



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:01 AM UTC

PDB ID : 6V74 / pdb_00006v74
Title : Crystal Structure of Human PKM2 in Complex with L-asparagine
Authors : Nandi, S.; Dey, M.
Deposited on : 2019-12-07
Resolution : 2.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

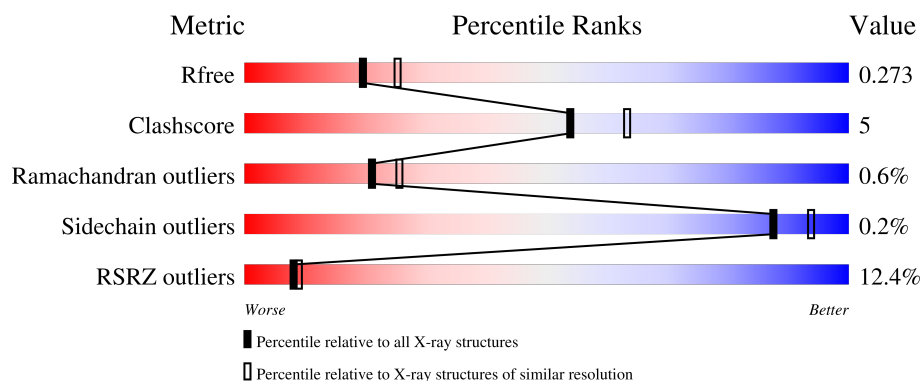
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	550	12% 85% 8% 7%
1	B	550	9% 83% 10% 6%
1	C	550	16% 78% 12% 9%
1	D	550	8% 67% 11% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	613	-	-	X	-
4	OXL	A	605	-	X	-	-
4	OXL	B	607	-	X	-	-
4	OXL	C	614	-	X	X	-
4	OXL	D	602	-	X	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14426 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 PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3681	2320	653	684	24			
1	B	516	Total	C	N	O	S	0	0	0
			3712	2334	653	700	25			
1	C	499	Total	C	N	O	S	0	0	0
			3543	2220	635	665	23			
1	D	427	Total	C	N	O	S	0	0	0
			3101	1949	549	581	22			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
B	-18	MET	-	initiating methionine	UNP P14618
B	-17	GLY	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
C	-18	MET	-	initiating methionine	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
D	-18	MET	-	initiating methionine	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618

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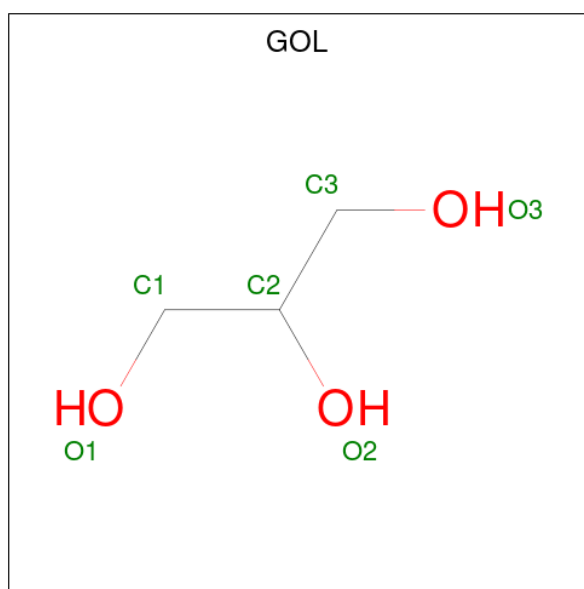
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

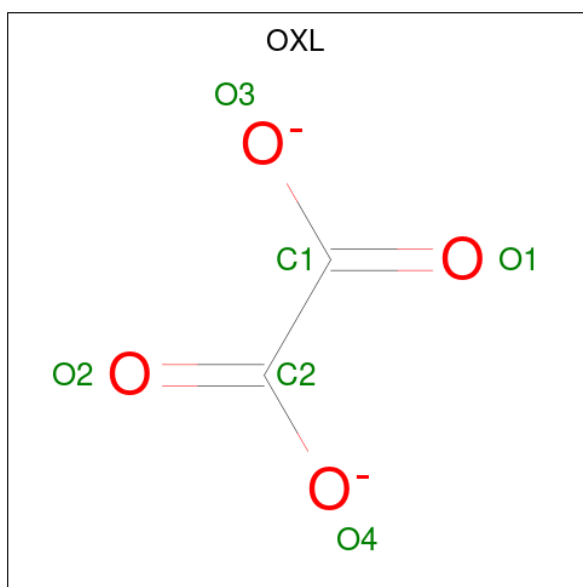
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	C	2	Total K 2 2	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



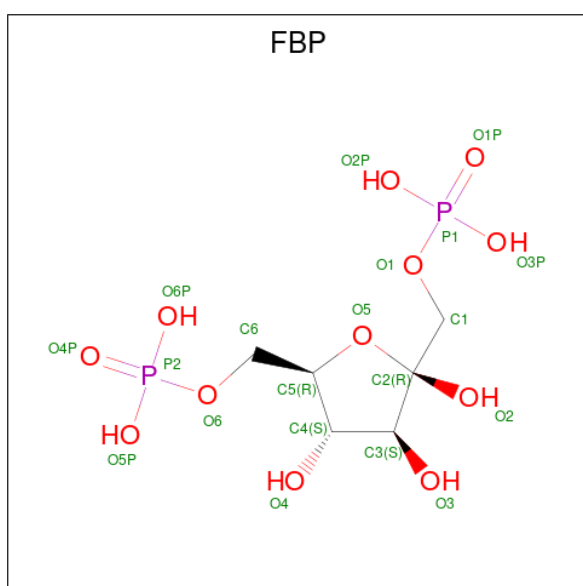
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	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		

- Molecule 5 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
5	A	1	Total	C	O	P	0	0
			20	6	12	2		
5	B	1	Total	C	O	P	0	0
			20	6	12	2		
5	C	1	Total	C	O	P	0	0
			20	6	12	2		
5	D	1	Total	C	O	P	0	0
			20	6	12	2		

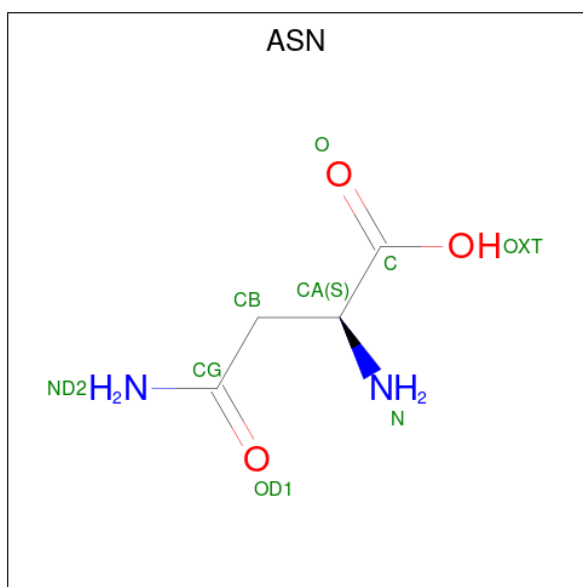
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

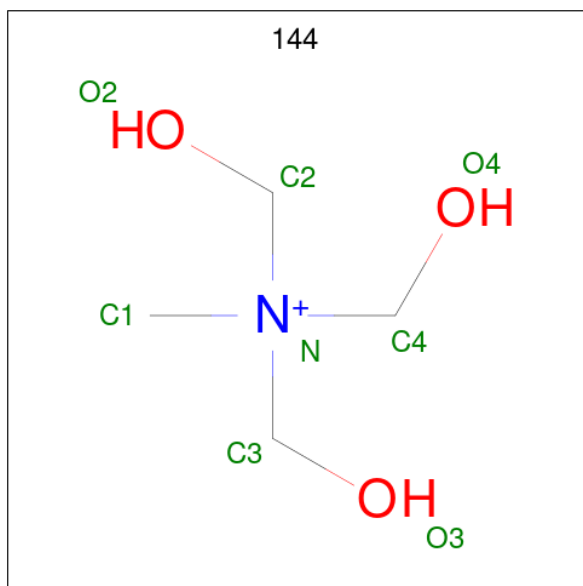
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is ASPARAGINE (CCD ID: ASN) (formula: C₄H₈N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 9 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (CCD ID: 144) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	O	0	0
			8	4	1	3		

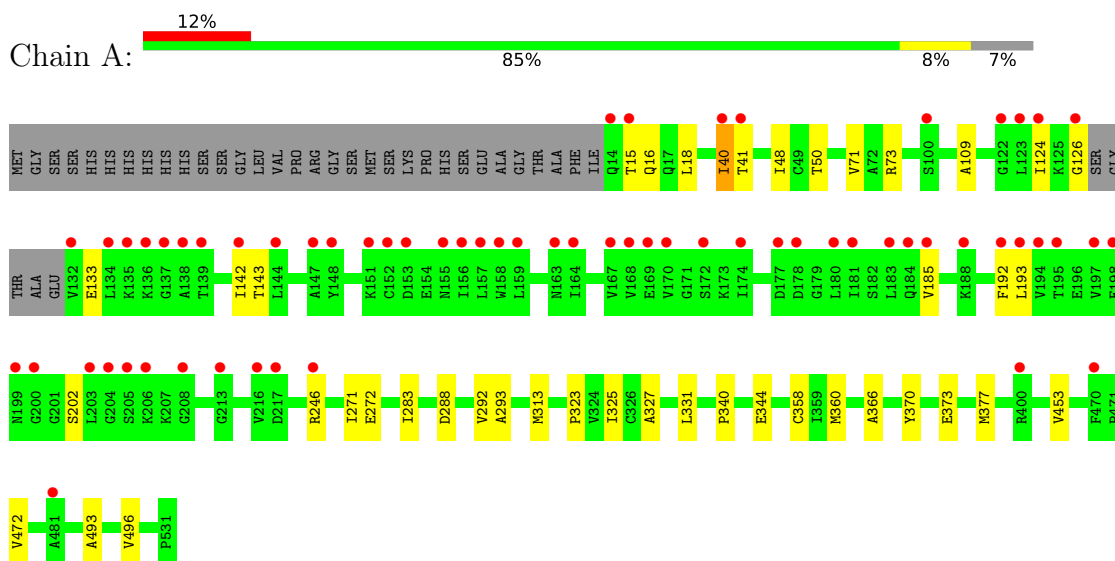
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	61	Total 61	O 61	0	0
10	B	31	Total 31	O 31	0	0
10	C	41	Total 41	O 41	0	0
10	D	23	Total 23	O 23	0	0

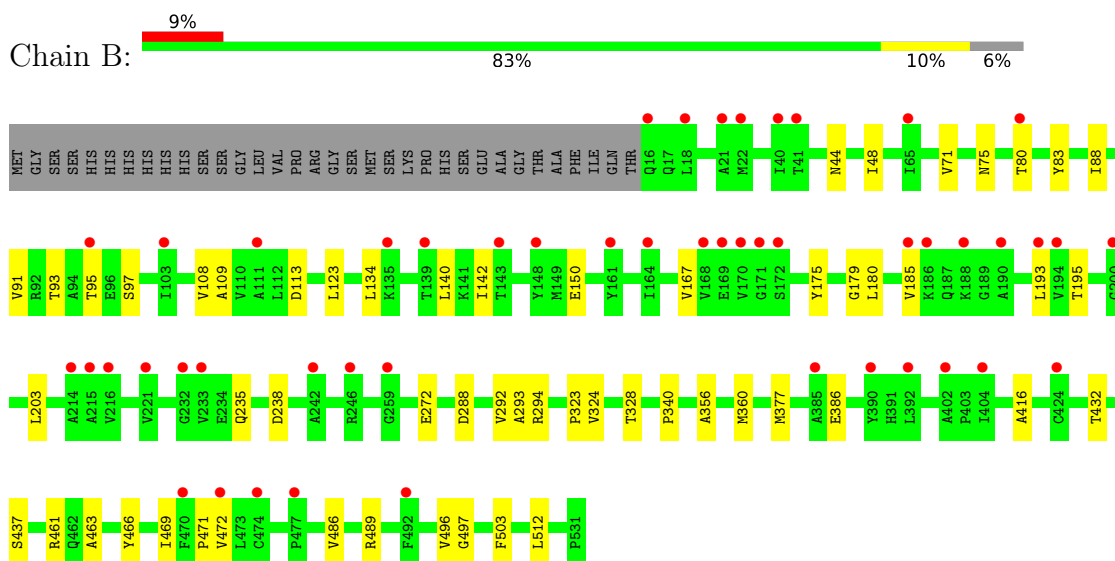
3 Residue-property plots [i](#)

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

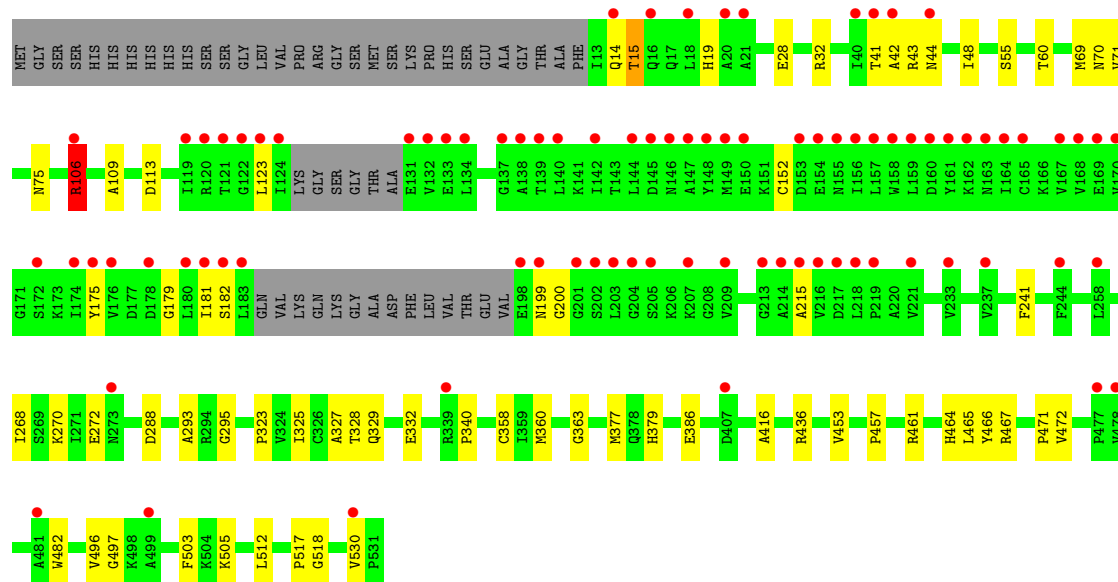
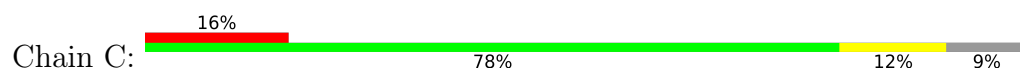
• Molecule 1: Pyruvate kinase PKM



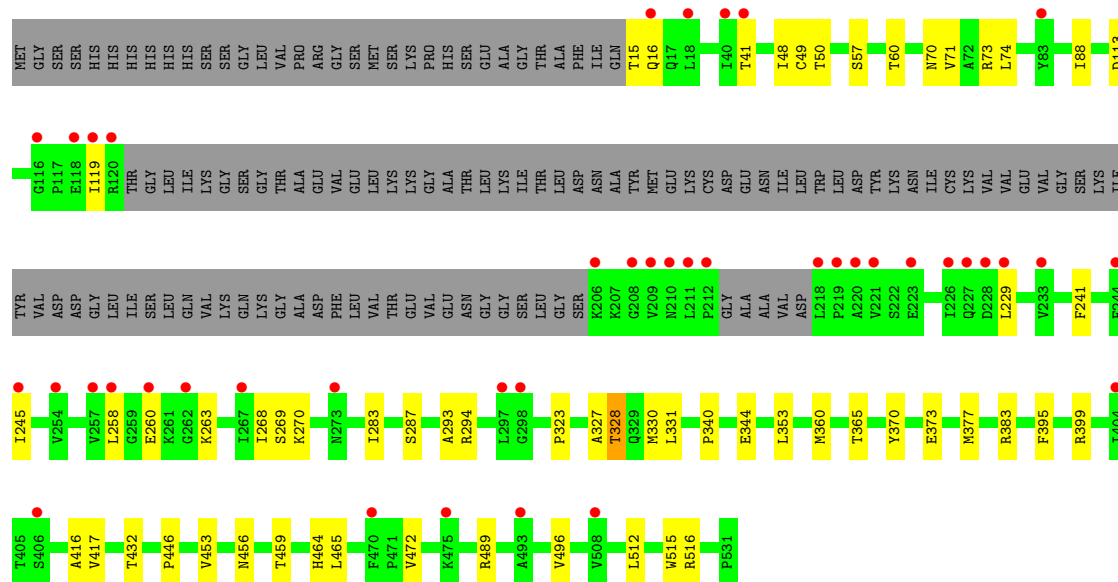
• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM



● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.99Å 154.58Å 92.15Å 90.00° 102.54° 90.00°	Depositor
Resolution (Å)	58.62 – 2.32 58.62 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.0 (58.62-2.32) 97.1 (58.62-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.233 , 0.275 0.236 , 0.273	Depositor DCC
R_{free} test set	4613 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14426	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: GOL, CL, 144, FBP, MG, OXL, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/3742	0.30	0/5084
1	B	0.09	0/3774	0.25	0/5135
1	C	0.57	12/3601 (0.3%)	0.40	4/4898 (0.1%)
1	D	0.10	0/3155	0.27	0/4290
All	All	0.31	12/14272 (0.1%)	0.31	4/19407 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	ASN	C-O	-17.87	1.00	1.24
1	C	70	ASN	C-N	16.13	1.54	1.33
1	C	106	ARG	C-O	-9.28	1.14	1.24
1	C	70	ASN	CG-OD1	-9.17	1.06	1.23
1	C	70	ASN	CG-ND2	-8.61	1.15	1.33
1	C	70	ASN	CA-CB	-6.59	1.43	1.53
1	C	106	ARG	CA-C	-6.19	1.46	1.52
1	C	69	MET	C-N	-6.16	1.24	1.33
1	C	70	ASN	N-CA	-5.79	1.38	1.46
1	C	70	ASN	CA-C	-5.70	1.44	1.52
1	C	15	THR	C-O	-5.24	1.17	1.23
1	C	70	ASN	CB-CG	-5.04	1.39	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	ASN	O-C-N	-10.82	106.99	122.36
1	C	70	ASN	CA-C-N	6.25	131.81	122.75
1	C	70	ASN	C-N-CA	6.25	131.81	122.75
1	C	69	MET	O-C-N	-5.43	115.44	122.77

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	3681	0	3486	25	0
1	B	3712	0	3524	31	0
1	C	3543	0	3291	45	0
1	D	3101	0	2961	35	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	12	0	16	2	0
3	B	30	0	40	1	0
3	C	54	0	72	10	0
3	D	6	0	8	0	0
4	A	6	0	0	1	0
4	B	6	0	0	1	0
4	C	6	0	0	2	0
4	D	6	0	0	2	0
5	A	20	0	10	0	0
5	B	20	0	10	2	0
5	C	20	0	10	1	0
5	D	20	0	10	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	C	9	0	5	3	0
9	D	8	0	12	2	0
10	A	61	0	0	0	0
10	B	31	0	0	0	0
10	C	41	0	0	0	0
10	D	23	0	0	0	0
All	All	14426	0	13455	137	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 (137) 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:C:43:ARG:H	3:C:613:GOL:H31	1.50	0.77
1:C:379:HIS:HE1	3:C:613:GOL:H32	1.51	0.75
1:A:272:GLU:HG2	1:A:293:ALA:HB3	1.67	0.74
1:C:44:ASN:O	1:C:467:ARG:HD3	1.90	0.70
1:C:464:HIS:HD1	8:C:604:ASN:N	1.89	0.69
1:A:16:GLN:HB3	1:A:18:LEU:HG	1.74	0.68
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.73	0.68
1:B:272:GLU:HG2	1:B:293:ALA:HB3	1.74	0.68
1:C:466:TYR:O	8:C:604:ASN:ND2	2.26	0.68
1:C:272:GLU:HG2	1:C:293:ALA:HB3	1.76	0.67
1:B:88:ILE:HD13	1:B:235:GLN:HG2	1.77	0.66
1:C:363:GLY:H	3:C:607:GOL:H11	1.63	0.64
1:A:292:VAL:HG22	1:A:313:MET:HE2	1.82	0.61
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.82	0.61
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.81	0.60
1:A:40:ILE:H	1:A:40:ILE:HD12	1.65	0.60
1:C:461:ARG:NH1	3:C:606:GOL:O1	2.34	0.60
1:D:241:PHE:HE1	1:D:268:ILE:HD11	1.68	0.59
1:D:241:PHE:CE1	1:D:268:ILE:HD11	2.38	0.59
1:A:340:PRO:HG3	1:A:377:MET:HG2	1.85	0.59
1:A:142:ILE:O	1:A:193:LEU:N	2.36	0.58
1:C:464:HIS:ND1	8:C:604:ASN:N	2.51	0.58
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.85	0.58
1:D:15:THR:HG22	1:D:16:GLN:HG2	1.85	0.57
1:B:80:THR:HG23	1:B:83:TYR:H	1.69	0.56
1:D:113:ASP:HA	1:D:241:PHE:HB2	1.88	0.56
1:B:142:ILE:HB	1:B:193:LEU:HB2	1.88	0.55
1:D:283:ILE:O	1:D:287:SER:OG	2.22	0.55
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.89	0.55
1:A:331:LEU:HD23	1:A:344:GLU:HB3	1.89	0.55
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.88	0.54
1:A:133:GLU:HA	1:A:202:SER:HA	1.90	0.54
1:B:95:THR:HG21	1:B:108:VAL:HB	1.90	0.54
1:D:353:LEU:HD13	9:D:606:144:H32	1.90	0.53
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.89	0.53
1:D:229:LEU:HD22	1:D:258:LEU:HD21	1.89	0.53
1:A:16:GLN:HG3	1:A:40:ILE:HG13	1.90	0.53
1:B:91:VAL:O	1:B:95:THR:HG23	2.08	0.53
1:B:134:LEU:HD11	1:B:203:LEU:HD22	1.91	0.53
1:B:140:LEU:O	1:B:195:THR:OG1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.91	0.52
1:B:293:ALA:HB1	4:B:607:OXL:C1	2.40	0.52
1:D:74:LEU:HD11	1:D:88:ILE:HG13	1.92	0.52
1:A:143:THR:HA	1:A:192:PHE:HA	1.91	0.52
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.93	0.51
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.91	0.51
1:D:50:THR:OG1	1:D:73:ARG:NH1	2.38	0.51
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.93	0.50
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.93	0.50
1:D:57:SER:OG	1:D:60:THR:HG23	2.12	0.50
1:C:329:GLN:HG3	3:C:607:GOL:H31	1.94	0.50
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.94	0.49
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.93	0.49
1:C:181:ILE:HA	1:C:200:GLY:HA2	1.94	0.49
1:C:482:TRP:CD1	1:C:517:PRO:HG3	2.46	0.49
1:D:49:CYS:HB3	1:D:365:THR:HG21	1.94	0.49
1:B:432:THR:HA	5:B:608:FBP:H61	1.94	0.49
1:D:245:ILE:HG13	1:D:269:SER:HB3	1.95	0.49
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.94	0.48
1:C:293:ALA:HB1	4:C:614:OXL:C2	2.43	0.48
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.95	0.48
1:C:43:ARG:N	3:C:613:GOL:H31	2.25	0.48
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.94	0.48
1:B:432:THR:HB	1:B:437:SER:HB2	1.94	0.48
1:A:325:ILE:HG12	1:A:358:CYS:HB2	1.96	0.48
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.97	0.47
1:A:366:ALA:HB3	3:A:603:GOL:H11	1.95	0.47
1:D:328:THR:HG21	4:D:602:OXL:O4	2.15	0.47
1:D:293:ALA:HB1	4:D:602:OXL:C2	2.45	0.47
1:D:515:TRP:CD2	1:D:516:ARG:HG2	2.50	0.47
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.97	0.47
1:C:270:LYS:NZ	4:C:614:OXL:O3	2.33	0.46
1:C:332:GLU:OE1	3:C:607:GOL:H12	2.15	0.46
1:B:48:ILE:HB	1:B:360:MET:HG3	1.97	0.46
1:A:142:ILE:N	1:A:193:LEU:O	2.37	0.46
1:C:75:ASN:HA	1:C:113:ASP:HB3	1.98	0.46
1:D:456:ASN:HB3	1:D:459:THR:HB	1.98	0.46
1:A:50:THR:OG1	1:A:73:ARG:HD3	2.16	0.45
1:C:379:HIS:CE1	3:C:613:GOL:H32	2.42	0.45
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.98	0.45
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASN:HD22	3:C:605:GOL:H11	1.81	0.45
1:D:395:PHE:CE1	1:D:399:ARG:HD2	2.52	0.45
1:A:271:ILE:HD11	1:A:283:ILE:HG21	1.98	0.45
1:B:489:ARG:NH1	5:B:608:FBP:O3P	2.43	0.45
1:C:55:SER:HA	1:C:60:THR:HG21	1.99	0.45
1:C:241:PHE:HD1	1:C:268:ILE:HB	1.81	0.45
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.51	0.45
9:D:606:144:O4	9:D:606:144:O2	2.29	0.44
1:B:123:LEU:HD13	1:B:150:GLU:HG2	1.99	0.44
1:D:119:ILE:HD12	1:D:119:ILE:H	1.81	0.44
1:D:453:VAL:HG11	1:D:489:ARG:HB3	1.99	0.44
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.52	0.44
1:D:327:ALA:HB1	1:D:360:MET:HE2	1.98	0.44
1:D:515:TRP:CE2	1:D:516:ARG:HG2	2.53	0.44
1:D:323:PRO:HB3	1:D:465:LEU:O	2.18	0.43
1:B:44:ASN:H	1:B:386:GLU:CD	2.26	0.43
1:B:463:ALA:HB3	1:B:471:PRO:HB3	1.99	0.43
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.99	0.43
1:A:293:ALA:HB1	4:A:605:OXL:C1	2.48	0.43
1:B:75:ASN:HA	1:B:113:ASP:HB3	2.01	0.43
1:D:70:ASN:HB3	1:D:464:HIS:CG	2.52	0.43
1:B:288:ASP:O	1:B:323:PRO:HD2	2.19	0.43
1:C:327:ALA:HB1	1:C:360:MET:HE2	2.00	0.43
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.48	0.43
1:C:28:GLU:O	1:C:32:ARG:HG3	2.19	0.43
1:C:295:GLY:HA3	1:C:328:THR:HG21	2.00	0.43
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.01	0.43
1:C:457:PRO:HB3	3:C:606:GOL:H2	2.01	0.43
1:D:370:TYR:HB3	1:D:373:GLU:HB2	2.01	0.43
1:C:453:VAL:HA	1:C:472:VAL:HG23	2.02	0.42
1:C:106:ARG:NE	1:C:106:ARG:HA	2.34	0.42
1:B:486:VAL:HG11	3:B:605:GOL:H32	2.01	0.42
1:C:106:ARG:HH12	1:C:471:PRO:HD2	1.84	0.42
1:D:294:ARG:NH2	1:D:330:MET:HG2	2.35	0.42
1:D:432:THR:HA	5:D:603:FBP:H61	2.00	0.42
1:A:246:ARG:NH2	3:A:604:GOL:H31	2.34	0.42
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.02	0.42
1:C:182:SER:N	1:C:199:ASN:O	2.50	0.42
1:B:292:VAL:HG12	1:B:294:ARG:HG2	2.01	0.41
1:B:93:THR:O	1:B:97:SER:OG	2.37	0.41
1:C:323:PRO:HB3	1:C:465:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:PHE:HB3	1:D:270:LYS:HD2	2.01	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.90	0.41
1:C:44:ASN:H	1:C:386:GLU:CD	2.27	0.41
1:C:106:ARG:HA	1:C:106:ARG:HE	1.85	0.41
1:C:288:ASP:O	1:C:323:PRO:HD2	2.21	0.41
1:A:124:ILE:C	1:A:126:GLY:H	2.29	0.41
1:A:288:ASP:O	1:A:323:PRO:HD2	2.21	0.41
1:B:238:ASP:OD1	1:B:461:ARG:NE	2.46	0.41
1:C:19:HIS:NE2	1:C:32:ARG:HD2	2.36	0.41
1:C:123:LEU:O	1:C:152:CYS:HB2	2.21	0.41
1:B:324:VAL:HG13	1:B:356:ALA:HA	2.02	0.40
1:C:505:LYS:HA	1:C:530:VAL:HG23	2.02	0.40
1:D:41:THR:HA	1:D:383:ARG:HH21	1.86	0.40
1:D:260:GLU:HA	1:D:263:LYS:HB3	2.03	0.40
1:C:518:GLY:O	5:C:615:FBP:O4	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	509/550 (92%)	490 (96%)	15 (3%)	4 (1%)	16	19
1	B	514/550 (94%)	499 (97%)	12 (2%)	3 (1%)	21	25
1	C	493/550 (90%)	467 (95%)	22 (4%)	4 (1%)	16	19
1	D	421/550 (76%)	407 (97%)	13 (3%)	1 (0%)	43	53
All	All	1937/2200 (88%)	1863 (96%)	62 (3%)	12 (1%)	21	25

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	40	ILE
1	A	41	THR
1	C	41	THR
1	C	215	ALA
1	C	14	GLN
1	B	167	VAL
1	C	42	ALA
1	A	185	VAL
1	D	328	THR
1	B	328	THR
1	B	185	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/452 (76%)	342 (100%)	0	100	100
1	B	351/452 (78%)	351 (100%)	0	100	100
1	C	323/452 (72%)	320 (99%)	3 (1%)	70	83
1	D	299/452 (66%)	299 (100%)	0	100	100
All	All	1315/1808 (73%)	1312 (100%)	3 (0%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	15	THR
1	C	106	ARG
1	C	436	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	458	GLN

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Mol	Chain	Res	Type
1	A	479	GLN
1	B	78	HIS
1	B	350	ASN
1	B	391	HIS
1	B	393	GLN
1	B	440	GLN
1	B	491	ASN
1	B	523	ASN
1	C	78	HIS
1	C	491	ASN
1	D	274	HIS

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 37 ligands modelled in this entry, 10 are monoatomic - leaving 27 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	$\# Z > 2$
3	GOL	C	612	-	5,5,5	0.93	0	5,5,5	1.07	0
5	FBP	B	608	-	18,20,20	0.93	1 (5%)	21,32,32	0.66	0
3	GOL	C	607	-	5,5,5	0.99	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FBP	C	615	-	18,20,20	0.92	1 (5%)	21,32,32	0.69	0
3	GOL	B	604	-	5,5,5	0.93	0	5,5,5	1.06	0
3	GOL	C	605	-	5,5,5	1.00	0	5,5,5	1.01	0
3	GOL	C	611	-	5,5,5	0.94	0	5,5,5	1.05	0
9	144	D	606	-	1,7,7	0.80	0	3,9,9	0.07	0
3	GOL	D	601	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	A	603	-	5,5,5	0.87	0	5,5,5	1.15	0
3	GOL	B	605	-	5,5,5	0.92	0	5,5,5	1.08	0
3	GOL	C	608	-	5,5,5	0.93	0	5,5,5	1.08	0
3	GOL	C	610	-	5,5,5	0.94	0	5,5,5	1.05	0
3	GOL	A	604	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	B	603	-	5,5,5	0.89	0	5,5,5	1.10	0
3	GOL	B	606	-	5,5,5	0.90	0	5,5,5	1.08	0
4	OXL	B	607	6	5,5,5	1.72	2 (40%)	6,6,6	1.69	2 (33%)
4	OXL	D	602	6	5,5,5	1.70	2 (40%)	6,6,6	1.68	2 (33%)
5	FBP	D	603	-	18,20,20	0.95	1 (5%)	21,32,32	0.67	0
4	OXL	C	614	2	5,5,5	1.70	2 (40%)	6,6,6	1.68	2 (33%)
3	GOL	C	606	-	5,5,5	0.97	0	5,5,5	1.07	0
3	GOL	C	613	-	5,5,5	0.92	0	5,5,5	1.06	0
3	GOL	C	609	-	5,5,5	0.94	0	5,5,5	1.05	0
4	OXL	A	605	6	5,5,5	1.42	0	6,6,6	2.45	2 (33%)
8	ASN	C	604	-	7,8,8	0.82	0	6,10,10	0.25	0
5	FBP	A	606	-	18,20,20	0.93	1 (5%)	21,32,32	0.69	0
3	GOL	B	602	-	5,5,5	0.96	0	5,5,5	1.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	612	-	-	2/4/4/4	-
5	FBP	B	608	-	-	4/13/32/32	0/1/1/1
3	GOL	C	607	-	-	4/4/4/4	-
5	FBP	C	615	-	-	4/13/32/32	0/1/1/1
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	C	605	-	-	3/4/4/4	-
3	GOL	C	611	-	-	4/4/4/4	-
9	144	D	606	-	-	0/0/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	601	-	-	2/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	B	605	-	-	3/4/4/4	-
3	GOL	C	608	-	-	1/4/4/4	-
3	GOL	C	610	-	-	0/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	B	606	-	-	0/4/4/4	-
4	OXL	B	607	6	-	4/4/4/4	-
4	OXL	D	602	6	-	4/4/4/4	-
5	FBP	D	603	-	-	5/13/32/32	0/1/1/1
4	OXL	C	614	2	-	4/4/4/4	-
3	GOL	C	606	-	-	0/4/4/4	-
3	GOL	C	613	-	-	0/4/4/4	-
3	GOL	C	609	-	-	4/4/4/4	-
4	OXL	A	605	6	-	4/4/4/4	-
8	ASN	C	604	-	-	3/8/8/8	-
5	FBP	A	606	-	-	2/13/32/32	0/1/1/1
3	GOL	B	602	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	603	FBP	O2-C2	2.83	1.45	1.40
5	C	615	FBP	O2-C2	2.70	1.45	1.40
5	A	606	FBP	O2-C2	2.69	1.45	1.40
5	B	608	FBP	O2-C2	2.68	1.45	1.40
4	B	607	OXL	O3-C1	-2.62	1.23	1.30
4	D	602	OXL	O4-C2	-2.58	1.23	1.30
4	B	607	OXL	O4-C2	-2.58	1.23	1.30
4	C	614	OXL	O4-C2	-2.57	1.23	1.30
4	D	602	OXL	O3-C1	-2.56	1.23	1.30
4	C	614	OXL	O3-C1	-2.56	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	OXL	O4-C2-C1	3.89	120.38	112.83
4	A	605	OXL	O3-C1-C2	3.87	120.35	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	OXL	O4-C2-C1	2.12	116.93	112.83
4	C	614	OXL	O4-C2-C1	2.11	116.93	112.83
4	B	607	OXL	O3-C1-C2	2.11	116.92	112.83
4	C	614	OXL	O3-C1-C2	2.09	116.88	112.83
4	B	607	OXL	O4-C2-C1	2.09	116.87	112.83
4	D	602	OXL	O3-C1-C2	2.08	116.85	112.83

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-C3
3	B	603	GOL	C1-C2-C3-O3
3	B	604	GOL	O1-C1-C2-O2
3	B	604	GOL	O1-C1-C2-C3
3	B	605	GOL	O1-C1-C2-C3
3	C	609	GOL	C1-C2-C3-O3
3	C	609	GOL	O2-C2-C3-O3
3	C	611	GOL	O1-C1-C2-C3
3	D	601	GOL	C1-C2-C3-O3
5	B	608	FBP	C4-C5-C6-O6
5	C	615	FBP	C1-O1-P1-O2P
5	C	615	FBP	C1-O1-P1-O3P
5	D	603	FBP	O1-C1-C2-O2
5	D	603	FBP	O1-C1-C2-C3
5	D	603	FBP	O1-C1-C2-O5
8	C	604	ASN	N-CA-CB-CG
5	A	606	FBP	C4-C5-C6-O6
5	C	615	FBP	C4-C5-C6-O6
5	D	603	FBP	C4-C5-C6-O6
5	B	608	FBP	O5-C5-C6-O6
5	D	603	FBP	O5-C5-C6-O6
5	C	615	FBP	O5-C5-C6-O6
8	C	604	ASN	OXT-C-CA-N
3	B	605	GOL	C1-C2-C3-O3
3	C	605	GOL	O1-C1-C2-C3
3	C	607	GOL	O1-C1-C2-C3
3	C	609	GOL	O1-C1-C2-C3
3	C	611	GOL	C1-C2-C3-O3
3	C	612	GOL	C1-C2-C3-O3
3	A	604	GOL	O1-C1-C2-O2
3	B	603	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	605	GOL	O1-C1-C2-O2
3	C	611	GOL	O2-C2-C3-O3
3	D	601	GOL	O2-C2-C3-O3
5	A	606	FBP	O5-C5-C6-O6
3	C	605	GOL	O1-C1-C2-O2
3	C	607	GOL	O1-C1-C2-O2
5	B	608	FBP	C6-O6-P2-O4P
3	C	605	GOL	O2-C2-C3-O3
8	C	604	ASN	O-C-CA-N
3	C	609	GOL	O1-C1-C2-O2
4	A	605	OXL	O3-C1-C2-O4
4	C	614	OXL	O3-C1-C2-O4
4	D	602	OXL	O3-C1-C2-O4
4	B	607	OXL	O3-C1-C2-O4
4	A	605	OXL	O1-C1-C2-O2
4	C	614	OXL	O1-C1-C2-O2
4	D	602	OXL	O1-C1-C2-O2
3	C	611	GOL	O1-C1-C2-O2
3	C	612	GOL	O2-C2-C3-O3
4	B	607	OXL	O1-C1-C2-O2
3	C	608	GOL	O1-C1-C2-C3
4	A	605	OXL	O1-C1-C2-O4
4	C	614	OXL	O1-C1-C2-O4
4	C	614	OXL	O3-C1-C2-O2
4	A	605	OXL	O3-C1-C2-O2
4	B	607	OXL	O1-C1-C2-O4
4	B	607	OXL	O3-C1-C2-O2
4	D	602	OXL	O1-C1-C2-O4
4	D	602	OXL	O3-C1-C2-O2
5	B	608	FBP	C6-O6-P2-O5P
3	C	607	GOL	C1-C2-C3-O3
3	C	607	GOL	O2-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 28 short contacts:

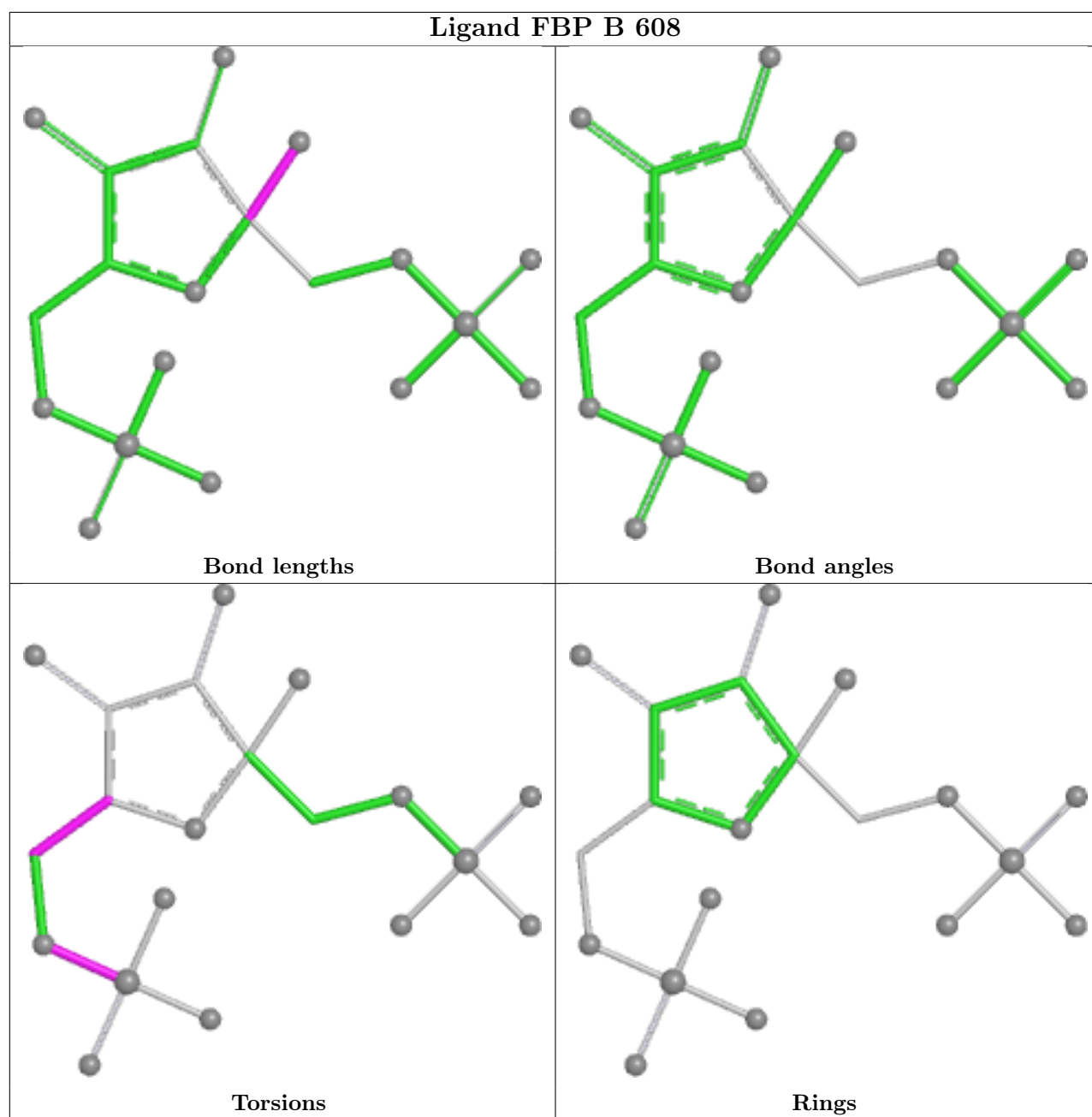
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	608	FBP	2	0
3	C	607	GOL	3	0
5	C	615	FBP	1	0
3	C	605	GOL	1	0
9	D	606	144	2	0

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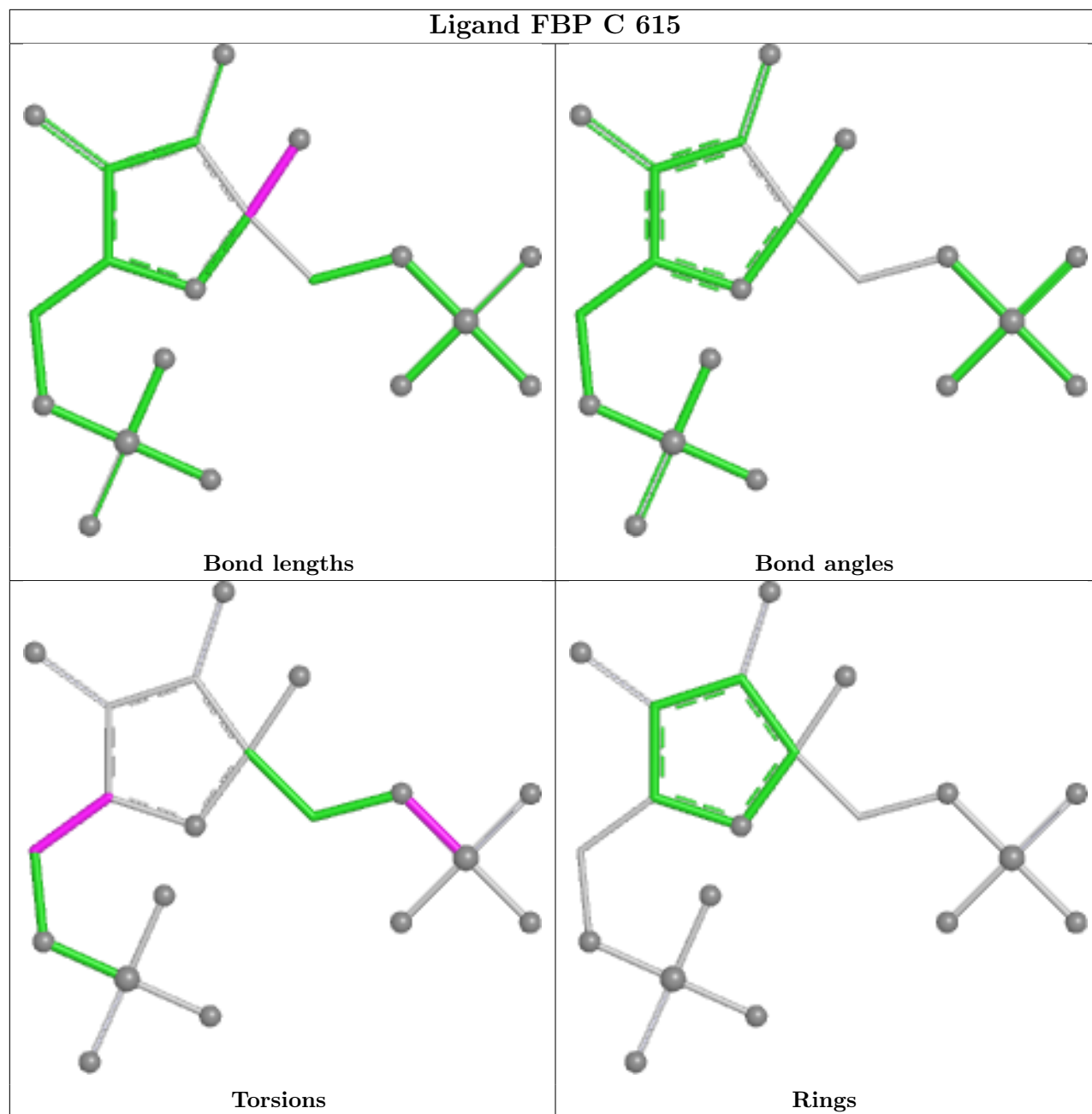
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	GOL	1	0
3	B	605	GOL	1	0
3	A	604	GOL	1	0
4	B	607	OXL	1	0
4	D	602	OXL	2	0
5	D	603	FBP	1	0
4	C	614	OXL	2	0
3	C	606	GOL	2	0
3	C	613	GOL	4	0
4	A	605	OXL	1	0
8	C	604	ASN	3	0

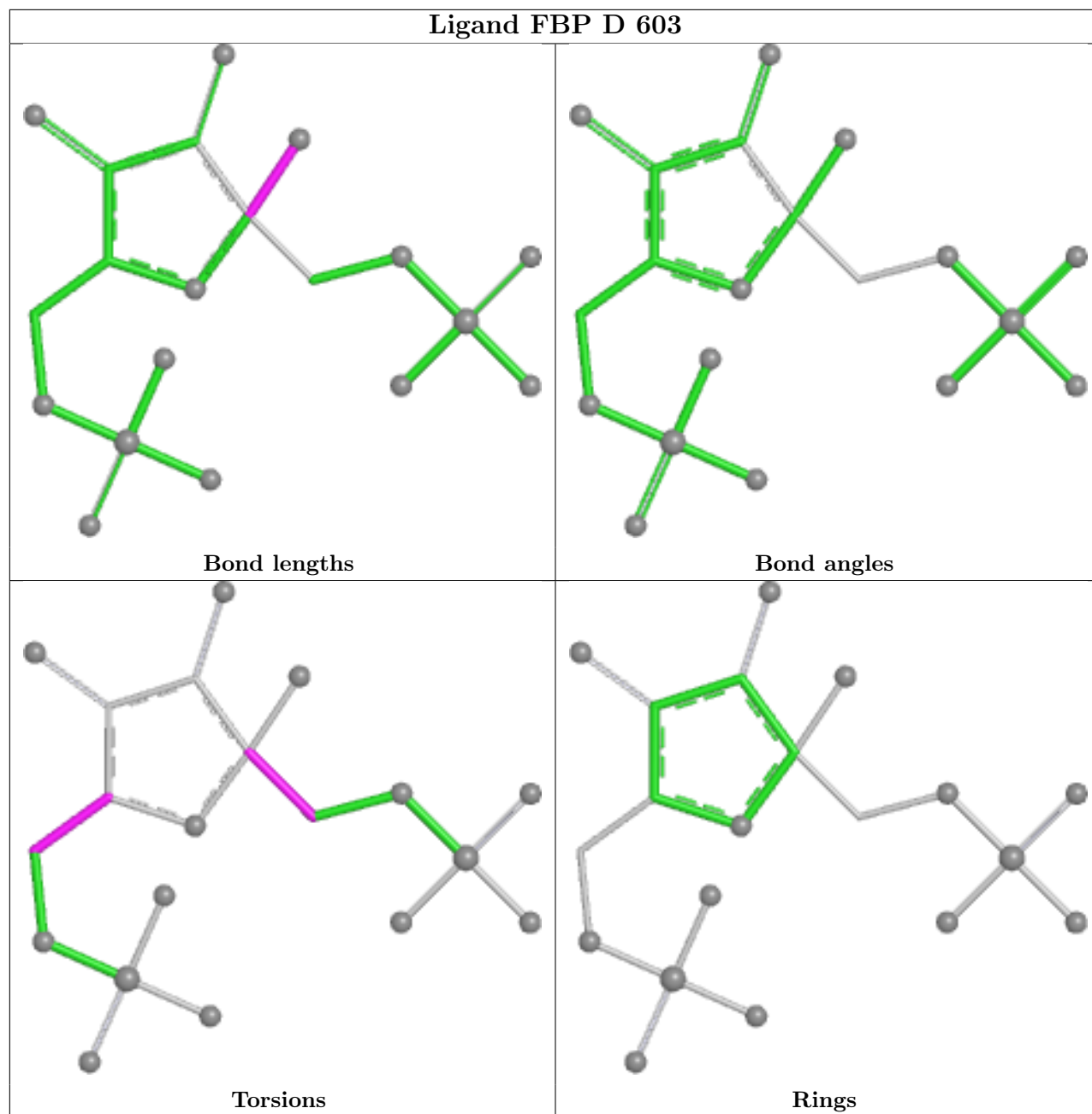
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

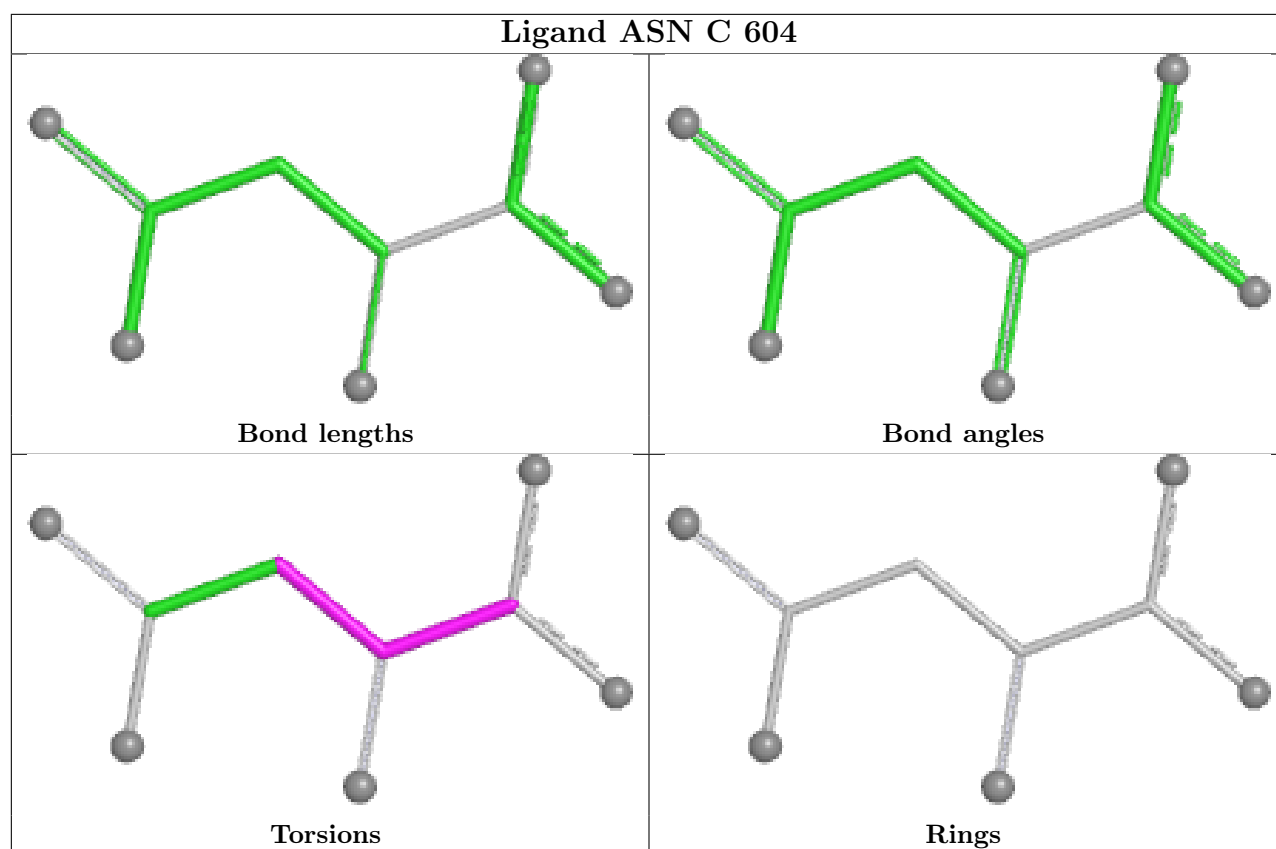


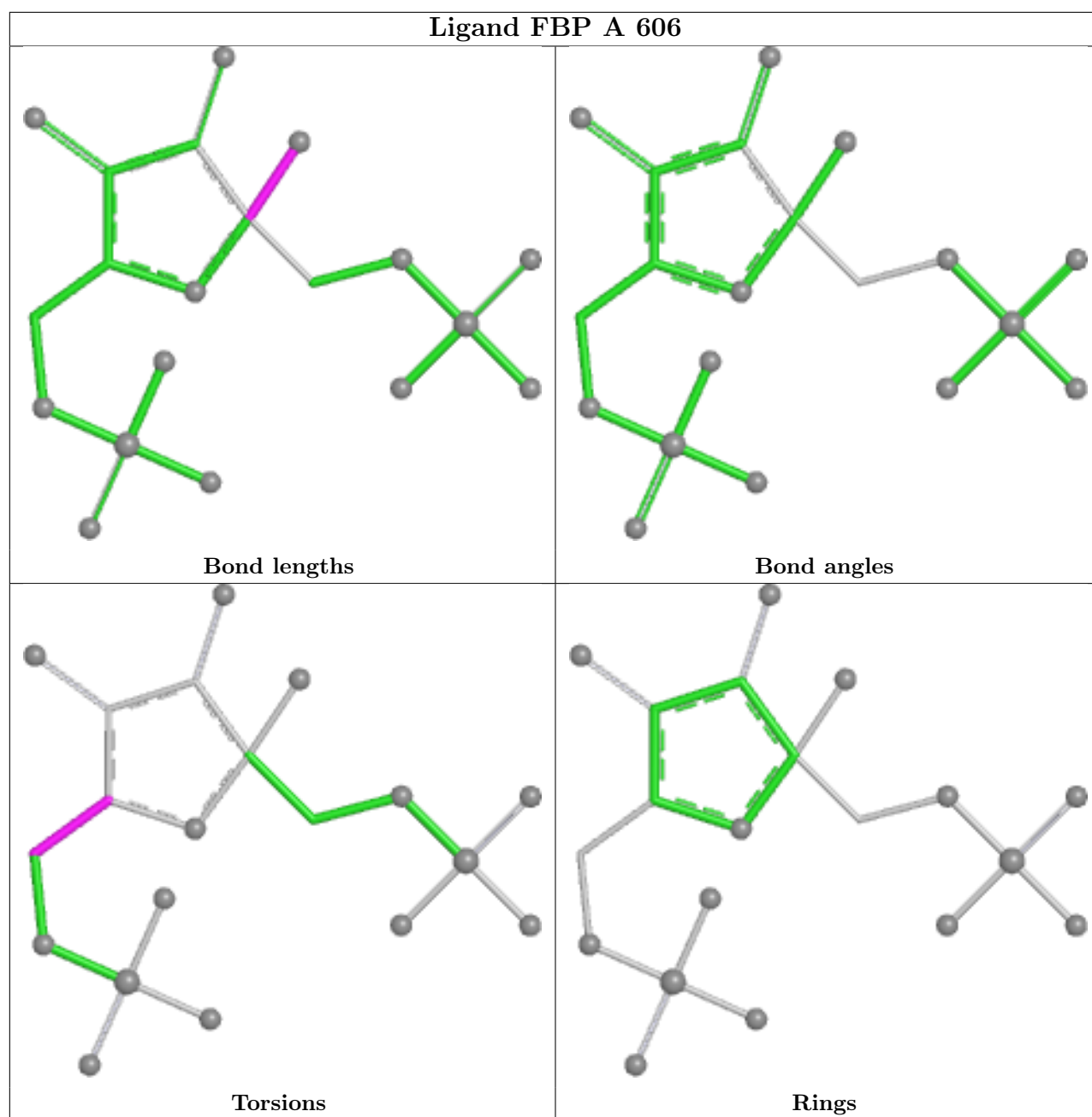
Ligand FBP C 615



Ligand FBP D 603







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	513/550 (93%)	0.85	64 (12%) 8 9	31, 43, 82, 92	0
1	B	516/550 (93%)	0.99	49 (9%) 14 16	36, 51, 70, 87	0
1	C	499/550 (90%)	1.09	87 (17%) 4 4	30, 46, 95, 105	0
1	D	427/550 (77%)	0.97	42 (9%) 13 15	36, 48, 66, 98	0
All	All	1955/2200 (88%)	0.97	242 (12%) 8 9	30, 47, 82, 105	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	GLY	7.5
1	A	41	THR	5.5
1	A	185	VAL	5.2
1	C	124	ILE	5.1
1	C	214	ALA	4.8
1	D	119	ILE	4.7
1	A	168	VAL	4.6
1	C	148	TYR	4.6
1	C	157	LEU	4.5
1	A	40	ILE	4.4
1	C	215	ALA	4.4
1	A	134	LEU	4.4
1	C	161	TYR	4.4
1	C	144	LEU	4.4
1	A	153	ASP	4.4
1	A	205	SER	4.3
1	C	140	LEU	4.3
1	C	165	CYS	4.2
1	B	16	GLN	4.1
1	A	136	LYS	4.1
1	C	172	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	164	ILE	4.0
1	A	203	LEU	4.0
1	B	168	VAL	4.0
1	C	216	VAL	4.0
1	C	14	GLN	3.9
1	C	167	VAL	3.9
1	C	163	ASN	3.8
1	C	123	LEU	3.8
1	D	120	ARG	3.8
1	D	218	LEU	3.8
1	A	139	THR	3.7
1	A	124	ILE	3.7
1	C	158	TRP	3.7
1	B	164	ILE	3.6
1	C	153	ASP	3.6
1	A	170	VAL	3.6
1	A	123	LEU	3.6
1	A	157	LEU	3.6
1	B	18	LEU	3.6
1	C	146	ASN	3.6
1	C	132	VAL	3.6
1	C	170	VAL	3.6
1	A	156	ILE	3.5
1	C	217	ASP	3.5
1	A	138	ALA	3.5
1	C	199	ASN	3.5
1	D	209	VAL	3.4
1	A	172	SER	3.4
1	A	148	TYR	3.4
1	A	193	LEU	3.4
1	C	159	LEU	3.4
1	C	18	LEU	3.4
1	A	198	GLU	3.4
1	C	139	THR	3.4
1	A	194	VAL	3.4
1	A	197	VAL	3.4
1	C	41	THR	3.3
1	D	244	PHE	3.3
1	A	177	ASP	3.3
1	D	40	ILE	3.3
1	A	178	ASP	3.2
1	C	181	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	212	PRO	3.2
1	A	137	GLY	3.2
1	D	41	THR	3.2
1	A	132	VAL	3.2
1	C	138	ALA	3.1
1	A	169	GLU	3.1
1	C	209	VAL	3.1
1	C	142	ILE	3.1
1	C	134	LEU	3.1
1	D	228	ASP	3.0
1	C	122	GLY	3.0
1	D	116	GLY	3.0
1	C	203	LEU	3.0
1	A	142	ILE	3.0
1	A	184	GLN	3.0
1	C	156	ILE	3.0
1	C	119	ILE	2.9
1	B	22	MET	2.9
1	A	164	ILE	2.9
1	D	226	ILE	2.9
1	B	259	GLY	2.9
1	C	204	GLY	2.9
1	A	167	VAL	2.9
1	D	257	VAL	2.9
1	B	80	THR	2.9
1	A	122	GLY	2.8
1	B	148	TYR	2.8
1	C	478	VAL	2.8
1	B	169	GLU	2.8
1	C	221	VAL	2.8
1	D	221	VAL	2.8
1	C	202	SER	2.8
1	B	40	ILE	2.8
1	C	205	SER	2.8
1	A	147	ALA	2.8
1	B	402	ALA	2.8
1	C	244	PHE	2.8
1	B	41	THR	2.7
1	B	65	ILE	2.7
1	C	40	ILE	2.7
1	C	121	THR	2.7
1	D	258	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	15	THR	2.7
1	B	404	ILE	2.7
1	A	204	GLY	2.7
1	C	213	GLY	2.7
1	C	183	LEU	2.7
1	A	199	ASN	2.7
1	D	118	GLU	2.7
1	D	211	LEU	2.7
1	B	185	VAL	2.7
1	D	210	ASN	2.7
1	C	169	GLU	2.7
1	D	219	PRO	2.7
1	A	144	LEU	2.7
1	A	481	ALA	2.6
1	B	385	ALA	2.6
1	C	42	ALA	2.6
1	C	44	ASN	2.6
1	C	168	VAL	2.6
1	C	237	VAL	2.6
1	C	137	GLY	2.6
1	A	14	GLN	2.6
1	A	200	GLY	2.6
1	B	103	ILE	2.6
1	B	193	LEU	2.6
1	A	217	ASP	2.6
1	A	195	THR	2.6
1	B	21	ALA	2.6
1	D	220	ALA	2.6
1	A	213	GLY	2.6
1	B	143	THR	2.6
1	B	221	VAL	2.6
1	B	135	LYS	2.5
1	C	339	ARG	2.5
1	C	147	ALA	2.5
1	C	530	VAL	2.5
1	D	223	GLU	2.5
1	C	162	LYS	2.5
1	B	161	TYR	2.5
1	A	152	CYS	2.4
1	C	154	GLU	2.4
1	C	174	ILE	2.4
1	D	267	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	163	ASN	2.4
1	B	111	ALA	2.4
1	B	190	ALA	2.4
1	B	200	GLY	2.4
1	A	159	LEU	2.4
1	C	155	ASN	2.4
1	C	21	ALA	2.4
1	C	481	ALA	2.4
1	D	475	LYS	2.4
1	D	83	TYR	2.4
1	C	201	GLY	2.4
1	C	182	SER	2.4
1	A	192	PHE	2.4
1	B	170	VAL	2.4
1	C	233	VAL	2.4
1	A	183	LEU	2.4
1	B	392	LEU	2.4
1	A	155	ASN	2.3
1	B	139	THR	2.3
1	C	176	VAL	2.3
1	B	246	ARG	2.3
1	A	206	LYS	2.3
1	C	149	MET	2.3
1	B	492	PHE	2.3
1	C	198	GLU	2.3
1	D	508	VAL	2.3
1	D	260	GLU	2.3
1	B	216	VAL	2.3
1	C	180	LEU	2.3
1	C	273	ASN	2.3
1	D	273	ASN	2.3
1	C	133	GLU	2.3
1	A	181	ILE	2.3
1	A	188	LYS	2.3
1	B	186	LYS	2.3
1	D	233	VAL	2.3
1	A	246	ARG	2.2
1	B	95	THR	2.2
1	C	150	GLU	2.2
1	C	175	TYR	2.2
1	B	474	CYS	2.2
1	B	171	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	499	ALA	2.2
1	A	158	TRP	2.2
1	C	218	LEU	2.2
1	B	194	VAL	2.2
1	D	298	GLY	2.2
1	B	470	PHE	2.2
1	D	227	GLN	2.2
1	D	493	ALA	2.2
1	C	106	ARG	2.1
1	D	18	LEU	2.1
1	D	245	ILE	2.1
1	A	216	VAL	2.1
1	A	151	LYS	2.1
1	D	206	LYS	2.1
1	A	208	GLY	2.1
1	B	172	SER	2.1
1	B	242	ALA	2.1
1	C	120	ARG	2.1
1	C	258	LEU	2.1
1	D	229	LEU	2.1
1	C	145	ASP	2.1
1	C	407	ASP	2.1
1	D	16	GLN	2.1
1	A	400	ARG	2.1
1	D	406	SER	2.1
1	C	131	GLU	2.1
1	A	174	ILE	2.1
1	D	297	LEU	2.1
1	B	472	VAL	2.1
1	A	470	PHE	2.1
1	D	262	GLY	2.1
1	D	404	ILE	2.1
1	C	219	PRO	2.1
1	C	477	PRO	2.1
1	B	233	VAL	2.1
1	D	254	VAL	2.1
1	B	188	LYS	2.0
1	B	214	ALA	2.0
1	C	178	ASP	2.0
1	B	477	PRO	2.0
1	B	390	TYR	2.0
1	B	232	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	208	GLY	2.0
1	D	470	PHE	2.0
1	C	207	LYS	2.0
1	A	100	SER	2.0
1	B	215	ALA	2.0
1	C	20	ALA	2.0
1	B	424	CYS	2.0
1	C	16	GLN	2.0
1	A	180	LEU	2.0
1	C	160	ASP	2.0
1	A	135	LYS	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
9	144	D	606	8/8	0.62	0.25	49,64,66,68	0
3	GOL	C	607	6/6	0.69	0.21	48,54,56,61	0
3	GOL	C	611	6/6	0.72	0.18	48,58,60,65	0
2	K	C	602	1/1	0.74	0.21	73,73,73,73	0
3	GOL	B	606	6/6	0.78	0.17	63,65,66,69	0
3	GOL	C	613	6/6	0.78	0.17	44,49,63,76	0
3	GOL	B	604	6/6	0.78	0.16	47,56,59,63	0
3	GOL	C	612	6/6	0.79	0.15	54,61,67,71	0
2	K	C	601	1/1	0.80	0.21	69,69,69,69	0
3	GOL	A	604	6/6	0.81	0.18	48,53,56,59	0
3	GOL	D	601	6/6	0.81	0.14	46,56,58,64	0
4	OXL	D	602	6/6	0.81	0.13	54,59,62,64	0

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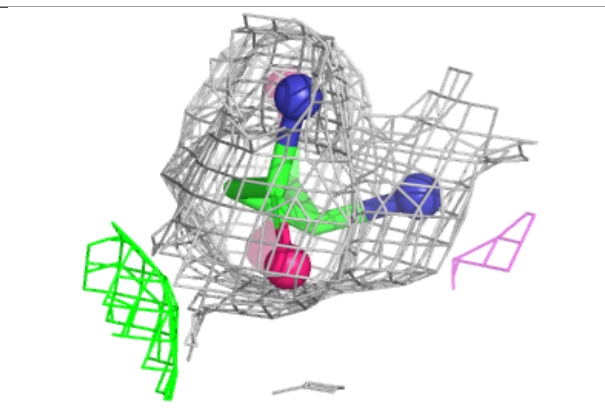
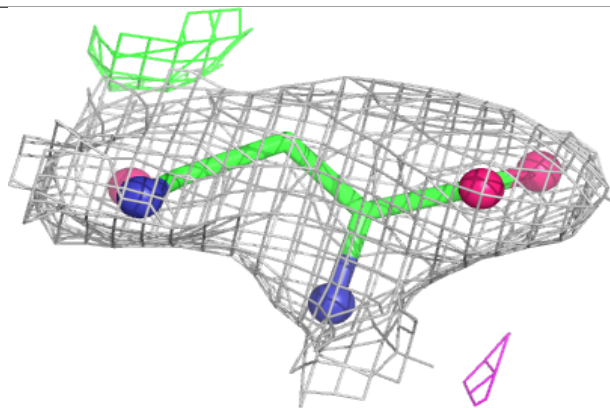
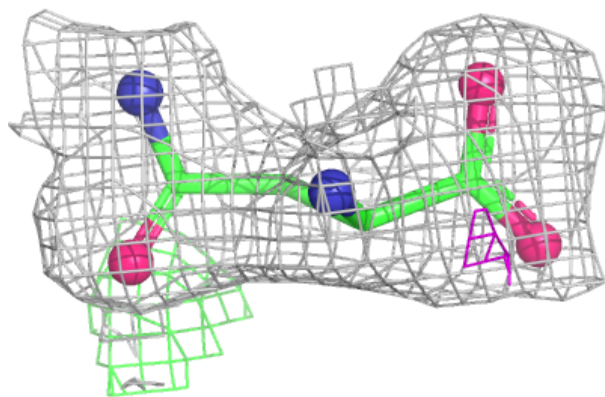
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	610	6/6	0.81	0.20	38,46,57,57	0
3	GOL	C	609	6/6	0.82	0.17	56,59,62,63	0
3	GOL	B	605	6/6	0.83	0.15	49,56,59,66	0
6	MG	D	604	1/1	0.84	0.13	57,57,57,57	0
3	GOL	B	603	6/6	0.85	0.15	46,51,59,62	0
3	GOL	A	603	6/6	0.86	0.17	28,45,52,56	0
8	ASN	C	604	9/9	0.86	0.13	48,51,54,62	0
3	GOL	C	605	6/6	0.86	0.16	46,55,64,66	0
3	GOL	C	606	6/6	0.87	0.14	47,55,57,58	0
4	OXL	C	614	6/6	0.87	0.13	47,52,56,59	0
6	MG	B	609	1/1	0.88	0.15	50,50,50,50	0
3	GOL	C	608	6/6	0.88	0.14	50,53,59,67	0
4	OXL	A	605	6/6	0.88	0.09	38,42,45,45	0
6	MG	A	607	1/1	0.88	0.19	42,42,42,42	0
3	GOL	B	602	6/6	0.90	0.10	47,51,52,62	0
6	MG	D	605	1/1	0.90	0.24	62,62,62,62	0
5	FBP	D	603	20/20	0.91	0.10	39,48,60,63	0
4	OXL	B	607	6/6	0.92	0.12	40,43,47,47	0
5	FBP	B	608	20/20	0.93	0.08	43,48,55,57	0
5	FBP	C	615	20/20	0.93	0.08	39,44,56,61	0
2	K	A	602	1/1	0.93	0.16	53,53,53,53	0
5	FBP	A	606	20/20	0.94	0.08	33,46,49,52	0
7	CL	B	601	1/1	0.95	0.14	56,56,56,56	0
2	K	A	601	1/1	0.97	0.06	56,56,56,56	0
7	CL	C	603	1/1	0.97	0.06	37,37,37,37	0

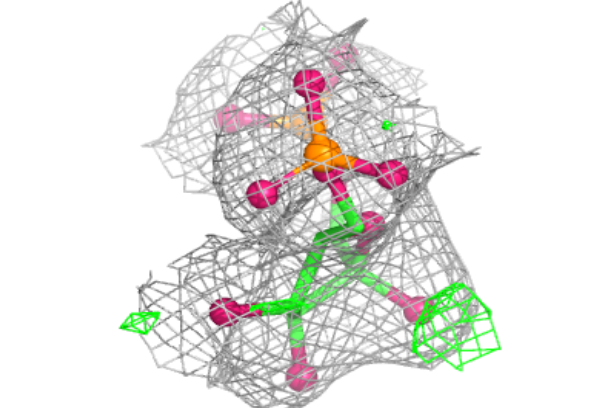
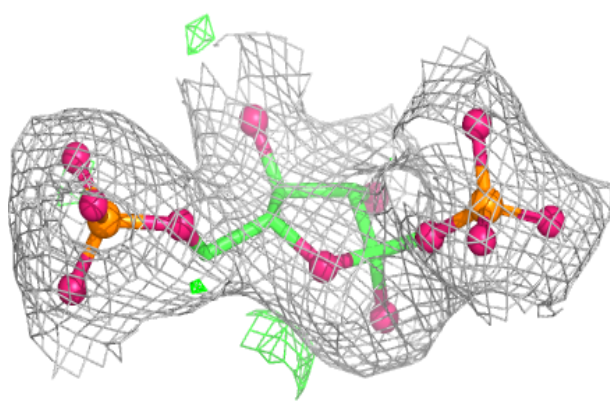
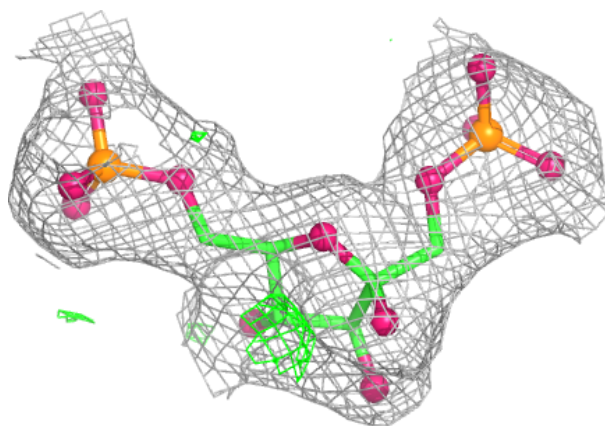
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ASN C 604:

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

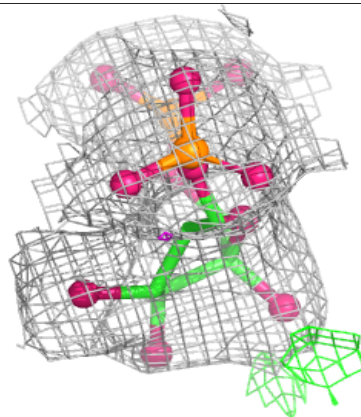
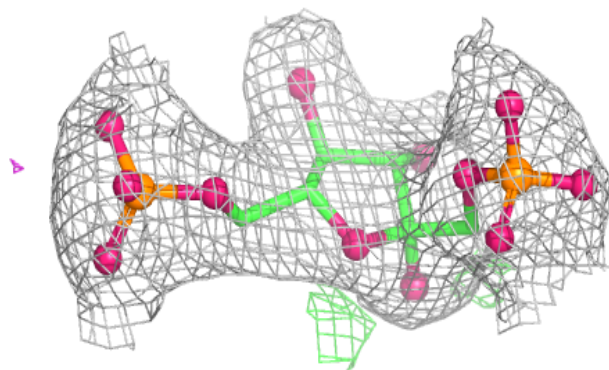
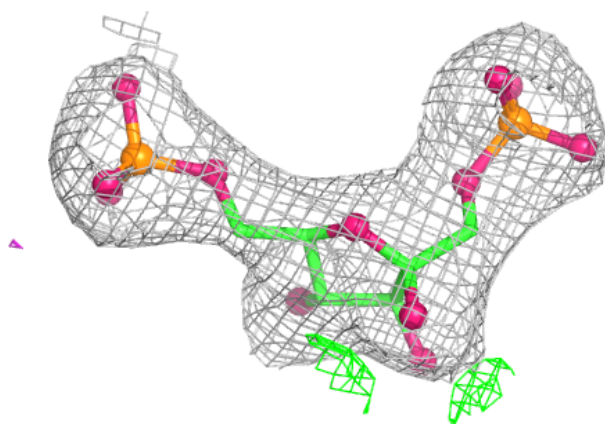
**Electron density around FBP D 603:**

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



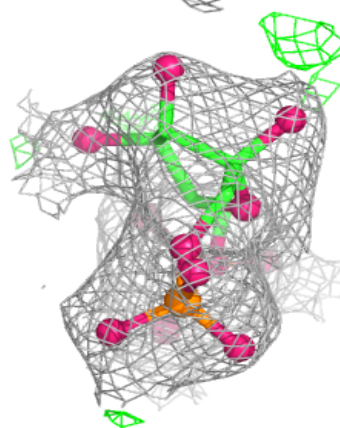
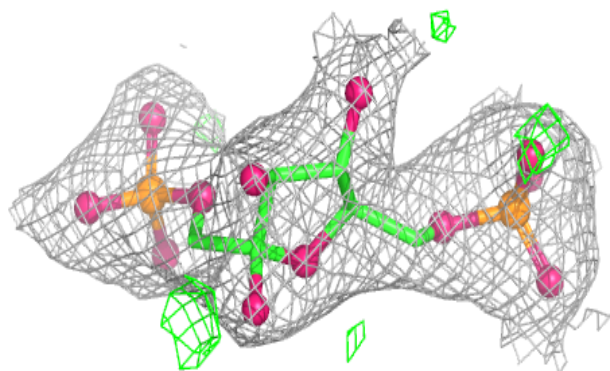
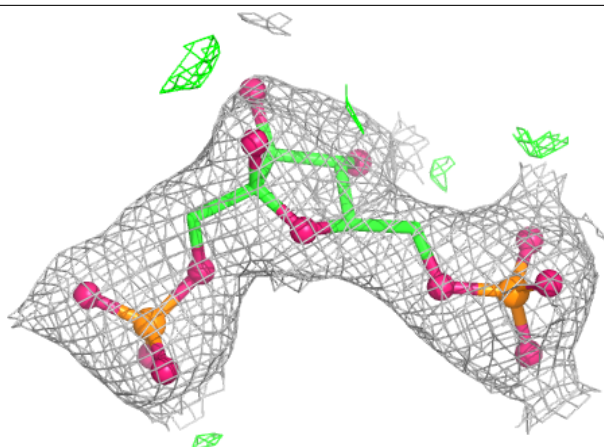
Electron density around FBP B 608:

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

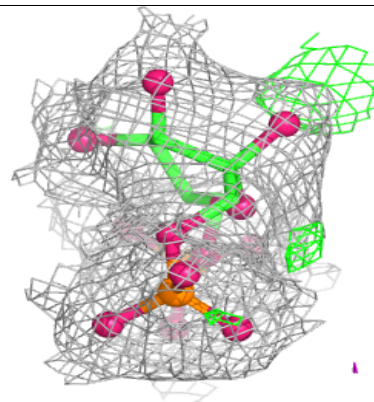
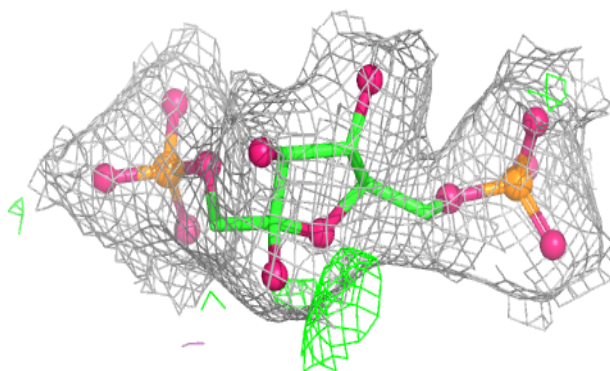
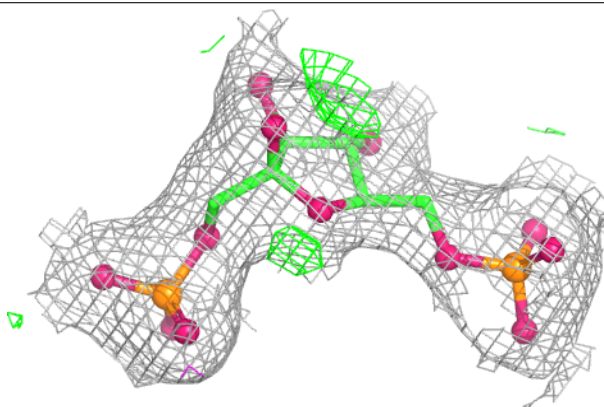


Electron density around FBP C 615:

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

**Electron density around FBP A 606:**

$2mF_o-DF_c$ (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.