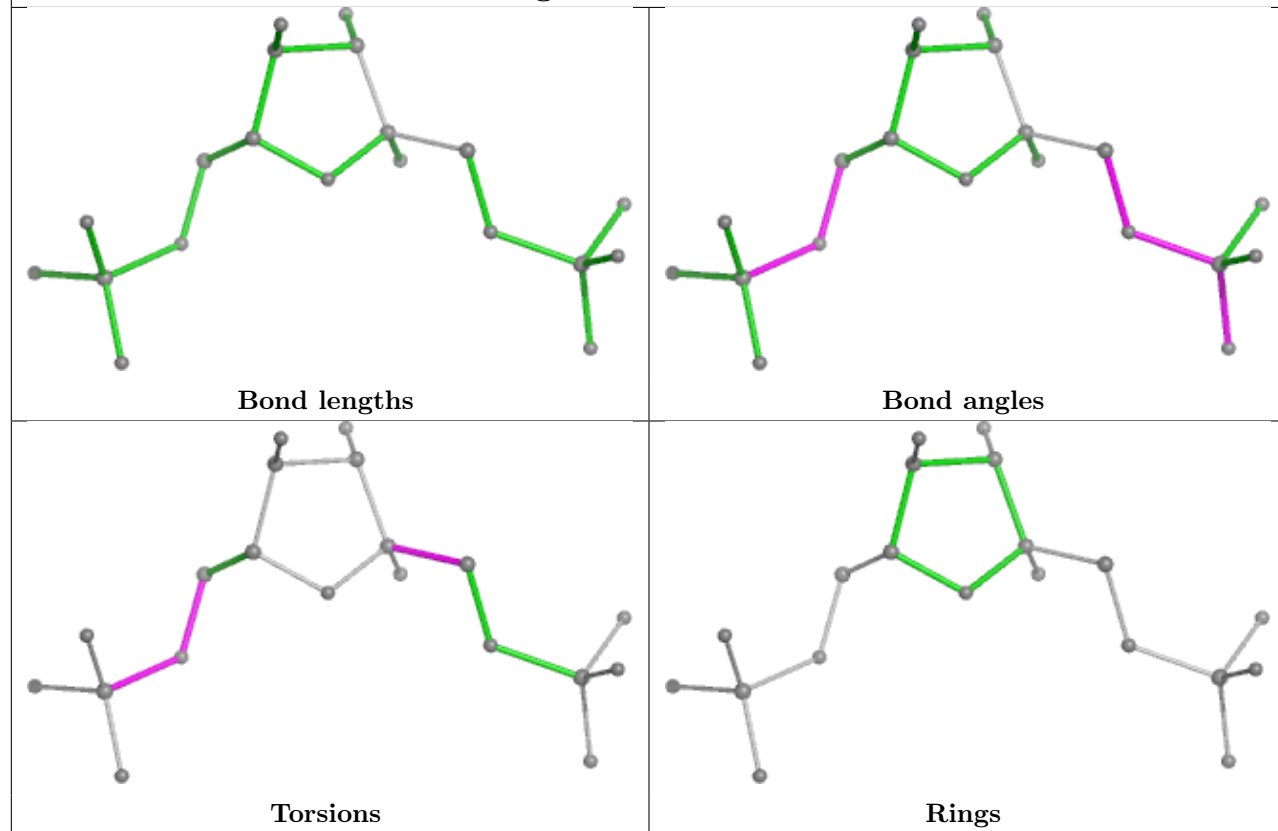




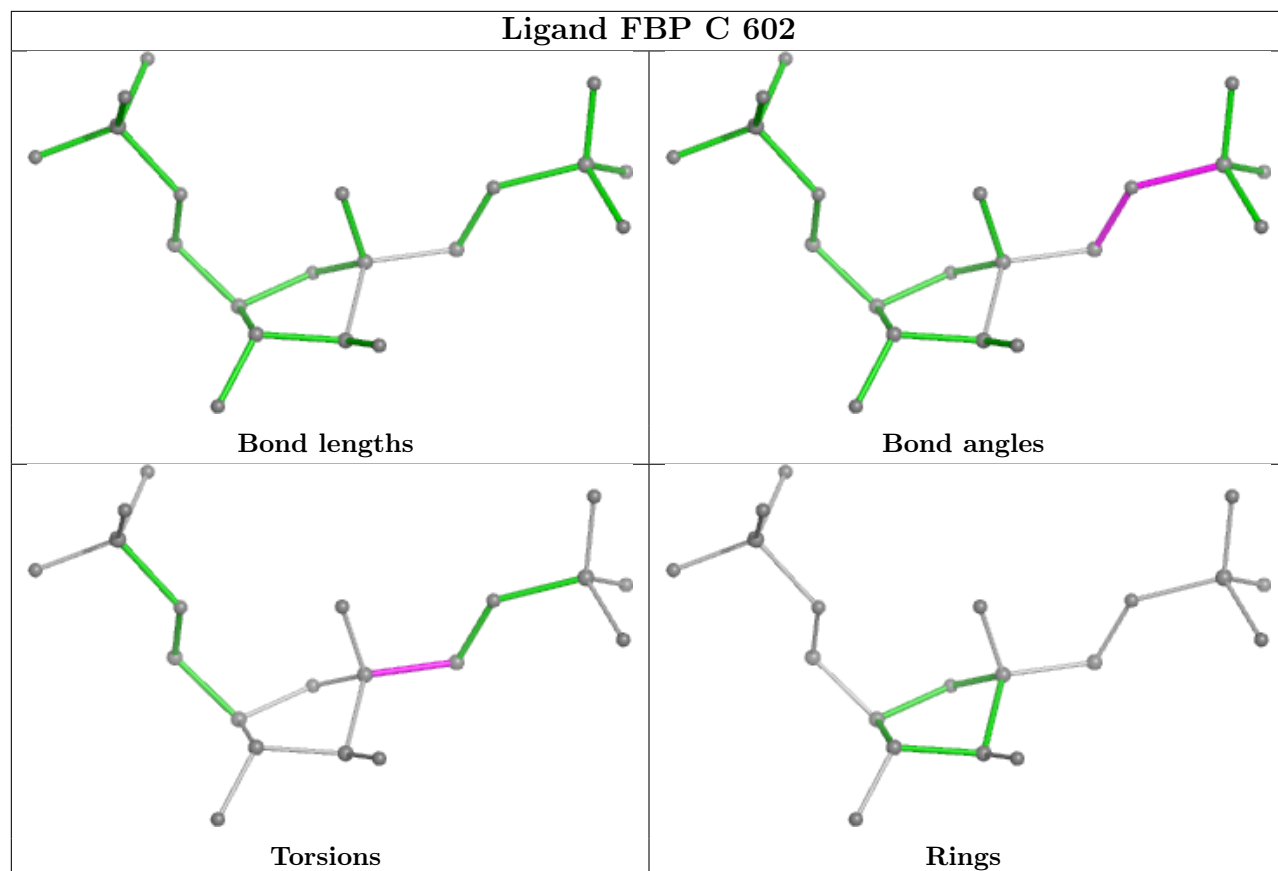
Ligand A1JB0 G 4001



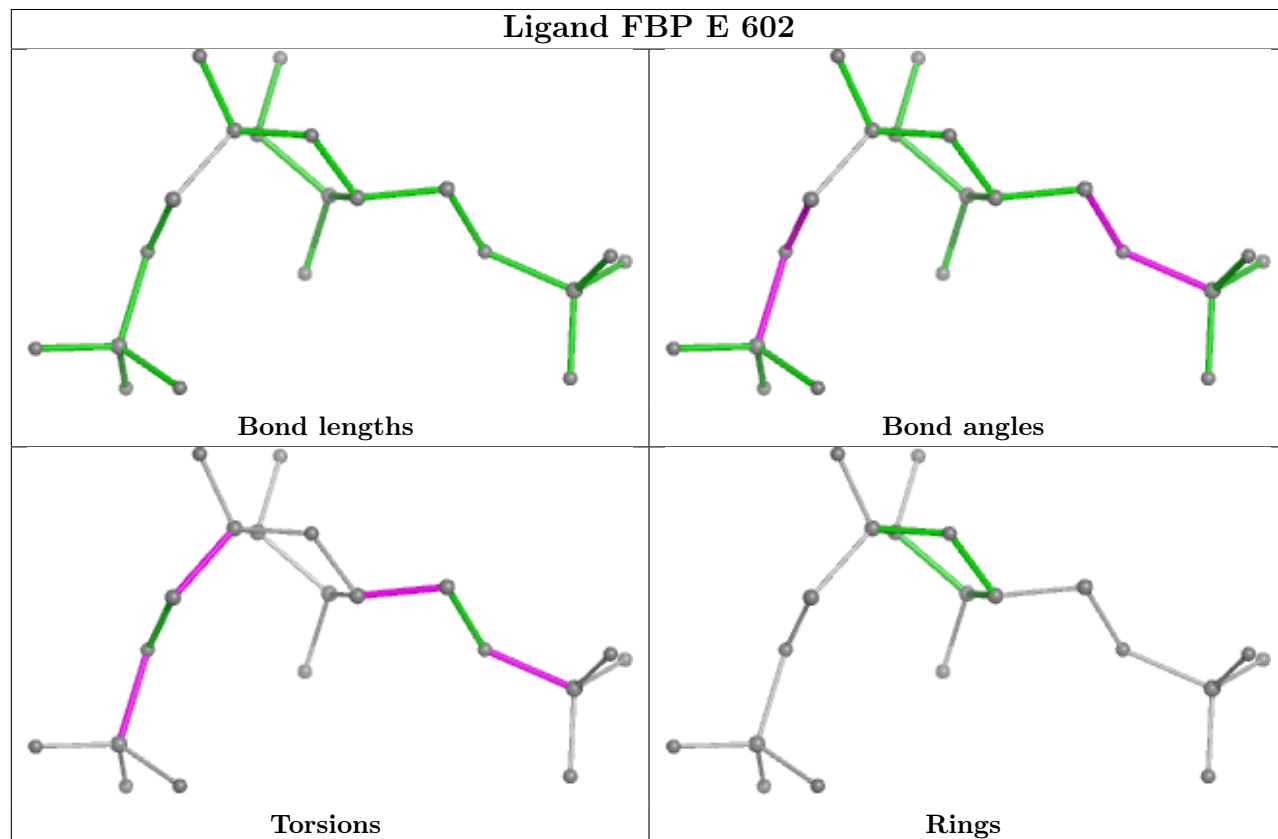
Ligand FBP F 603



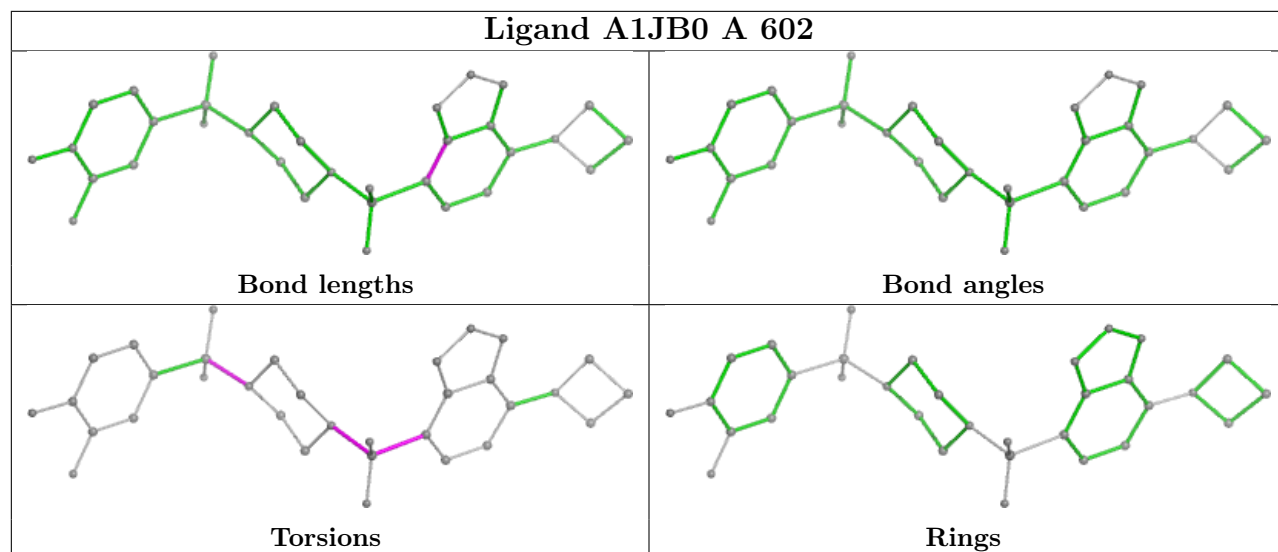
Ligand FBP C 602



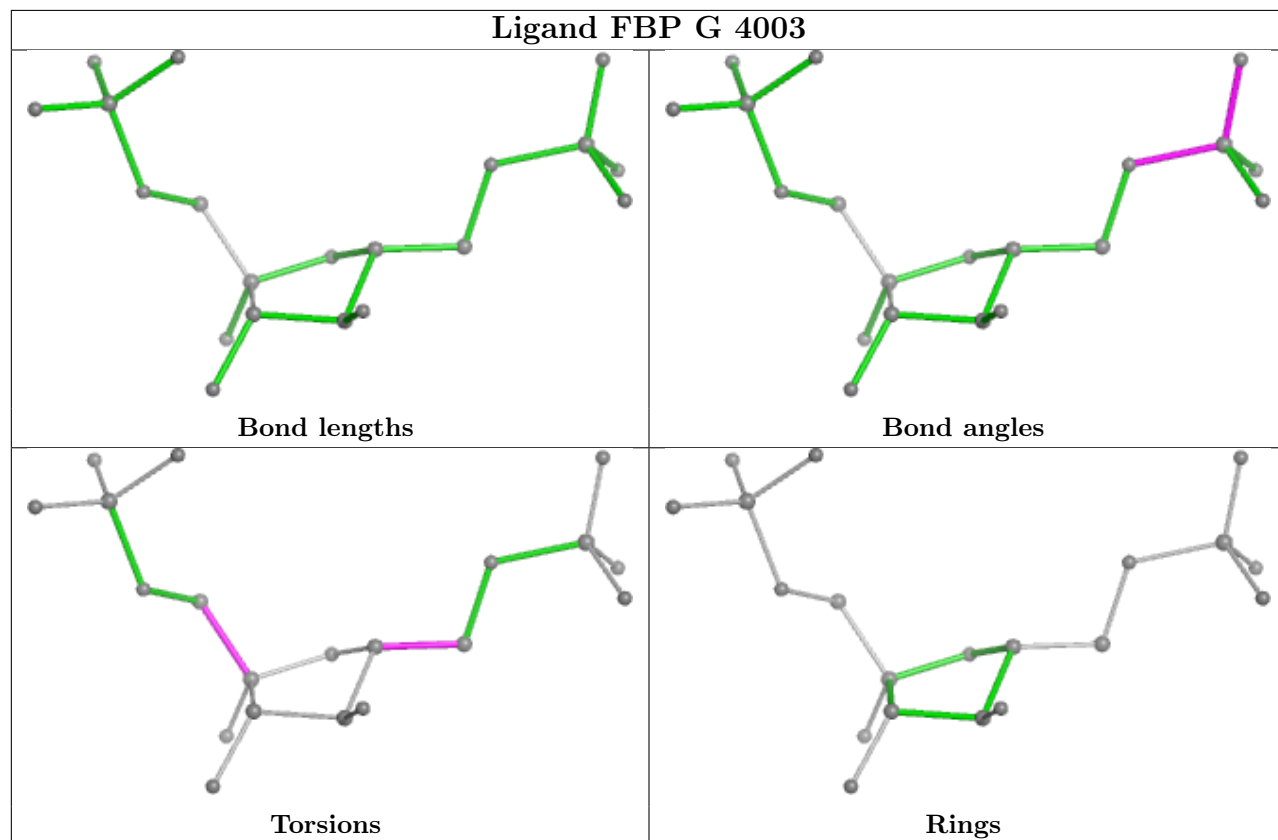
Ligand FBP E 602

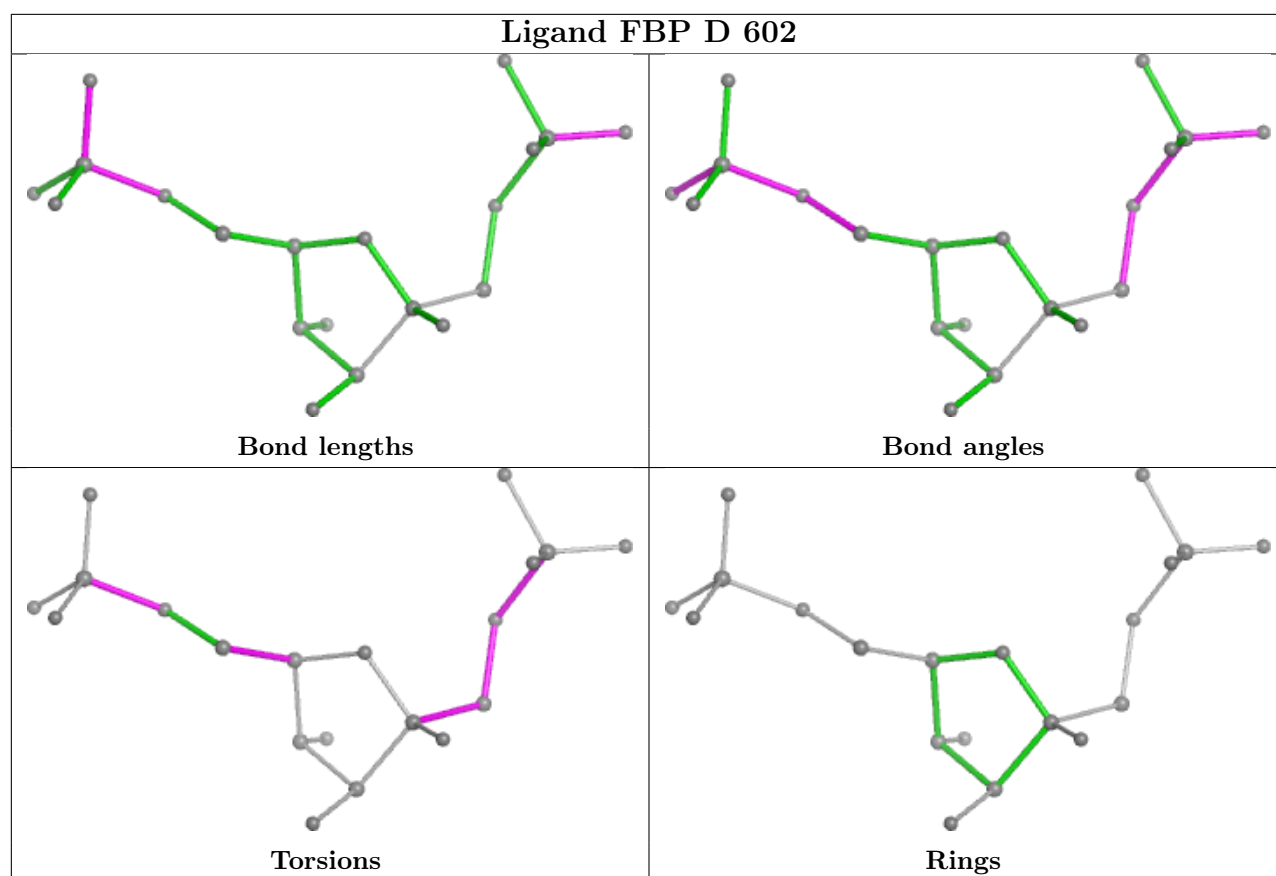


Ligand A1JB0 A 602



Ligand FBP G 4003





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	425/447 (95%)	-1.54	0 100 100	16, 34, 59, 90	1 (0%)
1	B	426/447 (95%)	-1.55	0 100 100	18, 34, 61, 93	0
1	C	424/447 (94%)	-1.54	0 100 100	16, 37, 65, 82	1 (0%)
1	D	424/447 (94%)	-1.49	0 100 100	15, 39, 69, 81	0
1	E	429/447 (95%)	-1.22	0 100 100	29, 62, 105, 116	0
1	F	433/447 (96%)	-1.22	0 100 100	31, 63, 99, 116	0
1	G	423/447 (94%)	-1.12	1 (0%) 92 93	40, 70, 99, 116	0
1	H	423/447 (94%)	-1.06	0 100 100	40, 70, 109, 131	0
All	All	3407/3576 (95%)	-1.34	1 (0%) 100 100	15, 51, 96, 131	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	504	PHE	2.9

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,

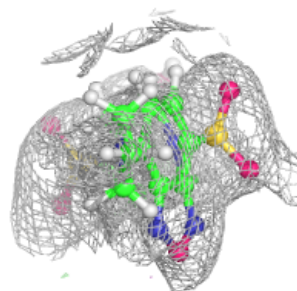
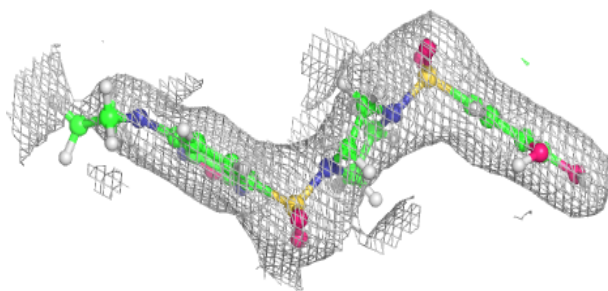
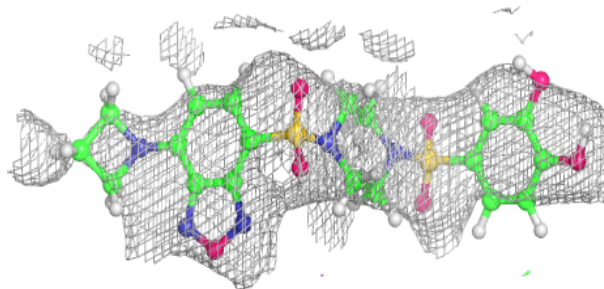
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	K	F	605	1/1	0.98	0.06	101,101,101,101	0
2	OXL	C	601	6/6	0.99	0.04	53,53,54,54	0
2	OXL	D	601	6/6	0.99	0.04	72,73,73,73	0
2	OXL	E	601	6/6	0.99	0.04	102,102,102,102	0
2	OXL	F	601	6/6	0.99	0.03	80,80,80,80	0
2	OXL	H	602	6/6	0.99	0.04	128,128,128,128	0
3	A1JB0	A	602	33/33	0.99	0.03	70,71,72,72	21
3	A1JB0	F	602	33/33	0.99	0.03	66,71,78,78	21
3	A1JB0	G	4001	33/33	0.99	0.03	68,70,76,76	21
3	A1JB0	H	601	33/33	0.99	0.03	56,61,64,64	21
4	FBP	E	602	20/20	0.99	0.03	79,79,81,81	10
4	FBP	F	603	20/20	0.99	0.03	74,75,75,75	10
4	FBP	G	4003	20/20	0.99	0.02	69,71,73,73	10
4	FBP	H	603	20/20	0.99	0.03	72,75,77,78	10
5	MG	A	605	1/1	0.99	0.02	45,45,45,45	0
5	MG	F	604	1/1	0.99	0.02	75,75,75,75	0
6	K	C	605	1/1	0.99	0.05	60,60,60,60	0
6	K	C	606	1/1	0.99	0.07	70,70,70,70	0
2	OXL	B	601	6/6	0.99	0.04	79,79,79,80	0
6	K	G	4005	1/1	0.99	0.08	78,78,78,78	0
5	MG	A	604	1/1	1.00	0.01	41,41,41,41	0
4	FBP	C	602	20/20	1.00	0.02	26,29,31,31	10
5	MG	B	603	1/1	1.00	0.01	45,45,45,45	0
5	MG	C	603	1/1	1.00	0.01	23,23,23,23	0
5	MG	C	604	1/1	1.00	0.01	22,22,22,22	0
5	MG	E	603	1/1	1.00	0.01	43,43,43,43	0
4	FBP	D	602	20/20	1.00	0.03	26,34,37,38	10
5	MG	G	4004	1/1	1.00	0.01	48,48,48,48	0
2	OXL	G	4002	6/6	1.00	0.02	72,72,72,72	0
2	OXL	A	601	6/6	1.00	0.02	62,62,63,63	0
4	FBP	A	603	20/20	1.00	0.02	26,31,33,34	10
4	FBP	B	602	20/20	1.00	0.01	19,22,23,24	10

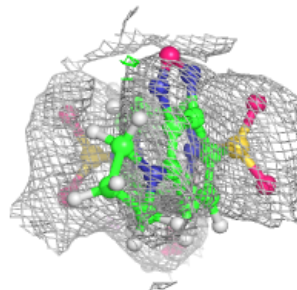
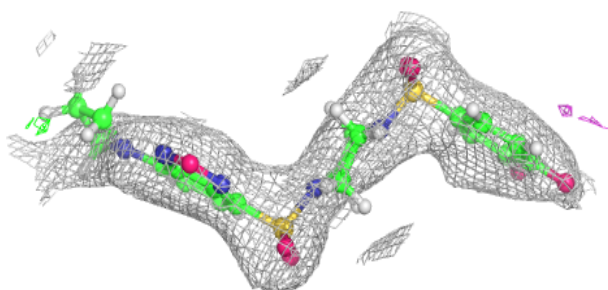
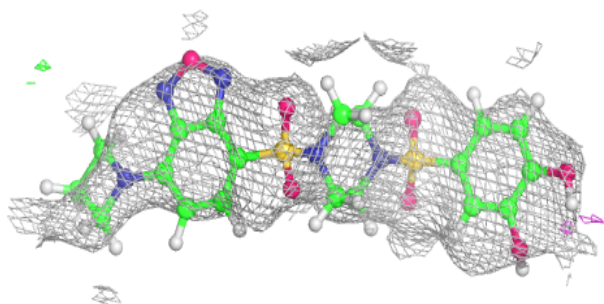
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1JB0 A 602:

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

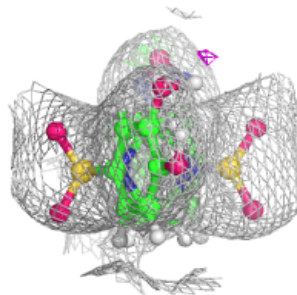
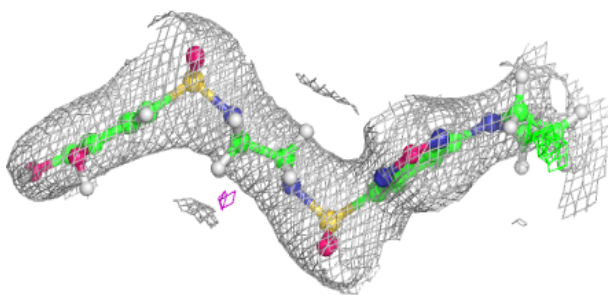
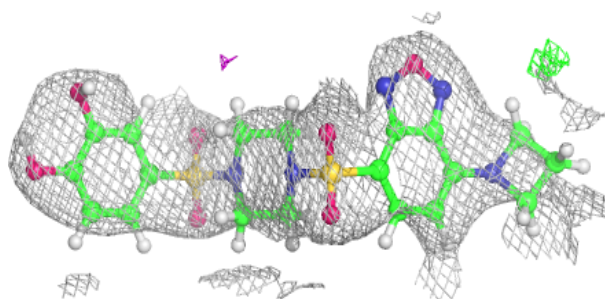
**Electron density around A1JB0 F 602:**

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

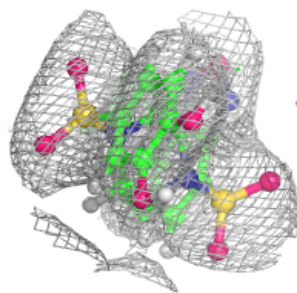
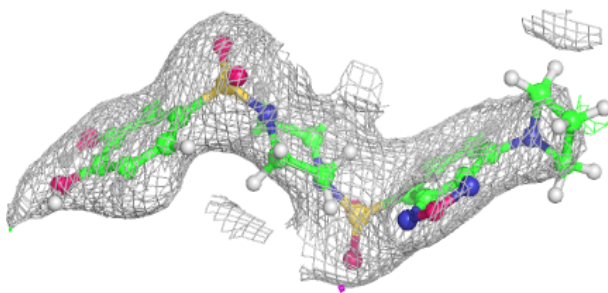
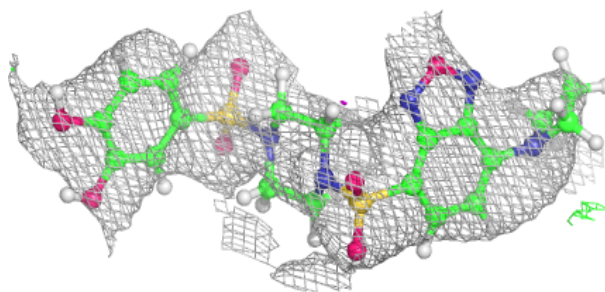


Electron density around A1JB0 G 4001:

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

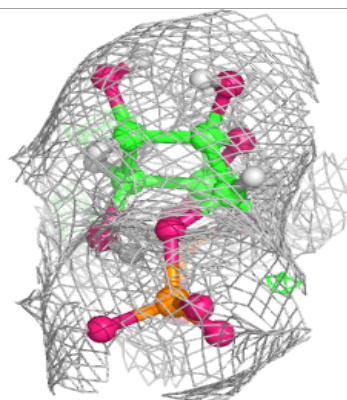
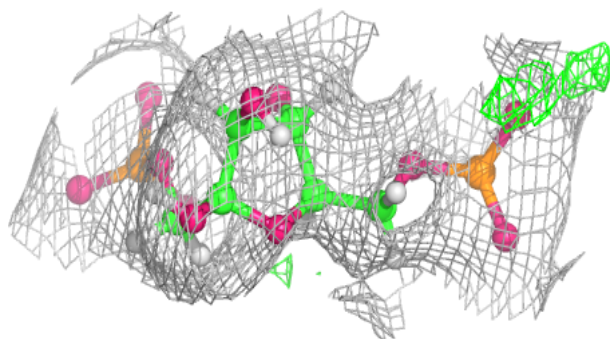
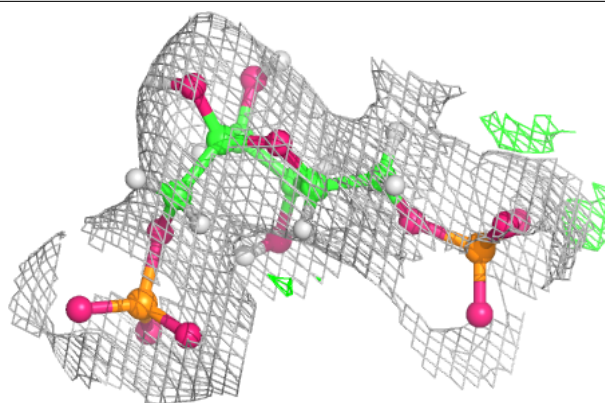
**Electron density around A1JB0 H 601:**

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

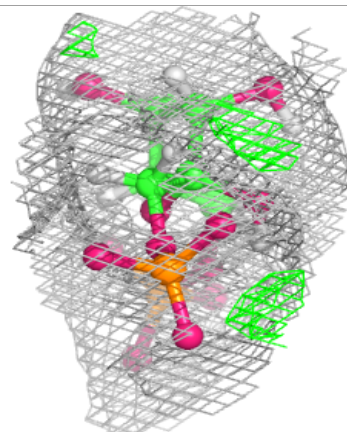
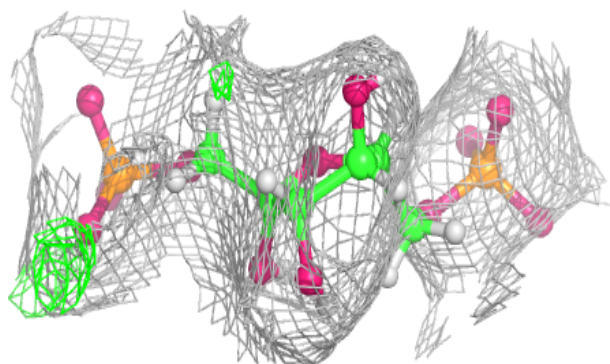
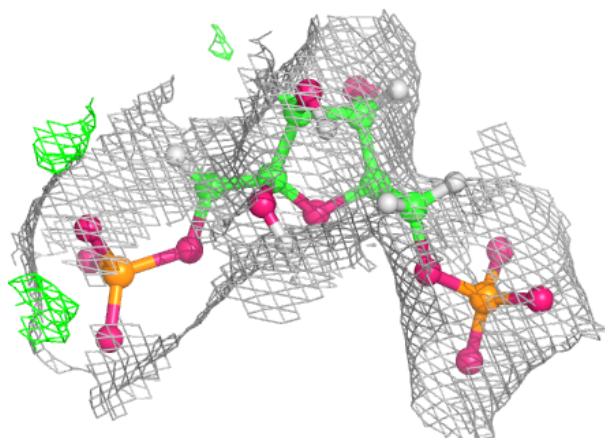


Electron density around FBP E 602:

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and green (positive)

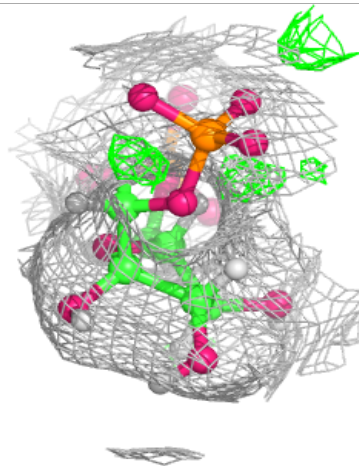
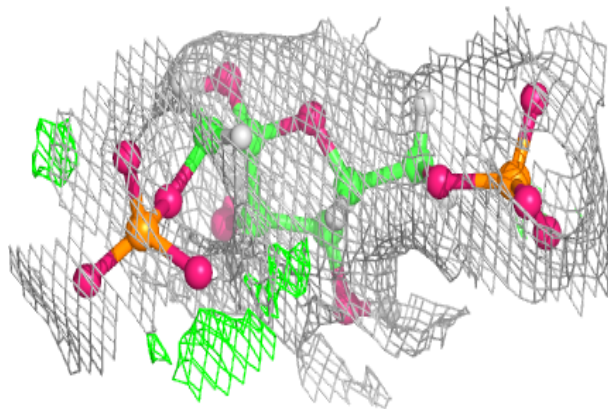
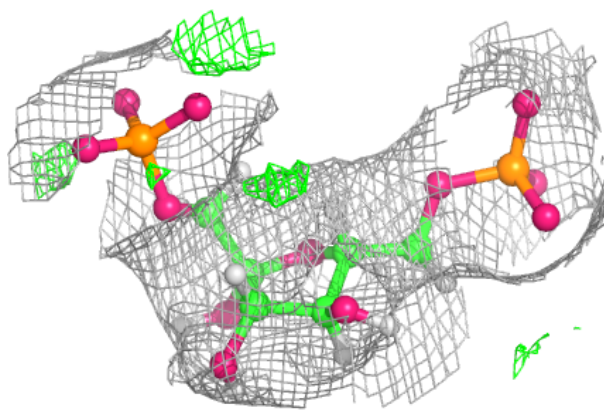
**Electron density around FBP F 603:**

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



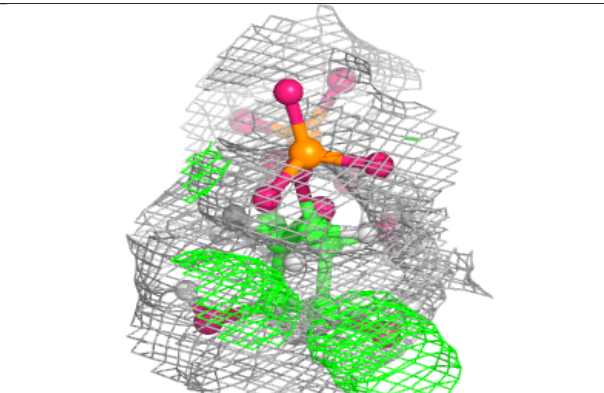
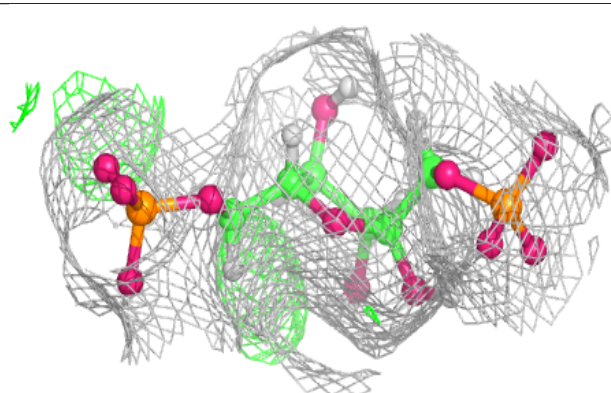
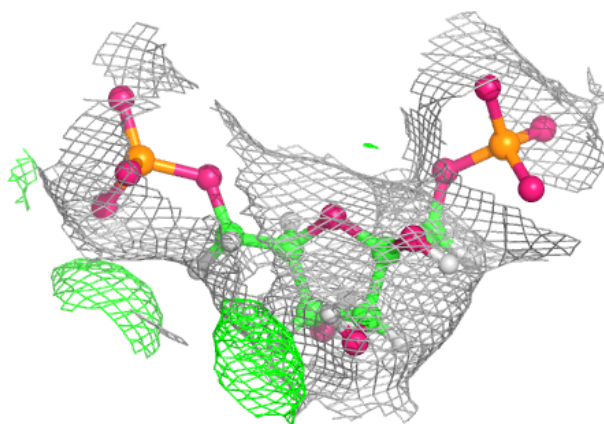
Electron density around FBP G 4003:

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and green (positive)

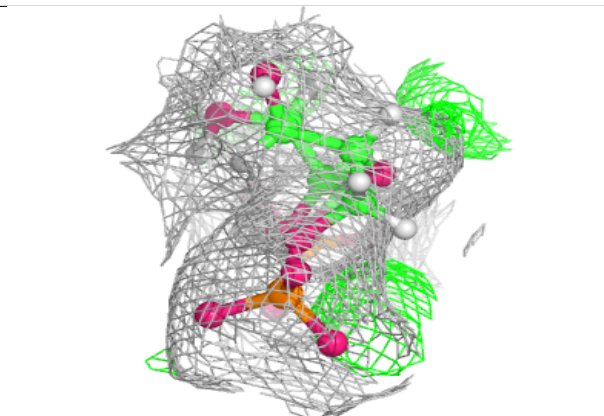
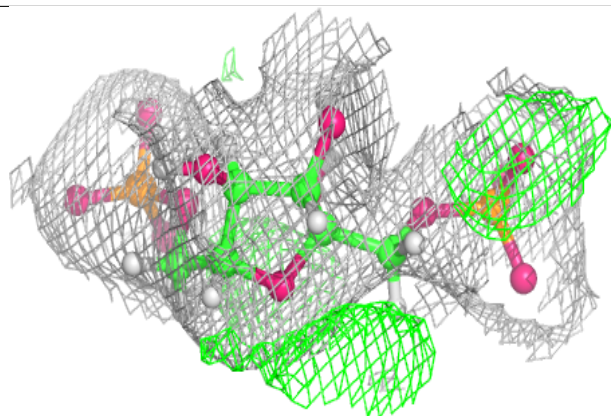
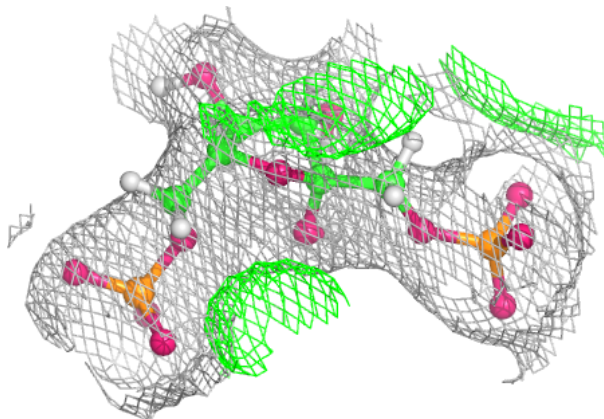


Electron density around FBP H 603:

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

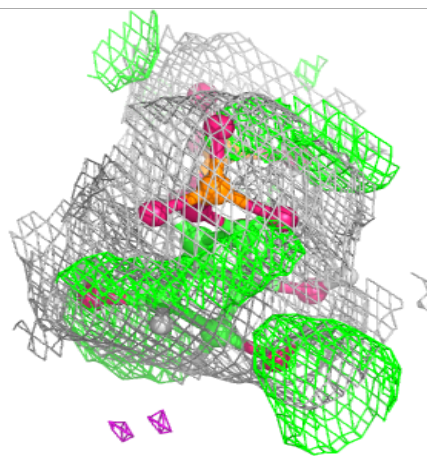
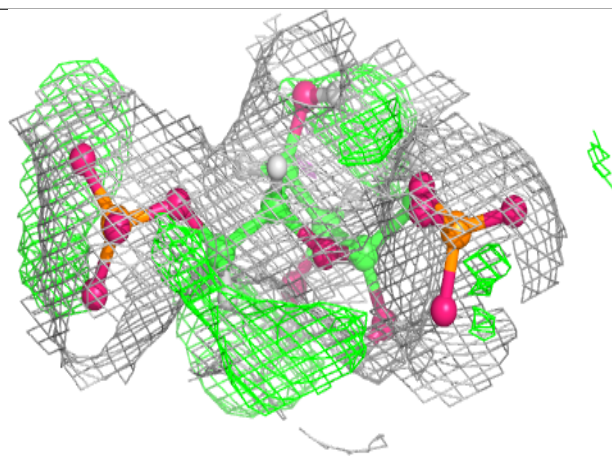
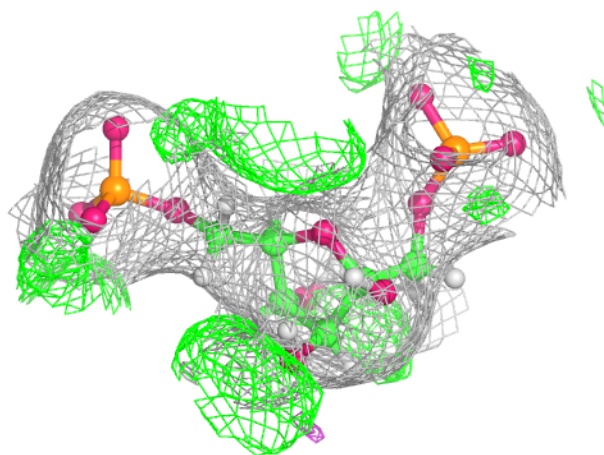
**Electron density around FBP C 602:**

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



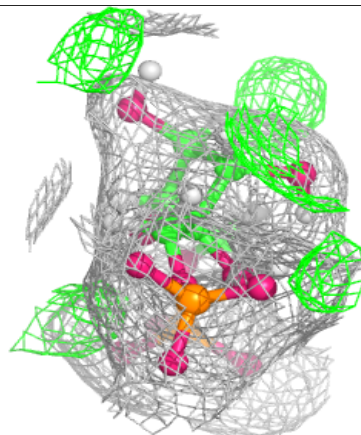
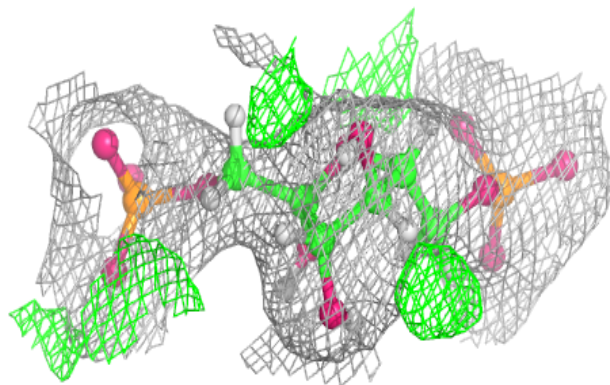
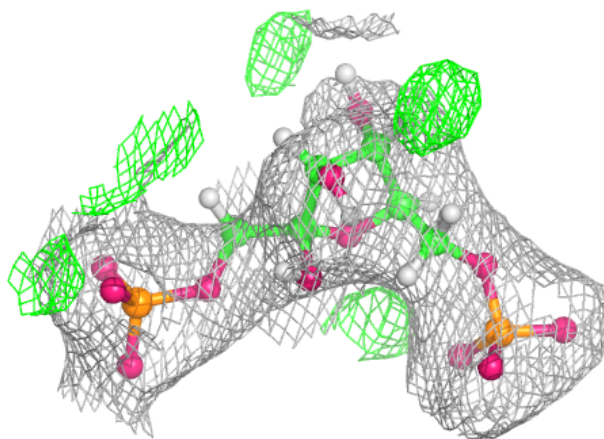
Electron density around FBP D 602:

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



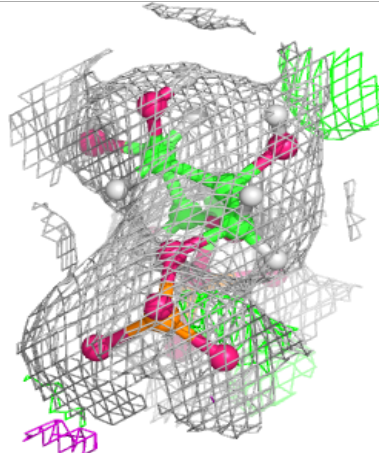
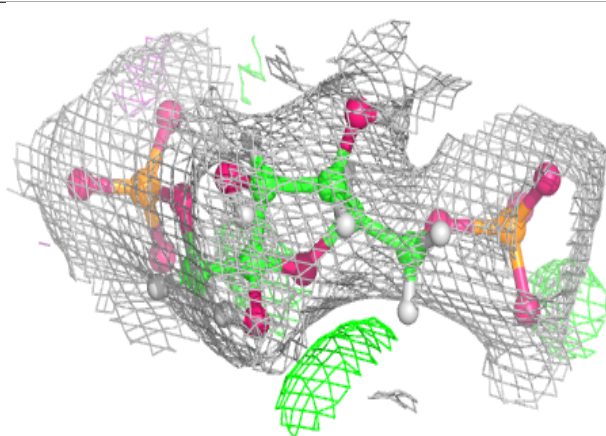
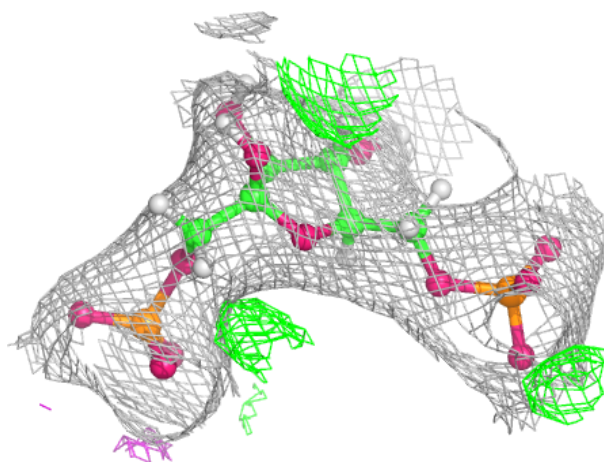
Electron density around FBP A 603:

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



Electron density around FBP B 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.