Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 01:54 pm GMT

PDB ID	:	4XZ2
Title	:	Human platelet phosphofructokinase in an R-state in complex with ADP and F6P, crystal form I
Authors	:	Kloos, M.; Strater, N.
Deposited on	:	2015-02-03
Resolution	:	2.67 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 (i) 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 (i)) were used in the production of this report:

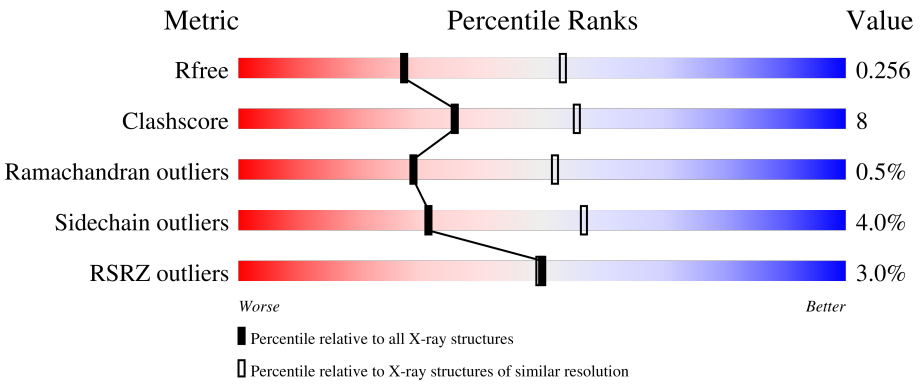
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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 <=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	761	2% 77% 14% • 7%
1	B	761	3% 81% 13% • •
1	C	761	2% 76% 14% • 7%
1	D	761	5% 78% 16% • 5%

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
2	PO4	C	802	-	-	X	-
5	F6P	B	803	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22132 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	708	5426	3410	961	1018	37	0	0	0
1	B	728	5568	3496	986	1048	38	0	0	0
1	C	704	5396	3389	957	1013	37	0	0	0
1	D	725	5546	3481	983	1044	38	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q01813
A	3	ALA	-	expression tag	UNP Q01813
A	4	SER	-	expression tag	UNP Q01813
A	5	TRP	-	expression tag	UNP Q01813
A	6	SER	-	expression tag	UNP Q01813
A	7	HIS	-	expression tag	UNP Q01813
A	8	PRO	-	expression tag	UNP Q01813
A	9	GLN	-	expression tag	UNP Q01813
A	10	PHE	-	expression tag	UNP Q01813
A	11	GLU	-	expression tag	UNP Q01813
A	12	LYS	-	expression tag	UNP Q01813
A	13	GLY	-	expression tag	UNP Q01813
A	14	ALA	-	expression tag	UNP Q01813
A	15	ASP	-	expression tag	UNP Q01813
A	16	ASP	-	expression tag	UNP Q01813
A	17	ASP	-	expression tag	UNP Q01813
A	18	ASP	-	expression tag	UNP Q01813
A	19	LYS	-	expression tag	UNP Q01813
A	20	VAL	-	expression tag	UNP Q01813
A	21	PRO	-	expression tag	UNP Q01813
A	22	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	PRO	-	expression tag	UNP Q01813
A	24	THR	-	expression tag	UNP Q01813
A	25	SER	-	expression tag	UNP Q01813
B	2	MET	-	initiating methionine	UNP Q01813
B	3	ALA	-	expression tag	UNP Q01813
B	4	SER	-	expression tag	UNP Q01813
B	5	TRP	-	expression tag	UNP Q01813
B	6	SER	-	expression tag	UNP Q01813
B	7	HIS	-	expression tag	UNP Q01813
B	8	PRO	-	expression tag	UNP Q01813
B	9	GLN	-	expression tag	UNP Q01813
B	10	PHE	-	expression tag	UNP Q01813
B	11	GLU	-	expression tag	UNP Q01813
B	12	LYS	-	expression tag	UNP Q01813
B	13	GLY	-	expression tag	UNP Q01813
B	14	ALA	-	expression tag	UNP Q01813
B	15	ASP	-	expression tag	UNP Q01813
B	16	ASP	-	expression tag	UNP Q01813
B	17	ASP	-	expression tag	UNP Q01813
B	18	ASP	-	expression tag	UNP Q01813
B	19	LYS	-	expression tag	UNP Q01813
B	20	VAL	-	expression tag	UNP Q01813
B	21	PRO	-	expression tag	UNP Q01813
B	22	ASP	-	expression tag	UNP Q01813
B	23	PRO	-	expression tag	UNP Q01813
B	24	THR	-	expression tag	UNP Q01813
B	25	SER	-	expression tag	UNP Q01813
C	2	MET	-	initiating methionine	UNP Q01813
C	3	ALA	-	expression tag	UNP Q01813
C	4	SER	-	expression tag	UNP Q01813
C	5	TRP	-	expression tag	UNP Q01813
C	6	SER	-	expression tag	UNP Q01813
C	7	HIS	-	expression tag	UNP Q01813
C	8	PRO	-	expression tag	UNP Q01813
C	9	GLN	-	expression tag	UNP Q01813
C	10	PHE	-	expression tag	UNP Q01813
C	11	GLU	-	expression tag	UNP Q01813
C	12	LYS	-	expression tag	UNP Q01813
C	13	GLY	-	expression tag	UNP Q01813
C	14	ALA	-	expression tag	UNP Q01813
C	15	ASP	-	expression tag	UNP Q01813
C	16	ASP	-	expression tag	UNP Q01813

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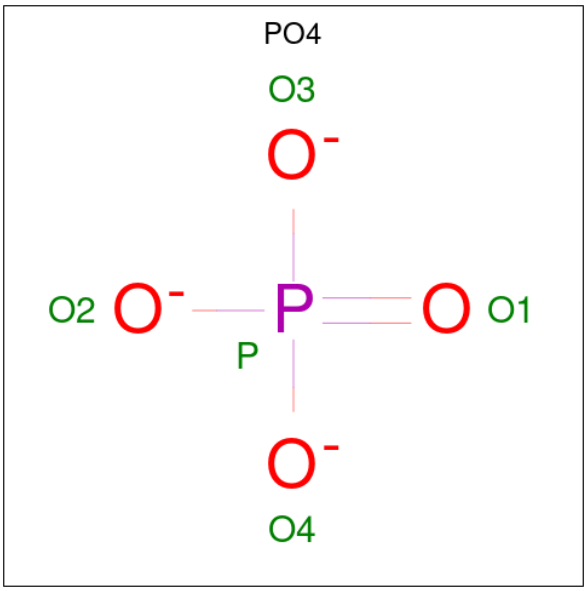
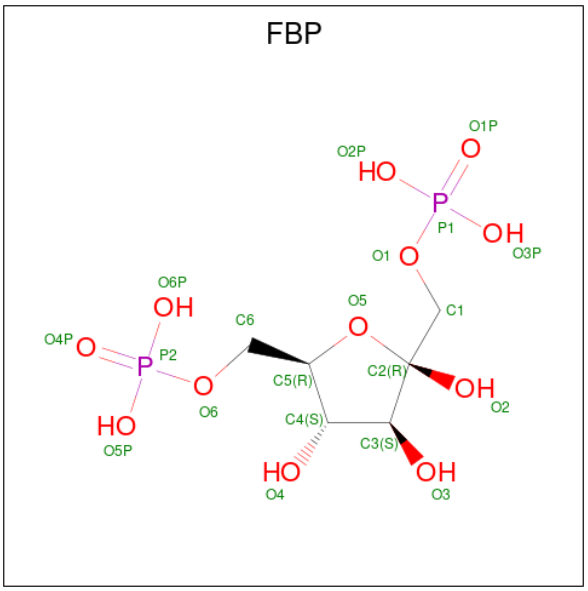
Chain	Residue	Modelled	Actual	Comment	Reference
C	17	ASP	-	expression tag	UNP Q01813
C	18	ASP	-	expression tag	UNP Q01813
C	19	LYS	-	expression tag	UNP Q01813
C	20	VAL	-	expression tag	UNP Q01813
C	21	PRO	-	expression tag	UNP Q01813
C	22	ASP	-	expression tag	UNP Q01813
C	23	PRO	-	expression tag	UNP Q01813
C	24	THR	-	expression tag	UNP Q01813
C	25	SER	-	expression tag	UNP Q01813
D	2	MET	-	initiating methionine	UNP Q01813
D	3	ALA	-	expression tag	UNP Q01813
D	4	SER	-	expression tag	UNP Q01813
D	5	TRP	-	expression tag	UNP Q01813
D	6	SER	-	expression tag	UNP Q01813
D	7	HIS	-	expression tag	UNP Q01813
D	8	PRO	-	expression tag	UNP Q01813
D	9	GLN	-	expression tag	UNP Q01813
D	10	PHE	-	expression tag	UNP Q01813
D	11	GLU	-	expression tag	UNP Q01813
D	12	LYS	-	expression tag	UNP Q01813
D	13	GLY	-	expression tag	UNP Q01813
D	14	ALA	-	expression tag	UNP Q01813
D	15	ASP	-	expression tag	UNP Q01813
D	16	ASP	-	expression tag	UNP Q01813
D	17	ASP	-	expression tag	UNP Q01813
D	18	ASP	-	expression tag	UNP Q01813
D	19	LYS	-	expression tag	UNP Q01813
D	20	VAL	-	expression tag	UNP Q01813
D	21	PRO	-	expression tag	UNP Q01813
D	22	ASP	-	expression tag	UNP Q01813
D	23	PRO	-	expression tag	UNP Q01813
D	24	THR	-	expression tag	UNP Q01813
D	25	SER	-	expression tag	UNP Q01813

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



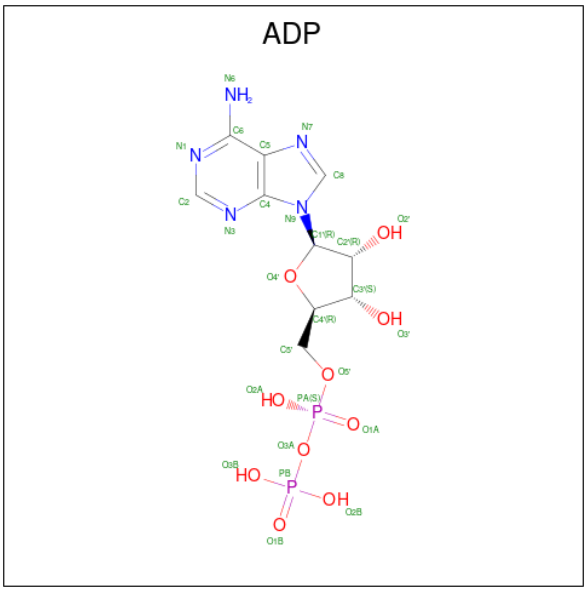
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



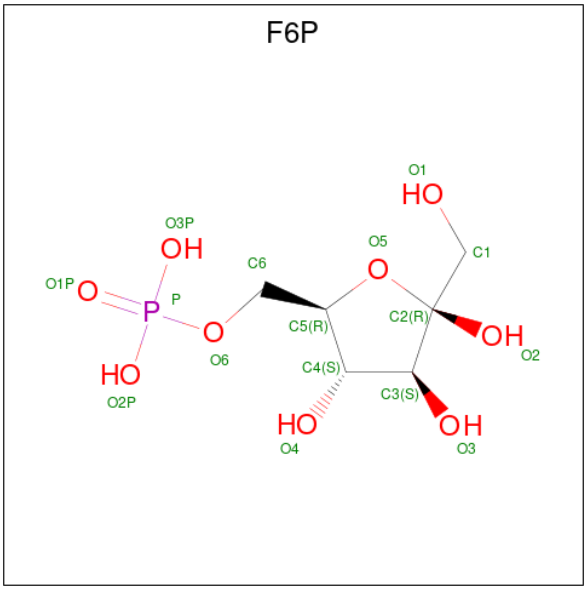
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		
3	C	1	Total	C	O	P	0	0
			20	6	12	2		
3	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).



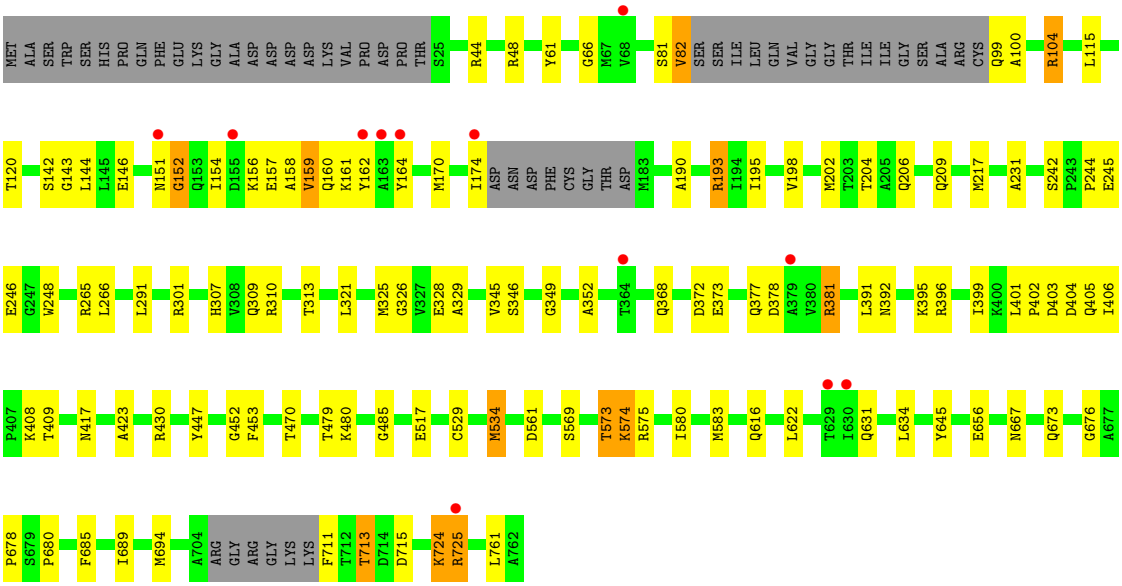
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			16	6	9	1		
5	D	1	Total	C	O	P	0	0
			16	6	9	1		

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.

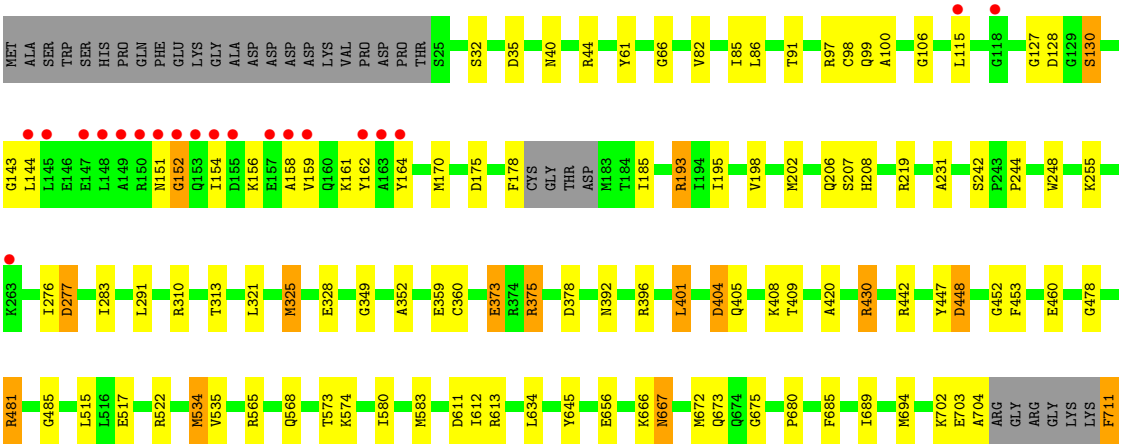
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

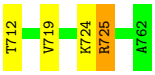
Chain A:



• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

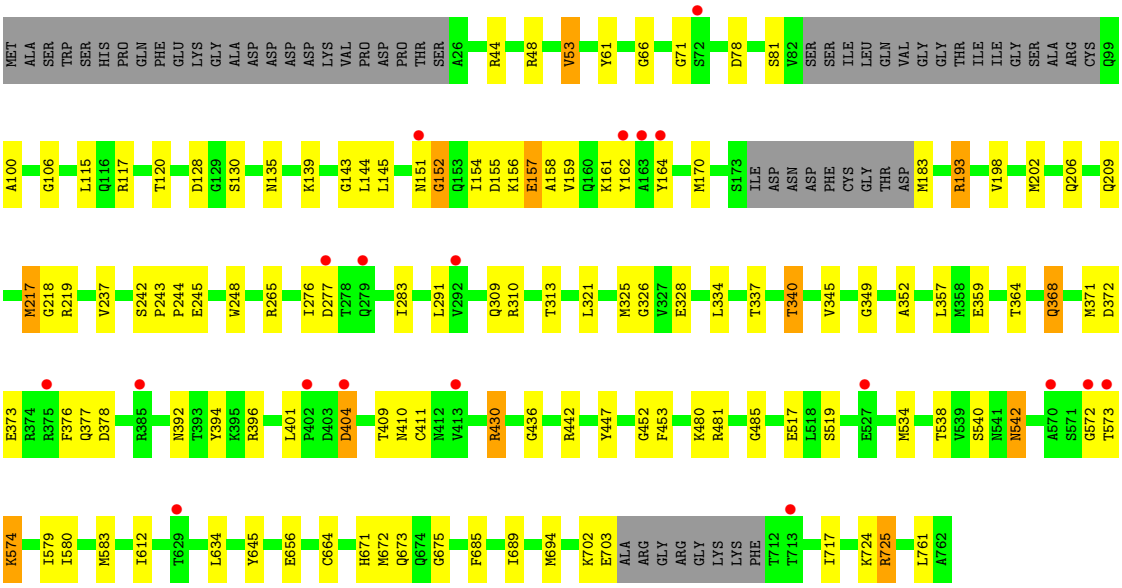
Chain B:





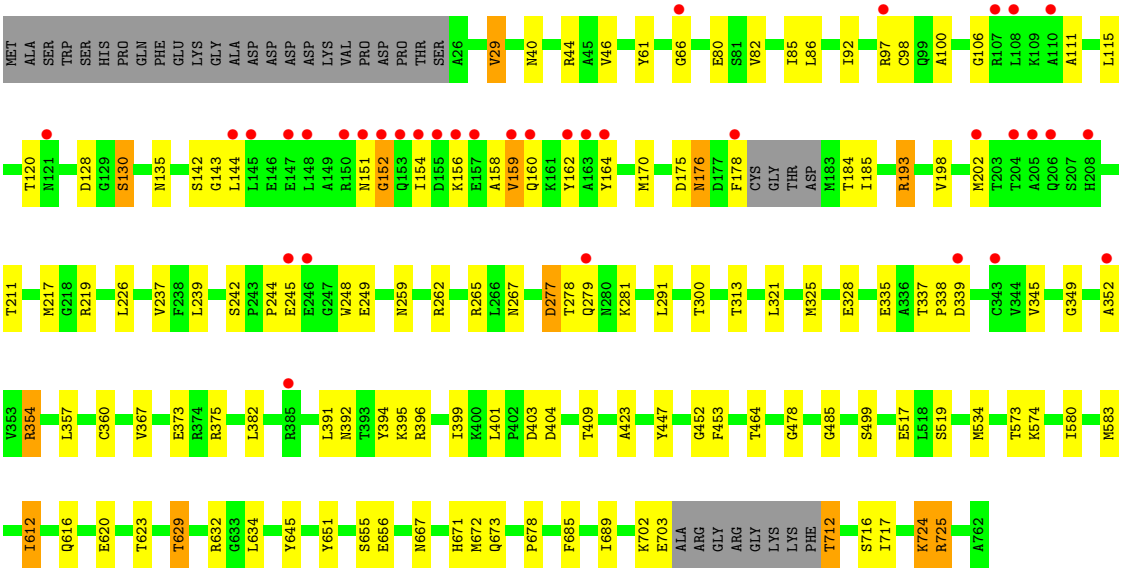
• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain C:



• Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.65Å 164.52Å 133.20Å 90.00° 102.96° 90.00°	Depositor
Resolution (Å)	46.03 – 2.67 46.04 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.03-2.67) 99.1 (46.04-2.67)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.216 , 0.255 0.218 , 0.256	Depositor DCC
R_{free} test set	4500 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22132	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, FBP, F6P, PO4

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	0.59	0/5513	0.77	7/7444 (0.1%)
1	B	0.58	0/5657	0.76	7/7640 (0.1%)
1	C	0.55	0/5482	0.76	5/7402 (0.1%)
1	D	0.54	0/5634	0.75	4/7609 (0.1%)
All	All	0.56	0/22286	0.76	23/30095 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	145	LEU	CB-CG-CD2	7.31	123.42	111.00
1	B	375	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	381	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	481	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	C	371	MET	CA-CB-CG	6.07	123.62	113.30
1	B	255	LYS	CD-CE-NZ	6.04	125.60	111.70
1	B	325	MET	CG-SD-CE	5.78	109.45	100.20
1	A	409	THR	N-CA-C	-5.73	95.53	111.00
1	D	354	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	561	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	D	403	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	C	371	MET	CG-SD-CE	5.48	108.97	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	277	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	D	265	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	481	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	381	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	534	MET	CG-SD-CE	-5.22	91.85	100.20
1	D	354	ARG	CG-CD-NE	5.22	122.76	111.80
1	A	48	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	565	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	561	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	219	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	375	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	143	GLY	Peptide

5.2 Too-close contacts (i)

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	5426	0	5453	95	1
1	B	5568	0	5595	96	0
1	C	5396	0	5426	86	1
1	D	5546	0	5576	105	0
2	A	5	0	0	0	0
2	B	10	0	0	2	0
2	C	5	0	0	2	0
2	D	10	0	0	1	0
3	A	20	0	10	1	0
3	B	20	0	10	0	0
3	C	20	0	10	1	0
3	D	20	0	10	3	0
4	B	27	0	12	7	0
4	D	27	0	12	2	0
5	B	16	0	11	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	16	0	11	4	0
All	All	22132	0	22136	360	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (360) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:NH1	1:A:631:GLN:NE2	1.62	1.45
1:D:111:ALA:O	1:D:115:LEU:HD12	1.54	1.06
1:A:529:CYS:O	1:A:711:PHE:N	1.88	1.06
1:B:373:GLU:HB3	1:B:375:ARG:HG3	1.34	1.05
1:B:534:MET:CE	1:B:719:VAL:HG22	1.93	0.99
1:D:44:ARG:HA	1:D:82:VAL:HG11	1.46	0.97
1:D:40:ASN:HB3	1:D:85:ILE:HG12	1.45	0.96
1:B:515:LEU:HD12	1:B:534:MET:HE2	1.49	0.95
1:A:417:ASN:CB	1:A:479:THR:HG22	1.97	0.94
1:D:219:ARG:HG3	5:D:803:F6P:O4	1.68	0.92
1:A:417:ASN:HB3	1:A:479:THR:HG22	1.49	0.92
1:B:219:ARG:HG3	5:B:803:F6P:O4	1.70	0.91
1:D:158:ALA:O	1:D:162:TYR:HB2	1.72	0.90
1:B:158:ALA:O	1:B:162:TYR:HB2	1.73	0.89
1:A:417:ASN:HB3	1:A:479:THR:CG2	2.02	0.88
1:C:277:ASP:OD1	1:C:283:ILE:HD11	1.72	0.88
1:A:158:ALA:O	1:A:162:TYR:HB2	1.73	0.88
1:B:98:CYS:N	4:B:801:ADP:O3'	2.08	0.87
1:B:534:MET:HE3	1:B:719:VAL:HG22	1.56	0.85
1:D:80:GLU:OE2	1:D:629:THR:HB	1.77	0.85
1:C:430:ARG:NH1	2:C:802:PO4:O3	2.10	0.85
1:C:158:ALA:O	1:C:162:TYR:HB2	1.78	0.84
1:A:573:THR:HG21	1:B:448:ASP:OD1	1.77	0.82
1:B:534:MET:HE1	1:B:719:VAL:HG22	1.60	0.81
1:D:178:PHE:CZ	1:D:360:CYS:HB3	2.15	0.81
1:B:40:ASN:HB3	1:B:85:ILE:HG22	1.63	0.80
1:D:111:ALA:O	1:D:115:LEU:CD1	2.32	0.78
1:B:130:SER:OG	4:B:801:ADP:O2B	2.03	0.77
1:D:82:VAL:HG12	1:D:85:ILE:HG21	1.66	0.77
1:D:82:VAL:CG1	1:D:85:ILE:HG21	2.14	0.76
1:B:583:MET:H	1:B:673:GLN:HE22	1.34	0.76
1:D:44:ARG:CA	1:D:82:VAL:HG11	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLU:HG2	1:B:375:ARG:HE	1.51	0.75
1:D:98:CYS:N	4:D:801:ADP:O3'	2.15	0.75
1:D:211:THR:HG22	1:D:267:ASN:HD22	1.50	0.75
1:A:44:ARG:HD2	1:A:82:VAL:HG22	1.68	0.74
1:A:244:PRO:O	1:A:245:GLU:HB3	1.87	0.74
1:B:82:VAL:HA	1:B:85:ILE:HD12	1.69	0.74
1:D:29:VAL:CG1	1:D:46:VAL:HG11	2.18	0.74
1:B:535:VAL:HG21	1:B:689:ILE:HG23	1.70	0.74
1:D:335:GLU:OE1	1:D:354:ARG:NH2	2.20	0.73
1:D:583:MET:H	1:D:673:GLN:HE22	1.33	0.73
1:D:85:ILE:HD12	1:D:92:ILE:HG21	1.70	0.73
1:C:542:ASN:H	1:C:542:ASN:HD22	1.35	0.72
1:D:82:VAL:O	1:D:85:ILE:HG22	1.89	0.72
1:A:529:CYS:C	1:A:711:PHE:N	2.42	0.72
1:C:325:MET:HE3	1:C:345:VAL:HG23	1.71	0.71
1:A:403:ASP:OD1	1:A:408:LYS:NZ	2.23	0.70
1:A:575:ARG:HG2	1:A:631:GLN:HB3	1.74	0.69
1:C:368:GLN:O	1:C:372:ASP:OD1	2.10	0.68
1:A:174:ILE:HD12	1:A:310:ARG:HD3	1.75	0.67
1:A:417:ASN:CB	1:A:479:THR:CG2	2.67	0.67
1:D:325:MET:HE3	1:D:345:VAL:O	1.95	0.67
1:A:573:THR:CG2	1:B:448:ASP:OD1	2.41	0.67
1:C:409:THR:HG22	1:C:411:CYS:H	1.59	0.67
1:A:301:ARG:NH1	5:B:803:F6P:P	2.68	0.67
1:A:104:ARG:NH1	1:A:146:GLU:OE1	2.28	0.66
1:B:401:LEU:CD2	1:B:405:GLN:OE1	2.42	0.66
1:C:583:MET:H	1:C:673:GLN:HE22	1.43	0.66
1:A:81:SER:O	1:A:82:VAL:HG12	1.96	0.66
1:B:535:VAL:HG21	1:B:689:ILE:CG2	2.26	0.65
1:B:97:ARG:HG3	4:B:801:ADP:H5'1	1.78	0.65
1:C:243:PRO:HG2	1:C:376:PHE:CZ	2.32	0.65
1:D:620:GLU:O	1:D:623:THR:HG22	1.97	0.65
1:A:616:GLN:HG3	1:D:612:ILE:HD13	1.77	0.65
1:D:226:LEU:HB2	1:D:239:LEU:HD21	1.78	0.64
1:C:206:GLN:HE21	1:C:265:ARG:HD3	1.62	0.64
1:A:195:ILE:HD12	1:A:680:PRO:HG3	1.80	0.64
1:D:328:GLU:OE2	1:D:354:ARG:NH1	2.30	0.64
1:D:82:VAL:HG12	1:D:82:VAL:O	1.99	0.63
1:D:259:ASN:HA	1:D:262:ARG:HD3	1.79	0.63
1:A:583:MET:SD	3:A:802:FBP:H3	2.38	0.63
1:A:583:MET:H	1:A:673:GLN:HE22	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:NH1	2:B:805:PO4:O4	2.32	0.63
1:B:401:LEU:HD23	1:B:405:GLN:OE1	1.98	0.63
1:D:130:SER:OG	4:D:801:ADP:O1B	2.17	0.63
1:A:480:LYS:NZ	1:B:573:THR:O	2.31	0.63
1:B:40:ASN:HB3	1:B:85:ILE:CG2	2.28	0.63
1:B:175:ASP:OD2	5:B:803:F6P:H12	1.99	0.63
1:C:573:THR:C	1:C:574:LYS:O	2.33	0.62
1:B:522:ARG:NH2	1:B:712:THR:HB	2.14	0.62
1:C:337:THR:H	1:C:340:THR:HB	1.65	0.62
1:B:373:GLU:HB3	1:B:375:ARG:CG	2.21	0.61
1:B:404:ASP:OD1	1:B:404:ASP:N	2.26	0.61
1:C:349:GLY:HA3	1:C:725:ARG:HD3	1.80	0.61
1:D:175:ASP:OD2	5:D:803:F6P:H11	2.00	0.61
1:C:724:LYS:O	1:C:725:ARG:HB3	2.00	0.61
1:C:409:THR:HG22	1:C:411:CYS:N	2.16	0.61
1:D:325:MET:HE3	1:D:345:VAL:HG23	1.81	0.61
1:D:82:VAL:HG12	1:D:85:ILE:CG2	2.31	0.60
1:A:417:ASN:HB2	1:A:479:THR:HG22	1.79	0.60
1:A:206:GLN:HE21	1:A:265:ARG:HD3	1.67	0.60
1:B:115:LEU:HD11	1:B:144:LEU:CD2	2.31	0.60
1:A:616:GLN:HG3	1:D:612:ILE:CD1	2.32	0.60
1:C:115:LEU:HD11	1:C:144:LEU:CD2	2.32	0.59
1:C:44:ARG:NH2	1:C:761:LEU:O	2.35	0.59
1:D:259:ASN:OD1	1:D:262:ARG:NH1	2.35	0.59
1:A:115:LEU:HD11	1:A:144:LEU:CD2	2.33	0.59
1:B:195:ILE:HD12	1:B:680:PRO:HG3	1.83	0.59
1:A:301:ARG:NH1	5:B:803:F6P:O2P	2.33	0.59
1:D:349:GLY:HA3	1:D:725:ARG:HB2	1.83	0.59
1:B:515:LEU:CD1	1:B:534:MET:HE2	2.30	0.59
1:C:154:ILE:HB	1:C:157:GLU:OE1	2.03	0.59
1:B:430:ARG:NH1	2:B:804:PO4:O3	2.36	0.58
1:A:44:ARG:NH2	1:A:761:LEU:O	2.36	0.58
1:C:206:GLN:NE2	1:C:265:ARG:HD3	2.18	0.58
1:B:442:ARG:NH1	1:B:460:GLU:OE1	2.37	0.58
1:C:349:GLY:CA	1:C:725:ARG:HD3	2.34	0.57
1:C:409:THR:CG2	1:C:411:CYS:SG	2.92	0.57
1:C:583:MET:SD	3:C:801:FBP:H3	2.44	0.57
1:D:583:MET:CE	3:D:802:FBP:H3	2.35	0.57
1:B:724:LYS:O	1:B:725:ARG:HB3	2.05	0.57
1:A:378:ASP:OD1	1:A:381:ARG:NH2	2.38	0.57
1:B:375:ARG:NH1	1:B:378:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:LYS:O	1:A:725:ARG:HB3	2.05	0.56
1:B:535:VAL:HG23	1:B:689:ILE:HG12	1.88	0.56
1:B:611:ASP:OD2	1:B:613:ARG:NH2	2.37	0.56
1:D:244:PRO:O	1:D:245:GLU:HB2	2.06	0.56
1:A:575:ARG:CZ	1:A:631:GLN:NE2	2.59	0.56
1:D:82:VAL:HG13	1:D:85:ILE:HG21	1.88	0.55
1:C:198:VAL:O	1:C:202:MET:HG3	2.06	0.55
1:A:206:GLN:NE2	1:A:265:ARG:HD3	2.21	0.55
1:D:176:ASN:HD22	1:D:184:THR:HB	1.71	0.55
1:A:301:ARG:HH12	5:B:803:F6P:P	2.29	0.55
1:D:632:ARG:NH2	2:D:805:PO4:O4	2.27	0.55
1:D:702:LYS:O	1:D:703:GLU:HG3	2.07	0.55
1:D:712:THR:HG22	1:D:716:SER:OG	2.07	0.55
1:C:340:THR:HG22	1:C:340:THR:O	2.07	0.55
1:C:671:HIS:H	1:D:667:ASN:HD21	1.55	0.54
1:C:573:THR:O	1:C:574:LYS:O	2.25	0.54
1:D:178:PHE:CE2	1:D:360:CYS:HB3	2.42	0.54
1:C:243:PRO:HG3	1:C:276:ILE:CD1	2.38	0.54
1:C:572:GLY:HA2	1:D:478:GLY:HA2	1.90	0.54
1:D:337:THR:HG22	1:D:338:PRO:HD2	1.90	0.54
1:D:277:ASP:OD2	1:D:281:LYS:HB2	2.08	0.54
1:C:538:THR:HG22	1:C:540:SER:H	1.73	0.54
1:C:183:MET:CE	1:C:183:MET:HA	2.38	0.54
1:C:325:MET:HE3	1:C:345:VAL:O	2.07	0.54
1:A:204:THR:HG21	1:B:310:ARG:HB2	1.90	0.54
1:C:115:LEU:HD11	1:C:144:LEU:HD21	1.90	0.54
1:A:195:ILE:HD11	1:A:231:ALA:CB	2.38	0.53
1:B:195:ILE:HD11	1:B:231:ALA:CB	2.38	0.53
1:B:115:LEU:HD11	1:B:144:LEU:HD21	1.89	0.53
1:B:195:ILE:HD11	1:B:231:ALA:HB3	1.90	0.53
1:C:183:MET:HA	1:C:183:MET:HE2	1.91	0.53
1:B:276:ILE:C	1:B:283:ILE:CD1	2.77	0.53
1:C:702:LYS:O	1:C:703:GLU:HG3	2.07	0.53
1:B:645:TYR:CE2	1:C:656:GLU:HG2	2.44	0.53
1:D:178:PHE:CZ	1:D:360:CYS:CB	2.91	0.53
1:C:373:GLU:O	1:C:373:GLU:HG2	2.08	0.53
1:A:195:ILE:HD11	1:A:231:ALA:HB3	1.91	0.52
1:C:209:GLN:HA	1:C:265:ARG:O	2.10	0.52
1:A:573:THR:HG21	1:B:448:ASP:CG	2.29	0.52
1:A:209:GLN:HA	1:A:265:ARG:O	2.10	0.52
1:A:115:LEU:HD11	1:A:144:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:VAL:HG23	1:D:394:TYR:CE2	2.44	0.52
1:C:573:THR:HG22	1:C:574:LYS:O	2.10	0.52
1:D:249:GLU:CG	1:D:291:LEU:HD11	2.39	0.52
1:A:245:GLU:HG2	1:A:246:GLU:N	2.24	0.52
1:A:307:HIS:CD2	1:A:310:ARG:NH1	2.78	0.52
1:B:349:GLY:HA3	1:B:725:ARG:HB2	1.92	0.52
1:C:244:PRO:O	1:C:245:GLU:HB2	2.10	0.52
1:D:244:PRO:O	1:D:245:GLU:CB	2.58	0.52
1:A:301:ARG:NH1	5:B:803:F6P:O1P	2.43	0.51
1:D:237:VAL:HG23	1:D:394:TYR:CZ	2.45	0.51
1:D:85:ILE:CD1	1:D:92:ILE:HG21	2.37	0.51
1:A:575:ARG:NH1	1:A:631:GLN:CD	2.52	0.51
1:C:71:GLY:O	1:C:117:ARG:NH2	2.44	0.51
1:D:325:MET:HE3	1:D:345:VAL:C	2.31	0.51
1:B:207:SER:O	1:B:208:HIS:HB3	2.09	0.51
1:D:40:ASN:CB	1:D:85:ILE:HG12	2.31	0.51
1:D:583:MET:SD	3:D:802:FBP:H3	2.51	0.51
1:A:391:LEU:O	1:A:395:LYS:HG3	2.11	0.50
1:A:711:PHE:N	1:A:711:PHE:CD1	2.78	0.50
1:B:244:PRO:HB2	1:B:248:TRP:CD1	2.46	0.50
1:B:408:LYS:HG2	1:B:409:THR:O	2.11	0.50
1:D:337:THR:CG2	1:D:338:PRO:HD2	2.41	0.50
1:C:328:GLU:HG2	1:C:352:ALA:HB1	1.94	0.50
1:A:325:MET:HE1	1:A:346:SER:HA	1.94	0.50
1:A:711:PHE:N	1:A:711:PHE:HD1	2.10	0.50
1:D:170:MET:CE	1:D:185:ILE:CD1	2.90	0.50
1:B:373:GLU:CB	1:B:375:ARG:HG3	2.24	0.49
1:C:237:VAL:HG23	1:C:394:TYR:CE2	2.47	0.49
1:C:244:PRO:O	1:C:245:GLU:CB	2.60	0.49
1:A:174:ILE:CD1	1:A:310:ARG:HD3	2.42	0.49
1:B:276:ILE:C	1:B:283:ILE:HD12	2.33	0.49
1:B:580:ILE:CD1	1:B:634:LEU:HD11	2.43	0.49
1:A:244:PRO:HB2	1:A:248:TRP:CD1	2.47	0.49
1:D:337:THR:HG22	1:D:339:ASP:H	1.78	0.49
1:C:447:TYR:O	1:C:452:GLY:HA3	2.13	0.49
1:D:120:THR:HB	1:D:164:TYR:O	2.13	0.49
1:D:193:ARG:NH2	1:D:313:THR:O	2.46	0.49
1:D:61:TYR:O	1:D:66:GLY:HA3	2.13	0.48
1:B:447:TYR:O	1:B:452:GLY:HA3	2.13	0.48
1:A:368:GLN:O	1:A:368:GLN:NE2	2.46	0.48
1:B:193:ARG:NH2	1:B:313:THR:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:PRO:HG3	1:C:276:ILE:HD12	1.94	0.48
1:D:29:VAL:HG13	1:D:46:VAL:HG11	1.94	0.48
1:D:447:TYR:O	1:D:452:GLY:HA3	2.13	0.48
1:D:82:VAL:O	1:D:85:ILE:CG2	2.58	0.48
1:D:724:LYS:O	1:D:725:ARG:HB3	2.14	0.48
1:B:127:GLY:HA3	4:B:801:ADP:O3B	2.13	0.48
1:B:277:ASP:N	1:B:283:ILE:CD1	2.76	0.48
1:B:98:CYS:H	4:B:801:ADP:HO3'	1.50	0.48
1:D:219:ARG:CG	5:D:803:F6P:O4	2.53	0.48
1:D:391:LEU:O	1:D:395:LYS:HG3	2.14	0.48
1:C:61:TYR:O	1:C:66:GLY:HA3	2.14	0.48
1:A:656:GLU:HG2	1:D:645:TYR:CE2	2.49	0.48
1:B:373:GLU:CG	1:B:375:ARG:HE	2.25	0.47
1:B:97:ARG:CG	4:B:801:ADP:H5'1	2.43	0.47
1:B:170:MET:CE	1:B:185:ILE:CD1	2.92	0.47
1:C:120:THR:HB	1:C:164:TYR:O	2.14	0.47
1:A:447:TYR:O	1:A:452:GLY:HA3	2.13	0.47
1:C:217:MET:HG3	1:C:309:GLN:CD	2.35	0.47
1:A:328:GLU:HG2	1:A:352:ALA:HB1	1.96	0.47
1:B:328:GLU:HG2	1:B:352:ALA:HB1	1.97	0.47
1:D:328:GLU:HG2	1:D:352:ALA:HB1	1.96	0.47
1:C:193:ARG:NH2	1:C:313:THR:O	2.48	0.47
1:C:237:VAL:HG23	1:C:394:TYR:CZ	2.50	0.47
1:A:120:THR:HB	1:A:164:TYR:O	2.15	0.47
1:D:321:LEU:O	1:D:325:MET:HG2	2.14	0.47
1:B:612:ILE:HD11	1:C:612:ILE:HD11	1.97	0.47
1:C:349:GLY:HA3	1:C:725:ARG:HB2	1.96	0.47
1:B:702:LYS:C	1:B:704:ALA:H	2.18	0.47
1:B:666:LYS:C	1:B:667:ASN:HD22	2.15	0.47
1:A:573:THR:HB	1:B:478:GLY:HA3	1.96	0.46
1:A:713:THR:HB	1:A:715:ASP:OD1	2.15	0.46
1:B:321:LEU:O	1:B:325:MET:HG2	2.16	0.46
1:A:430:ARG:HD3	1:A:470:THR:HG22	1.97	0.46
1:B:656:GLU:HG2	1:C:645:TYR:CE2	2.51	0.46
1:B:522:ARG:CZ	1:B:712:THR:HB	2.45	0.46
1:D:135:ASN:HB2	1:D:357:LEU:HD21	1.96	0.46
1:B:685:PHE:O	1:B:689:ILE:HG22	2.15	0.46
1:D:44:ARG:CB	1:D:82:VAL:HG11	2.46	0.46
1:A:195:ILE:HD12	1:A:680:PRO:CG	2.45	0.46
1:A:645:TYR:CE2	1:D:656:GLU:HG2	2.50	0.46
1:B:61:TYR:O	1:B:66:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:PHE:O	1:A:689:ILE:HG22	2.16	0.46
1:D:580:ILE:CD1	1:D:634:LEU:HD11	2.45	0.46
1:B:310:ARG:HD3	5:B:803:F6P:O2	2.15	0.46
1:B:115:LEU:HD23	1:B:161:LYS:HG3	1.98	0.46
1:C:155:ASP:OD1	1:C:156:LYS:N	2.49	0.45
1:A:485:GLY:N	1:A:517:GLU:OE1	2.49	0.45
1:A:575:ARG:NH1	1:A:631:GLN:HG2	2.31	0.45
1:C:430:ARG:NH1	2:C:802:PO4:P	2.89	0.45
1:B:711:PHE:HD1	1:B:711:PHE:O	1.98	0.45
1:A:61:TYR:O	1:A:66:GLY:HA3	2.16	0.45
1:A:349:GLY:HA3	1:A:725:ARG:HB2	1.97	0.45
1:B:535:VAL:CG2	1:B:689:ILE:CG2	2.95	0.45
1:C:243:PRO:HG2	1:C:376:PHE:CE2	2.52	0.45
1:A:193:ARG:NH2	1:A:313:THR:O	2.48	0.45
1:C:580:ILE:CD1	1:C:634:LEU:HD11	2.47	0.45
1:D:217:MET:SD	5:D:803:F6P:O3	2.75	0.45
1:A:321:LEU:O	1:A:325:MET:HG2	2.17	0.45
1:B:178:PHE:CE2	1:B:360:CYS:HB3	2.52	0.45
1:B:193:ARG:HA	1:B:193:ARG:HD3	1.63	0.45
1:C:485:GLY:N	1:C:517:GLU:OE1	2.49	0.45
1:D:176:ASN:HD22	1:D:184:THR:CB	2.30	0.45
1:D:244:PRO:HB2	1:D:248:TRP:CD1	2.52	0.45
1:B:195:ILE:HD12	1:B:680:PRO:CG	2.47	0.45
1:C:321:LEU:O	1:C:325:MET:HG2	2.17	0.45
1:D:29:VAL:HG11	1:D:46:VAL:HG11	1.96	0.45
1:D:651:TYR:O	1:D:655:SER:HB3	2.17	0.45
1:D:685:PHE:O	1:D:689:ILE:HG22	2.17	0.45
1:D:485:GLY:N	1:D:517:GLU:OE1	2.50	0.44
1:C:685:PHE:O	1:C:689:ILE:HG22	2.17	0.44
1:C:48:ARG:NH1	1:C:761:LEU:O	2.50	0.44
1:D:373:GLU:CD	1:D:375:ARG:HH11	2.20	0.44
1:D:144:LEU:HD12	1:D:162:TYR:HD1	1.83	0.44
1:D:249:GLU:HG2	1:D:291:LEU:HD11	1.98	0.44
1:A:156:LYS:O	1:A:159:VAL:HG12	2.18	0.44
1:C:372:ASP:OD1	1:C:372:ASP:N	2.51	0.44
1:A:406:ILE:O	1:A:408:LYS:HE3	2.18	0.44
1:C:672:MET:O	1:C:675:GLY:HA2	2.18	0.44
1:D:85:ILE:CD1	1:D:92:ILE:CG2	2.95	0.44
1:A:193:ARG:HA	1:A:193:ARG:HD3	1.67	0.44
1:A:144:LEU:HD12	1:A:162:TYR:HD1	1.81	0.44
1:A:580:ILE:CD1	1:A:634:LEU:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:O	1:D:202:MET:HG3	2.17	0.44
1:A:667:ASN:HD21	1:B:672:MET:H	1.65	0.44
1:B:144:LEU:HD12	1:B:162:TYR:HD1	1.83	0.43
1:C:276:ILE:HD12	1:C:276:ILE:O	2.18	0.43
1:C:724:LYS:O	1:C:725:ARG:CB	2.62	0.43
1:D:156:LYS:O	1:D:159:VAL:HG12	2.18	0.43
1:D:392:ASN:O	1:D:396:ARG:HG3	2.18	0.43
1:B:392:ASN:O	1:B:396:ARG:HG3	2.18	0.43
1:D:583:MET:HE2	3:D:802:FBP:H3	2.00	0.43
1:D:193:ARG:HD3	1:D:193:ARG:HA	1.63	0.43
1:A:569:SER:HB3	1:B:675:GLY:O	2.18	0.43
1:C:135:ASN:HB2	1:C:357:LEU:HD21	2.01	0.43
1:A:115:LEU:HD23	1:A:161:LYS:HG3	1.99	0.43
1:A:616:GLN:OE1	1:D:616:GLN:OE1	2.35	0.43
1:C:115:LEU:HD23	1:C:161:LYS:HG3	1.99	0.43
1:C:193:ARG:HA	1:C:193:ARG:HD3	1.66	0.43
1:C:244:PRO:HB2	1:C:248:TRP:CD1	2.54	0.43
1:A:198:VAL:O	1:A:202:MET:HG3	2.18	0.43
1:B:485:GLY:N	1:B:517:GLU:OE1	2.51	0.43
1:A:307:HIS:CD2	1:A:310:ARG:HH12	2.37	0.42
1:D:237:VAL:CG2	1:D:394:TYR:CZ	3.02	0.42
1:B:277:ASP:N	1:B:283:ILE:HD11	2.34	0.42
1:B:645:TYR:CZ	1:C:656:GLU:HG2	2.54	0.42
1:C:154:ILE:HG22	1:C:156:LYS:H	1.84	0.42
1:D:337:THR:HG22	1:D:338:PRO:CD	2.49	0.42
1:A:217:MET:H	1:A:309:GLN:HE22	1.65	0.42
1:A:329:ALA:HA	1:A:345:VAL:HG21	2.01	0.42
1:A:423:ALA:HB1	1:A:678:PRO:HB3	2.01	0.42
1:B:198:VAL:O	1:B:202:MET:HG3	2.18	0.42
1:D:277:ASP:HB3	1:D:279:GLN:H	1.84	0.42
1:C:53:VAL:HG11	1:C:334:LEU:HD11	2.02	0.42
1:C:325:MET:HE3	1:C:345:VAL:C	2.40	0.42
1:C:392:ASN:O	1:C:396:ARG:HG3	2.20	0.42
1:B:151:ASN:O	1:B:152:GLY:C	2.58	0.42
1:D:178:PHE:CD1	1:D:178:PHE:C	2.92	0.41
1:D:357:LEU:C	1:D:357:LEU:HD23	2.40	0.41
1:D:423:ALA:HB1	1:D:678:PRO:HB3	2.02	0.41
1:A:170:MET:CE	1:A:326:GLY:HA2	2.49	0.41
1:B:97:ARG:HA	4:B:801:ADP:O3'	2.21	0.41
1:C:78:ASP:OD1	1:C:81:SER:N	2.53	0.41
1:D:367:VAL:HG22	1:D:382:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:GLY:HA2	1:C:694:MET:CE	2.49	0.41
1:A:99:GLN:CG	1:A:100:ALA:H	2.33	0.41
1:A:574:LYS:HG3	1:A:575:ARG:N	2.34	0.41
1:A:99:GLN:CG	1:A:100:ALA:N	2.84	0.41
1:A:160:GLN:O	1:A:164:TYR:HD2	2.03	0.41
1:C:151:ASN:O	1:C:152:GLY:C	2.59	0.41
1:C:170:MET:CE	1:C:326:GLY:HA2	2.51	0.41
1:B:277:ASP:HB3	1:B:283:ILE:HD11	2.03	0.41
1:C:519:SER:HB2	1:C:717:ILE:HD12	2.03	0.41
1:D:154:ILE:HG22	1:D:156:LYS:H	1.86	0.41
1:D:176:ASN:HD21	1:D:184:THR:H	1.68	0.41
1:A:151:ASN:O	1:A:152:GLY:C	2.59	0.41
1:A:174:ILE:HG23	1:A:190:ALA:CB	2.51	0.41
1:A:392:ASN:O	1:A:396:ARG:HG3	2.21	0.41
1:A:713:THR:CB	1:A:715:ASP:OD1	2.68	0.41
1:B:206:GLN:O	1:B:208:HIS:O	2.40	0.41
1:B:420:ALA:HB2	1:B:481:ARG:NH1	2.35	0.41
1:C:480:LYS:NZ	1:D:573:THR:O	2.53	0.41
1:C:542:ASN:HD22	1:C:542:ASN:N	2.09	0.41
1:D:100:ALA:O	1:D:106:GLY:HA3	2.21	0.41
1:A:115:LEU:CD2	1:A:161:LYS:HG3	2.51	0.40
1:A:402:PRO:O	1:A:405:GLN:HB2	2.21	0.40
1:B:175:ASP:OD2	5:B:803:F6P:C1	2.68	0.40
1:B:580:ILE:HD12	1:B:634:LEU:HD11	2.02	0.40
1:C:115:LEU:CD2	1:C:161:LYS:HG3	2.51	0.40
1:D:160:GLN:O	1:D:164:TYR:HD2	2.03	0.40
1:A:154:ILE:N	1:A:157:GLU:OE2	2.55	0.40
1:B:32:SER:HB3	1:B:130:SER:HB3	2.03	0.40
1:B:724:LYS:O	1:B:725:ARG:CB	2.67	0.40
1:D:151:ASN:O	1:D:152:GLY:C	2.59	0.40
1:D:211:THR:OG1	1:D:300:THR:HG23	2.21	0.40
1:B:100:ALA:O	1:B:106:GLY:HA3	2.22	0.40
1:B:154:ILE:HG22	1:B:156:LYS:H	1.86	0.40
1:C:579:ILE:CD1	1:C:664:CYS:HB3	2.51	0.40
1:D:519:SER:HB2	1:D:717:ILE:HD12	2.04	0.40
1:C:409:THR:HG22	1:C:410:ASN:N	2.37	0.40
1:D:373:GLU:CD	1:D:375:ARG:NH1	2.75	0.40
1:A:204:THR:HA	1:B:35:ASP:OD2	2.21	0.40
1:A:676:GLY:H	1:B:568:GLN:NE2	2.19	0.40
1:C:100:ALA:O	1:C:106:GLY:HA3	2.22	0.40
1:C:404:ASP:OD1	1:C:404:ASP:N	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASP:OD2	1:C:139:LYS:NZ[1_554]	2.17	0.03

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	700/761 (92%)	686 (98%)	11 (2%)	3 (0%)	34	58
1	B	722/761 (95%)	698 (97%)	20 (3%)	4 (1%)	25	47
1	C	696/761 (92%)	682 (98%)	11 (2%)	3 (0%)	34	58
1	D	719/761 (94%)	695 (97%)	20 (3%)	4 (1%)	25	47
All	All	2837/3044 (93%)	2761 (97%)	62 (2%)	14 (0%)	29	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	GLY
1	A	152	GLY
1	B	152	GLY
1	C	574	LYS
1	D	152	GLY
1	D	724	LYS
1	A	724	LYS
1	B	703	GLU
1	D	574	LYS
1	B	574	LYS
1	A	143	GLY
1	B	143	GLY
1	C	218	GLY
1	D	143	GLY

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	571/614 (93%)	550 (96%)	21 (4%)	34	60
1	B	587/614 (96%)	565 (96%)	22 (4%)	34	60
1	C	568/614 (92%)	544 (96%)	24 (4%)	30	55
1	D	585/614 (95%)	559 (96%)	26 (4%)	28	53
All	All	2311/2456 (94%)	2218 (96%)	93 (4%)	31	57

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	104	ARG
1	A	142	SER
1	A	159	VAL
1	A	193	ARG
1	A	242	SER
1	A	266	LEU
1	A	291	LEU
1	A	373	GLU
1	A	377	GLN
1	A	399	ILE
1	A	401	LEU
1	A	404	ASP
1	A	453	PHE
1	A	534	MET
1	A	573	THR
1	A	574	LYS
1	A	622	LEU
1	A	694	MET
1	A	713	THR
1	A	725	ARG
1	B	86	LEU
1	B	91	THR
1	B	99	GLN

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Mol	Chain	Res	Type
1	B	128	ASP
1	B	130	SER
1	B	159	VAL
1	B	164	TYR
1	B	193	ARG
1	B	242	SER
1	B	291	LEU
1	B	359	GLU
1	B	373	GLU
1	B	401	LEU
1	B	404	ASP
1	B	430	ARG
1	B	448	ASP
1	B	453	PHE
1	B	534	MET
1	B	667	ASN
1	B	694	MET
1	B	711	PHE
1	B	725	ARG
1	C	53	VAL
1	C	128	ASP
1	C	130	SER
1	C	157	GLU
1	C	159	VAL
1	C	193	ARG
1	C	217	MET
1	C	242	SER
1	C	291	LEU
1	C	310	ARG
1	C	340	THR
1	C	359	GLU
1	C	364	THR
1	C	368	GLN
1	C	377	GLN
1	C	378	ASP
1	C	401	LEU
1	C	404	ASP
1	C	430	ARG
1	C	442	ARG
1	C	453	PHE
1	C	534	MET
1	C	542	ASN

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Mol	Chain	Res	Type
1	C	725	ARG
1	D	29	VAL
1	D	86	LEU
1	D	97	ARG
1	D	128	ASP
1	D	130	SER
1	D	142	SER
1	D	159	VAL
1	D	176	ASN
1	D	193	ARG
1	D	242	SER
1	D	277	ASP
1	D	278	THR
1	D	399	ILE
1	D	401	LEU
1	D	404	ASP
1	D	409	THR
1	D	453	PHE
1	D	464	THR
1	D	499	SER
1	D	534	MET
1	D	612	ILE
1	D	629	THR
1	D	671	HIS
1	D	672	MET
1	D	712	THR
1	D	725	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	206	GLN
1	A	309	GLN
1	A	368	GLN
1	A	494	GLN
1	A	644	ASN
1	A	652	GLN
1	A	673	GLN
1	B	65	GLN
1	B	267	ASN
1	B	351	HIS

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Mol	Chain	Res	Type
1	B	417	ASN
1	B	494	GLN
1	B	568	GLN
1	B	616	GLN
1	B	644	ASN
1	B	652	GLN
1	B	671	HIS
1	B	673	GLN
1	B	730	GLN
1	C	206	GLN
1	C	494	GLN
1	C	542	ASN
1	C	652	GLN
1	C	673	GLN
1	D	176	ASN
1	D	307	HIS
1	D	362	GLN
1	D	501	ASN
1	D	616	GLN
1	D	644	ASN
1	D	667	ASN
1	D	673	GLN
1	D	749	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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	FBP	D	802	-	18,20,20	0.97	1 (5%)	23,32,32	0.98	0
2	PO4	D	805	-	4,4,4	0.95	0	6,6,6	0.67	0
4	ADP	B	801	-	24,29,29	1.17	3 (12%)	29,45,45	1.61	7 (24%)
4	ADP	D	801	-	24,29,29	1.05	2 (8%)	29,45,45	1.57	5 (17%)
5	F6P	B	803	-	15,16,16	0.85	1 (6%)	17,25,25	1.34	2 (11%)
5	F6P	D	803	-	15,16,16	0.86	1 (6%)	17,25,25	1.14	1 (5%)
2	PO4	D	804	-	4,4,4	0.81	0	6,6,6	0.85	0
2	PO4	B	804	-	4,4,4	1.16	0	6,6,6	0.69	0
2	PO4	C	802	-	4,4,4	1.34	0	6,6,6	0.68	0
3	FBP	A	802	-	18,20,20	1.29	1 (5%)	23,32,32	1.52	1 (4%)
3	FBP	B	802	-	18,20,20	1.18	1 (5%)	23,32,32	1.07	1 (4%)
2	PO4	A	801	-	4,4,4	1.11	0	6,6,6	0.75	0
3	FBP	C	801	-	18,20,20	1.10	1 (5%)	23,32,32	1.39	2 (8%)
2	PO4	B	805	-	4,4,4	1.12	0	6,6,6	0.76	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
4	ADP	B	801	-	-	0/12/32/32	0/3/3/3
3	FBP	D	802	-	-	4/13/32/32	0/1/1/1
4	ADP	D	801	-	-	4/12/32/32	0/3/3/3
5	F6P	D	803	-	-	5/9/28/28	0/1/1/1
3	FBP	B	802	-	-	6/13/32/32	0/1/1/1
5	F6P	B	803	-	-	3/9/28/28	0/1/1/1
3	FBP	C	801	-	-	4/13/32/32	0/1/1/1
3	FBP	A	802	-	-	5/13/32/32	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	FBP	O2-C2	4.00	1.47	1.40
3	B	802	FBP	O2-C2	3.03	1.45	1.40
3	D	802	FBP	O2-C2	2.97	1.45	1.40
4	B	801	ADP	C2-N3	2.86	1.36	1.32
4	B	801	ADP	O4'-C1'	2.62	1.44	1.41
4	D	801	ADP	C2-N3	2.51	1.36	1.32
4	D	801	ADP	C5-C4	2.47	1.47	1.40
3	C	801	FBP	O5-C2	-2.42	1.39	1.43
5	B	803	F6P	O2-C2	2.17	1.44	1.40
4	B	801	ADP	C5-C4	2.13	1.46	1.40
5	D	803	F6P	O2-C2	2.02	1.44	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	FBP	O2-C2-O5	5.20	119.55	109.50
4	B	801	ADP	N3-C2-N1	-3.71	122.88	128.68
4	D	801	ADP	N3-C2-N1	-3.53	123.16	128.68
5	B	803	F6P	O1-C1-C2	3.30	118.89	111.86
4	D	801	ADP	PA-O3A-PB	-3.29	121.53	132.83
4	D	801	ADP	C3'-C2'-C1'	3.07	105.60	100.98
4	B	801	ADP	PA-O3A-PB	-3.05	122.36	132.83
3	C	801	FBP	O2P-P1-O1	2.77	114.10	106.73
3	C	801	FBP	O2-C2-O5	2.67	114.66	109.50
4	B	801	ADP	O2B-PB-O1B	2.67	121.12	110.68
4	B	801	ADP	C3'-C2'-C1'	2.62	104.93	100.98
4	B	801	ADP	O3B-PB-O2B	2.48	117.10	107.64
3	B	802	FBP	O6-P2-O4P	2.47	113.41	106.47
4	B	801	ADP	C2'-C3'-C4'	2.41	107.33	102.64
4	D	801	ADP	N6-C6-N1	2.27	123.29	118.57
4	D	801	ADP	C2'-C3'-C4'	2.19	106.89	102.64
5	D	803	F6P	O3P-P-O2P	2.07	115.55	107.64
5	B	803	F6P	O3-C3-C4	-2.02	106.36	113.32
4	B	801	ADP	C4-C5-N7	-2.02	107.30	109.40

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	FBP	O1-C1-C2-O2
3	A	802	FBP	O1-C1-C2-C3
3	A	802	FBP	O1-C1-C2-O5

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Mol	Chain	Res	Type	Atoms
3	A	802	FBP	C4-C5-C6-O6
3	B	802	FBP	O1-C1-C2-O2
3	B	802	FBP	O1-C1-C2-O5
3	C	801	FBP	C4-C5-C6-O6
3	C	801	FBP	O5-C5-C6-O6
3	D	802	FBP	O1-C1-C2-O2
3	D	802	FBP	O1-C1-C2-C3
3	D	802	FBP	C4-C5-C6-O6
3	D	802	FBP	O5-C5-C6-O6
4	D	801	ADP	PA-O3A-PB-O2B
4	D	801	ADP	PA-O3A-PB-O3B
5	D	803	F6P	C6-O6-P-O1P
3	A	802	FBP	O5-C5-C6-O6
5	D	803	F6P	O1-C1-C2-O5
3	B	802	FBP	C1-O1-P1-O1P
5	B	803	F6P	O1-C1-C2-C3
5	D	803	F6P	O1-C1-C2-C3
5	B	803	F6P	O1-C1-C2-O2
3	B	802	FBP	C4-C5-C6-O6
5	B	803	F6P	O1-C1-C2-O5
3	B	802	FBP	O5-C5-C6-O6
3	C	801	FBP	O1-C1-C2-C3
5	D	803	F6P	O1-C1-C2-O2
4	D	801	ADP	O4'-C4'-C5'-O5'
4	D	801	ADP	C3'-C4'-C5'-O5'
3	B	802	FBP	C6-O6-P2-O6P
5	D	803	F6P	C6-O6-P-O2P
3	C	801	FBP	C6-O6-P2-O4P

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	802	FBP	3	0
2	D	805	PO4	1	0
4	B	801	ADP	7	0
4	D	801	ADP	2	0
5	B	803	F6P	8	0
5	D	803	F6P	4	0
2	B	804	PO4	1	0
2	C	802	PO4	2	0
3	A	802	FBP	1	0

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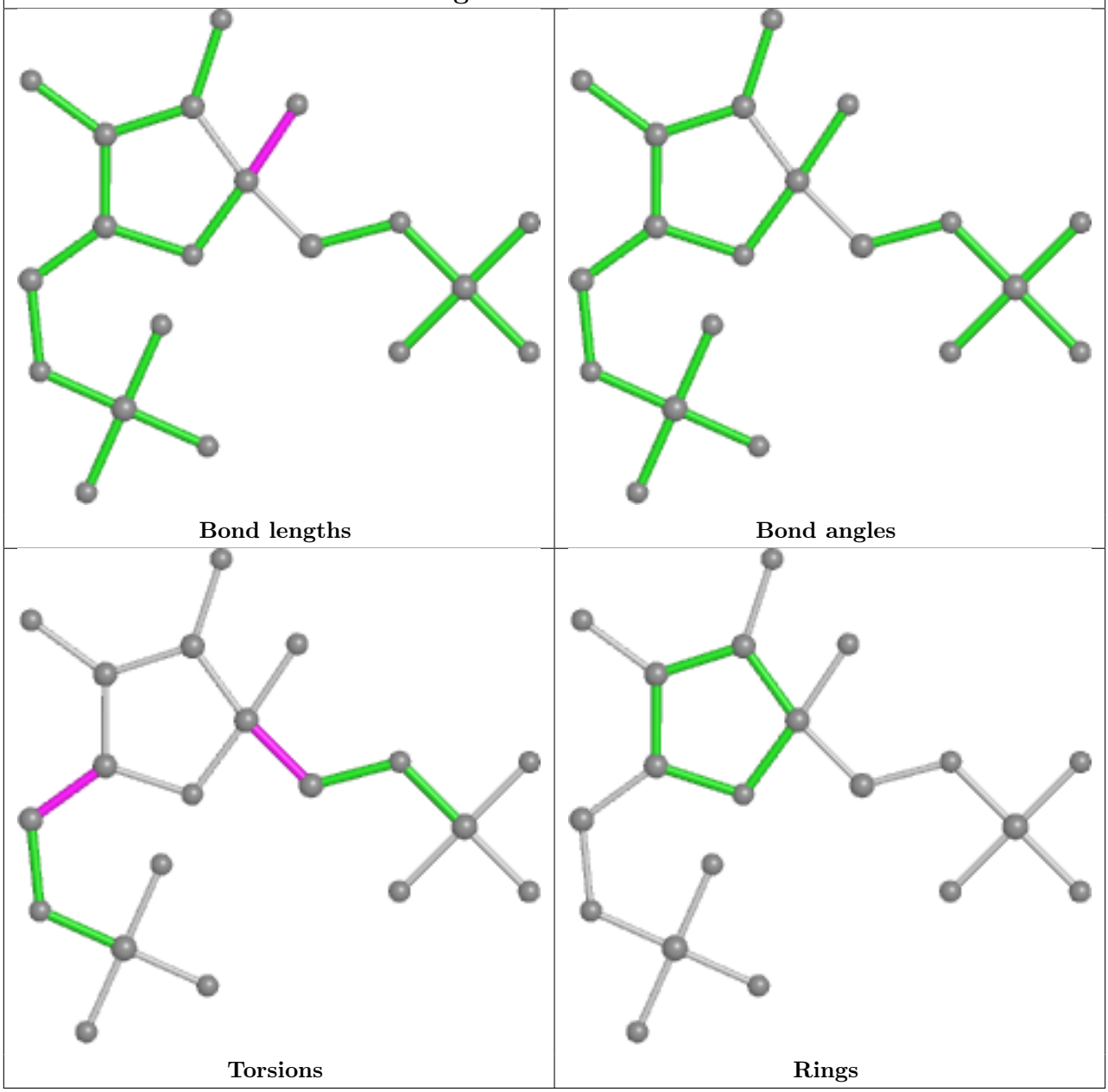
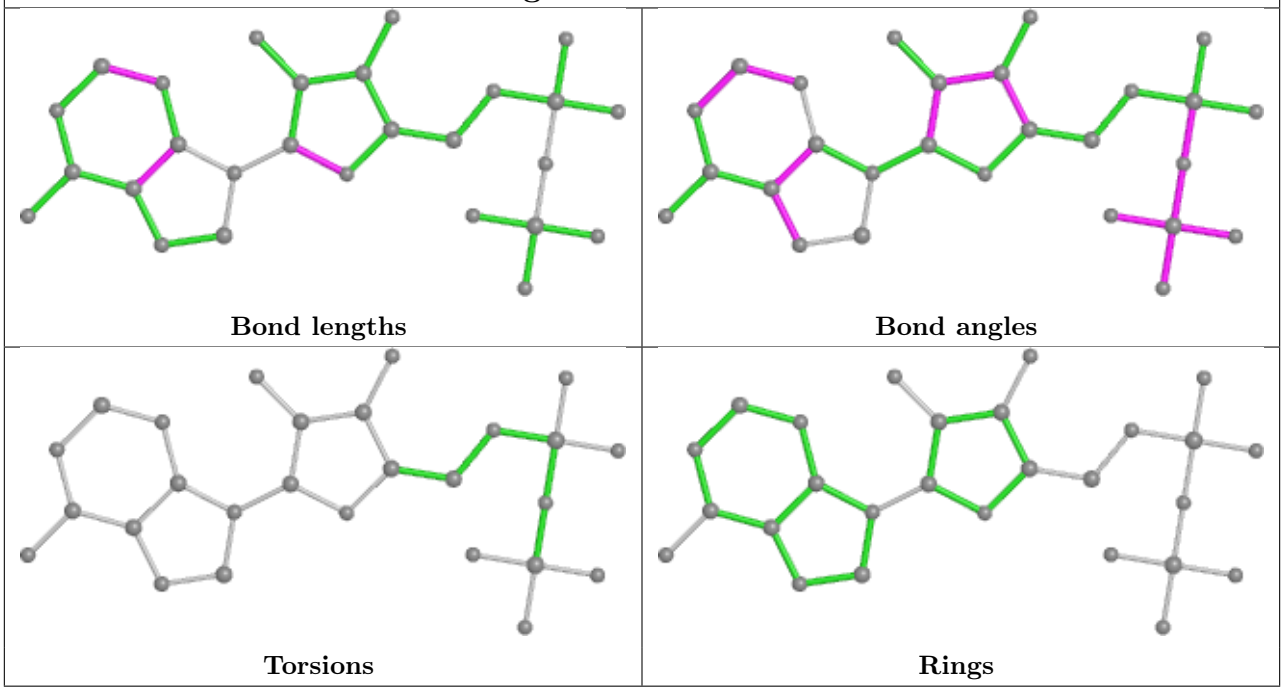
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	FBP	1	0
2	B	805	PO4	1	0

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

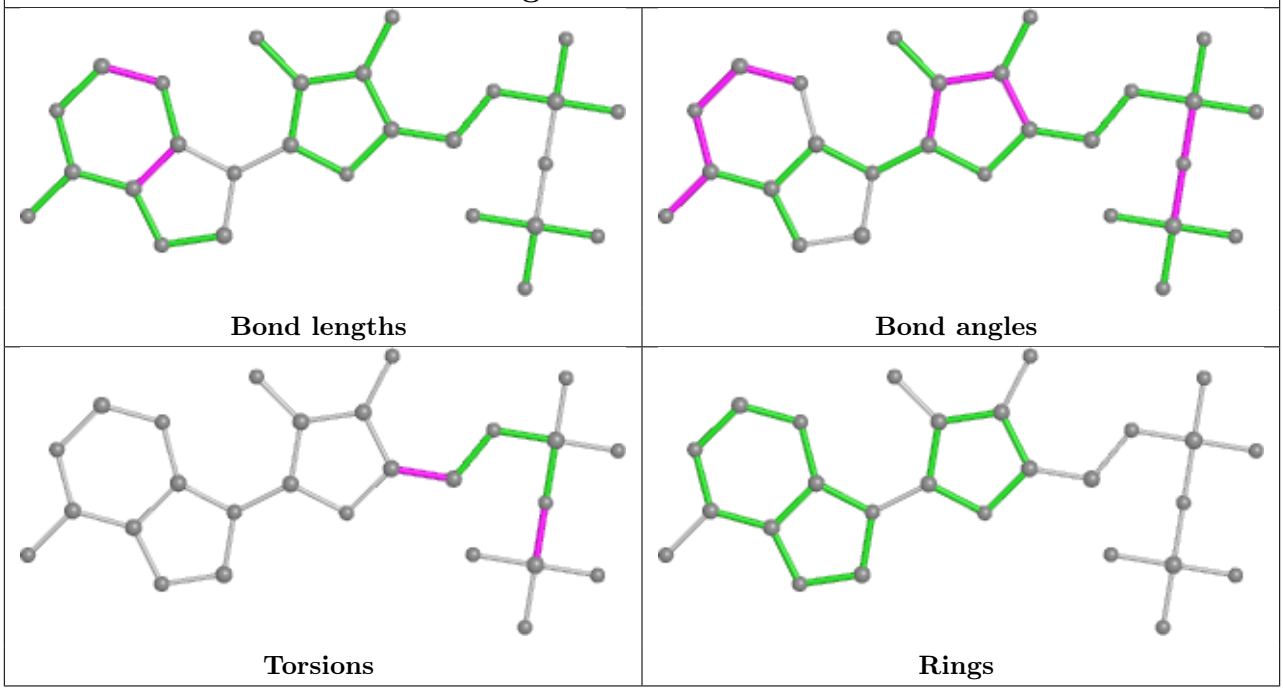
Ligand FBP D 802



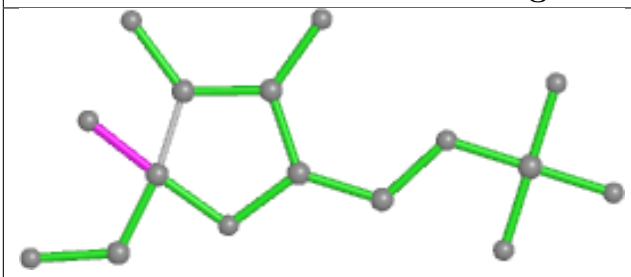
Ligand ADP B 801



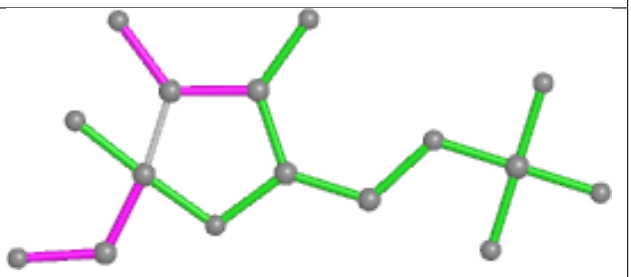
Ligand ADP D 801



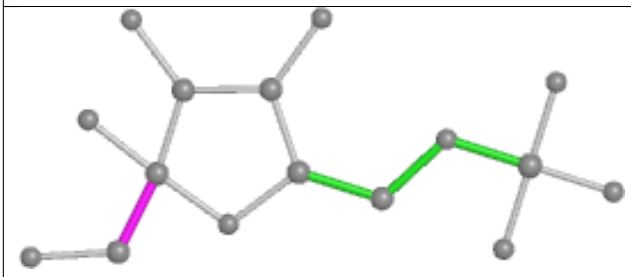
Ligand F6P B 803



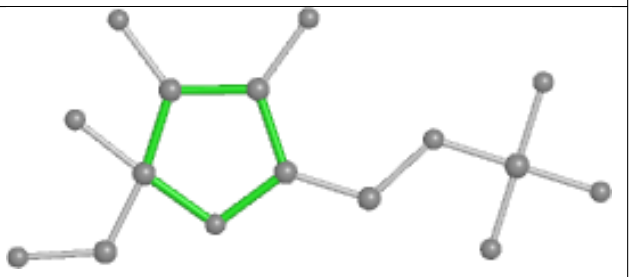
Bond lengths



Bond angles

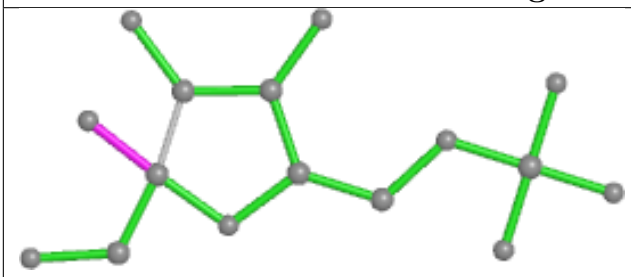


Torsions

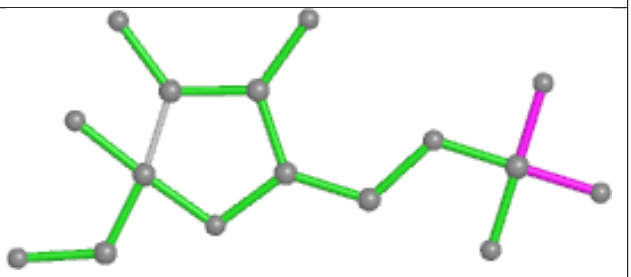


Rings

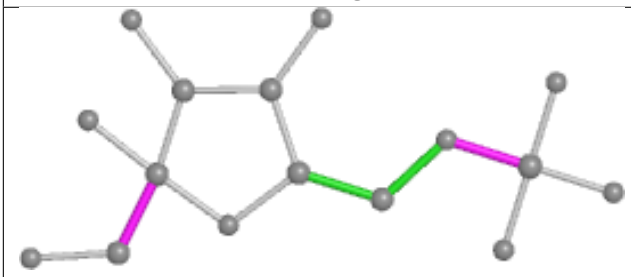
Ligand F6P D 803



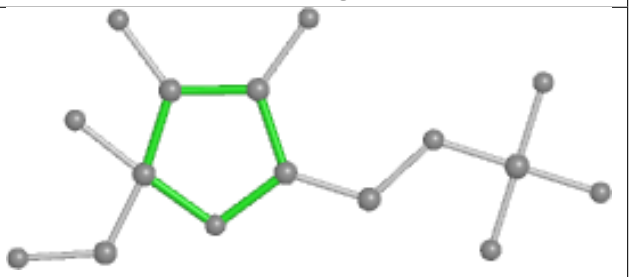
Bond lengths



Bond angles

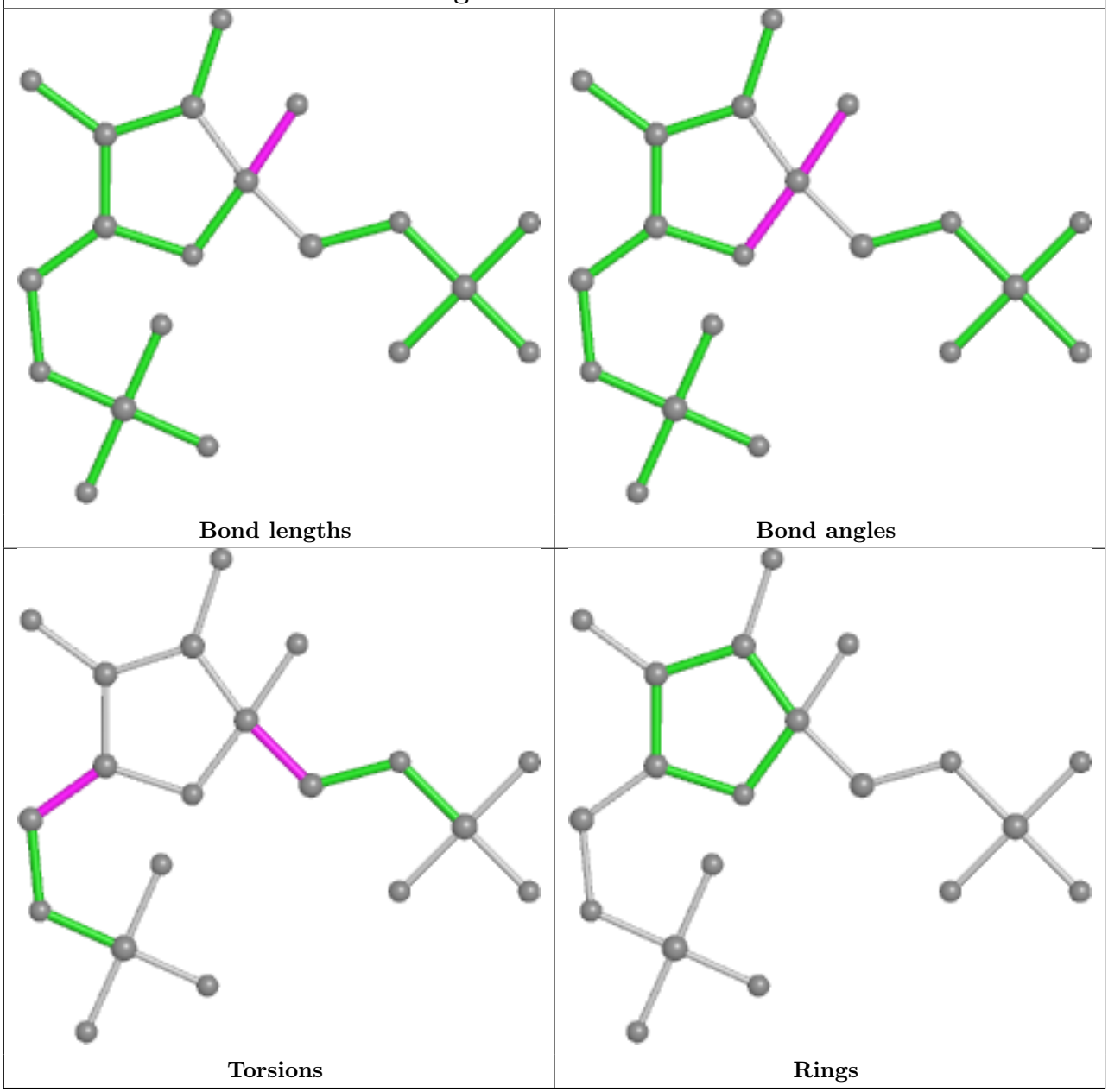


Torsions

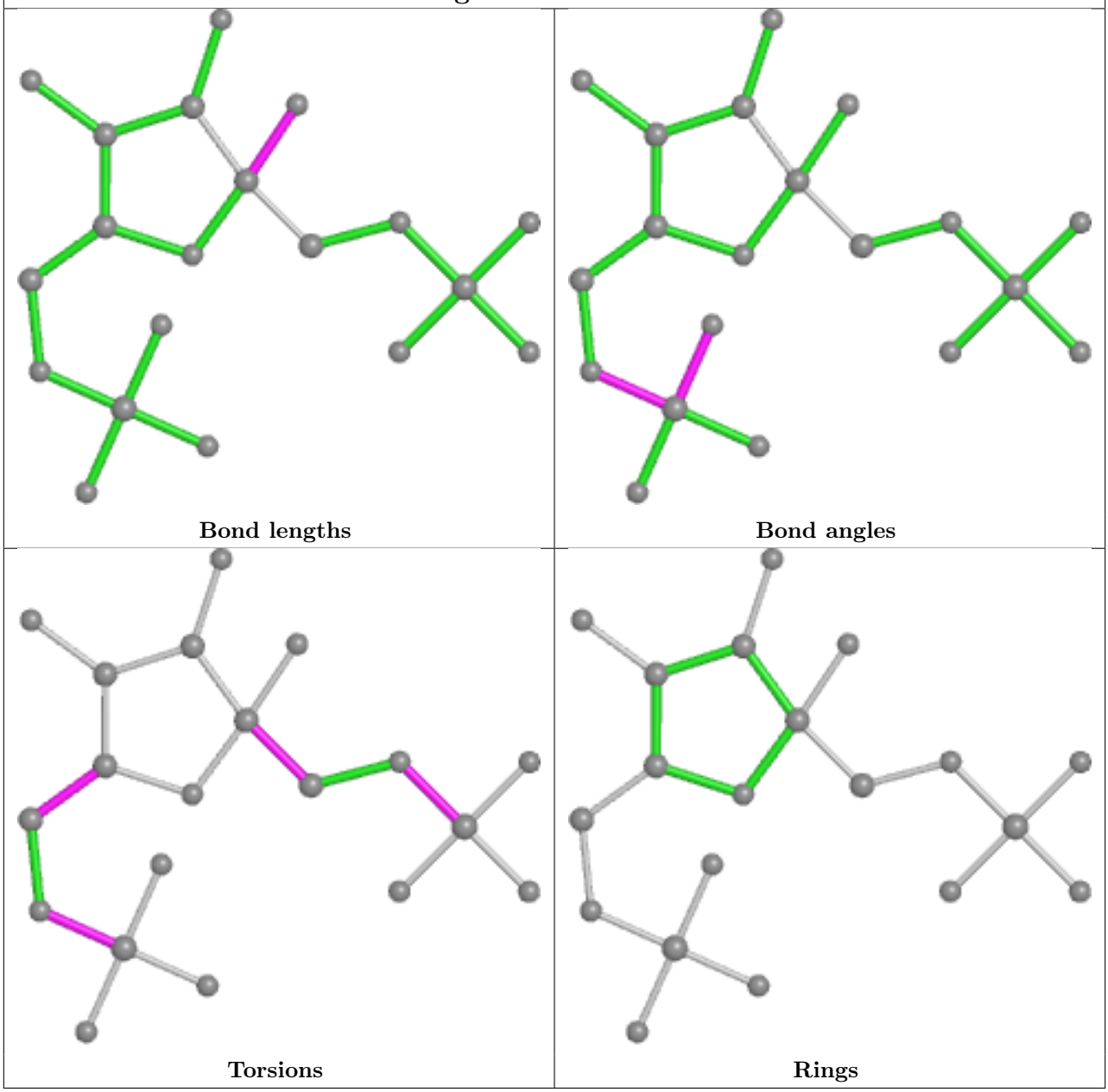


Rings

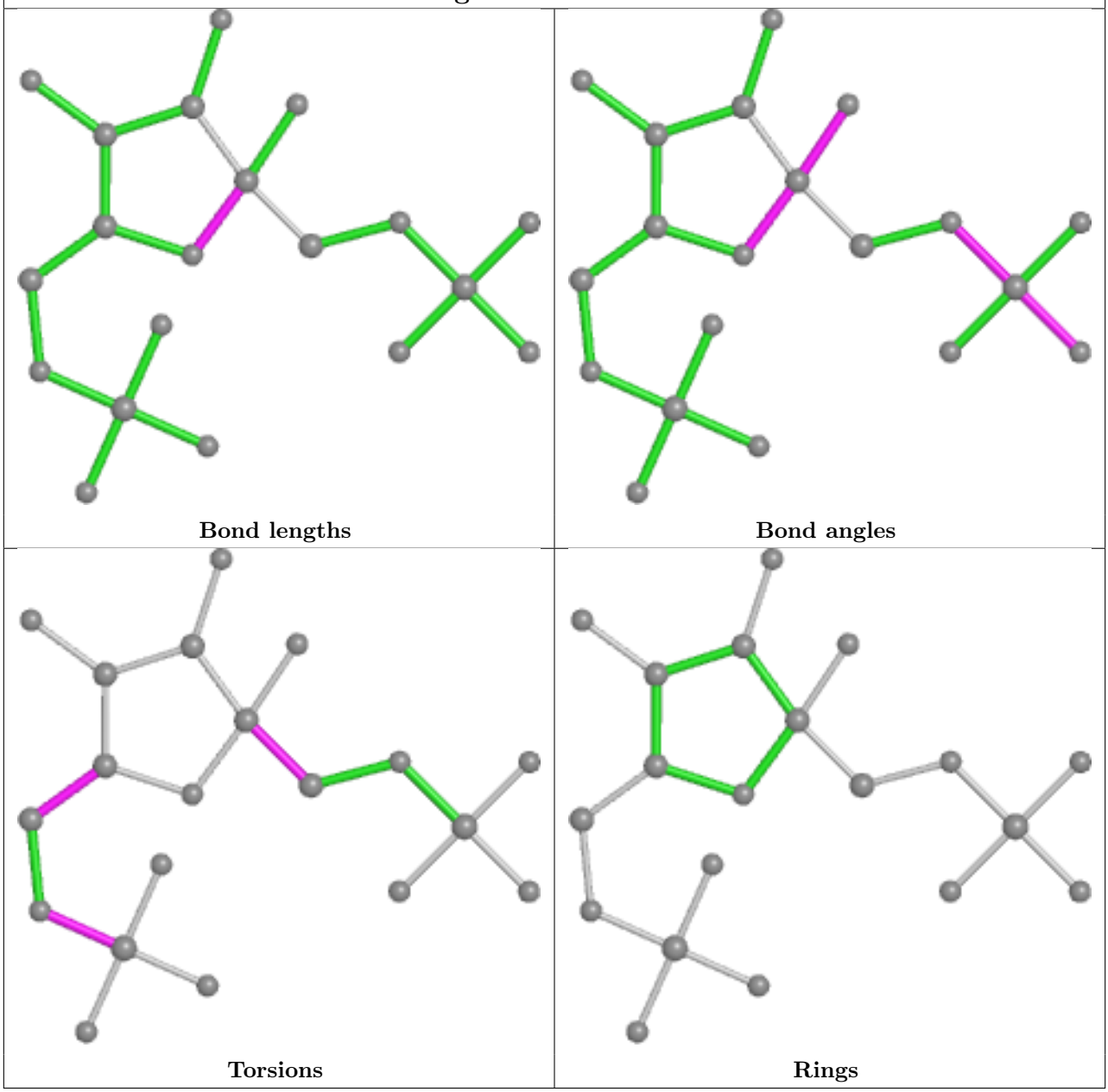
Ligand FBP A 802



Ligand FBP B 802



Ligand FBP C 801



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	708/761 (93%)	-0.14	12 (1%)	70	71	27, 48, 94, 158	0
1	B	728/761 (95%)	-0.01	20 (2%)	54	54	30, 51, 100, 194	0
1	C	704/761 (92%)	0.09	19 (2%)	54	54	35, 66, 108, 138	0
1	D	725/761 (95%)	0.16	36 (4%)	28	26	35, 66, 115, 174	0
All	All	2865/3044 (94%)	0.02	87 (3%)	50	49	27, 57, 108, 194	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	TYR	13.9
1	B	162	TYR	13.9
1	D	162	TYR	11.5
1	D	163	ALA	9.4
1	B	157	GLU	9.2
1	C	629	THR	9.0
1	D	205	ALA	7.5
1	B	155	ASP	7.5
1	D	153	GLN	7.1
1	D	164	TYR	6.6
1	C	162	TYR	6.4
1	B	148	LEU	6.2
1	B	164	TYR	5.9
1	B	149	ALA	5.8
1	C	573	THR	5.6
1	D	151	ASN	5.1
1	A	164	TYR	4.8
1	B	147	GLU	4.7
1	B	153	GLN	4.4
1	A	629	THR	4.3
1	B	163	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	144	LEU	4.1
1	D	154	ILE	4.1
1	A	163	ALA	4.1
1	B	154	ILE	4.1
1	B	159	VAL	4.0
1	C	164	TYR	3.9
1	D	147	GLU	3.8
1	B	115	LEU	3.8
1	D	206	GLN	3.7
1	D	155	ASP	3.6
1	D	108	LEU	3.6
1	D	157	GLU	3.5
1	A	151	ASN	3.5
1	C	151	ASN	3.3
1	D	159	VAL	3.3
1	D	178	PHE	3.3
1	C	163	ALA	3.2
1	D	150	ARG	3.2
1	B	145	LEU	3.2
1	C	385	ARG	3.1
1	D	160	GLN	3.1
1	C	277	ASP	3.0
1	D	97	ARG	2.9
1	C	527	GLU	2.8
1	C	72	SER	2.7
1	B	151	ASN	2.7
1	D	208	HIS	2.7
1	C	570	ALA	2.6
1	A	725	ARG	2.6
1	D	204	THR	2.6
1	A	174	ILE	2.6
1	A	364	THR	2.6
1	C	572	GLY	2.6
1	A	155	ASP	2.6
1	C	404	ASP	2.6
1	A	68	VAL	2.5
1	D	152	GLY	2.5
1	B	150	ARG	2.5
1	A	630	ILE	2.5
1	B	144	LEU	2.5
1	D	339	ASP	2.5
1	D	279	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	713	THR	2.4
1	D	148	LEU	2.4
1	D	66	GLY	2.4
1	D	107	ARG	2.3
1	B	152	GLY	2.3
1	C	375	ARG	2.3
1	D	202	MET	2.3
1	D	110	ALA	2.3
1	D	156	LYS	2.3
1	B	263	LYS	2.3
1	C	413	VAL	2.3
1	D	343	CYS	2.2
1	B	118	GLY	2.2
1	D	385	ARG	2.2
1	D	246	GLU	2.1
1	D	352	ALA	2.1
1	D	121	ASN	2.1
1	D	145	LEU	2.1
1	A	379	ALA	2.0
1	B	158	ALA	2.0
1	C	279	GLN	2.0
1	C	292	VAL	2.0
1	D	245	GLU	2.0
1	C	402	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

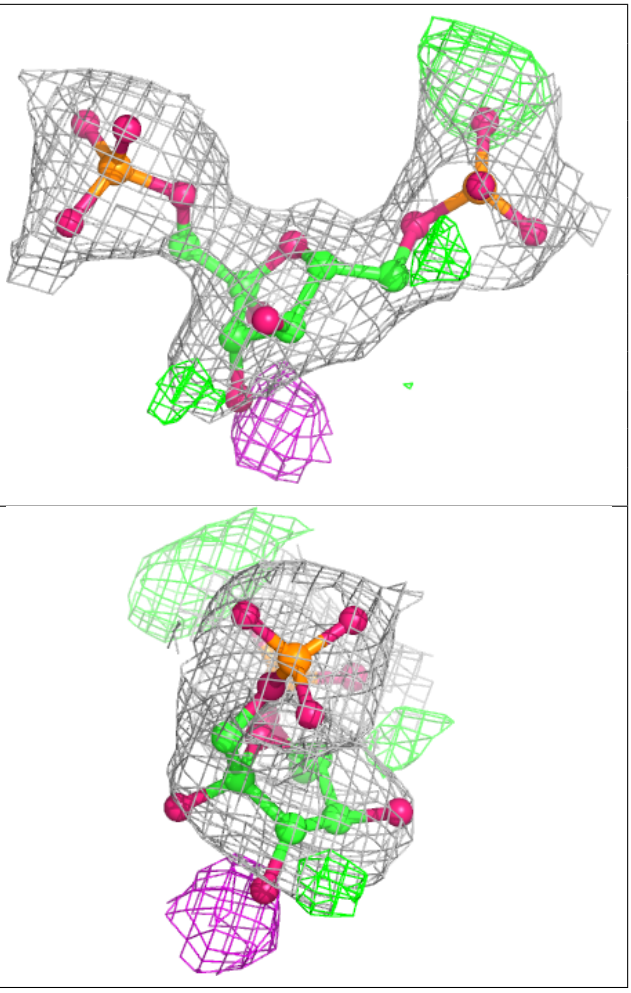
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FBP	B	802	20/20	0.87	0.17	70,89,99,100	0
4	ADP	D	801	27/27	0.90	0.15	84,89,96,102	0
4	ADP	B	801	27/27	0.91	0.15	59,69,78,81	0
3	FBP	D	802	20/20	0.91	0.17	65,84,105,119	0
2	PO4	D	804	5/5	0.93	0.14	62,72,76,76	0
5	F6P	B	803	16/16	0.93	0.13	43,54,61,69	0
3	FBP	C	801	20/20	0.95	0.15	38,54,61,70	0
5	F6P	D	803	16/16	0.95	0.11	65,72,77,77	0
3	FBP	A	802	20/20	0.97	0.15	36,43,44,46	0
2	PO4	B	805	5/5	0.98	0.13	39,39,40,42	0
2	PO4	C	802	5/5	0.98	0.15	54,55,59,61	0
2	PO4	B	804	5/5	0.98	0.12	49,49,51,54	0
2	PO4	D	805	5/5	0.98	0.12	48,54,57,59	0
2	PO4	A	801	5/5	0.99	0.13	33,33,34,36	0

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

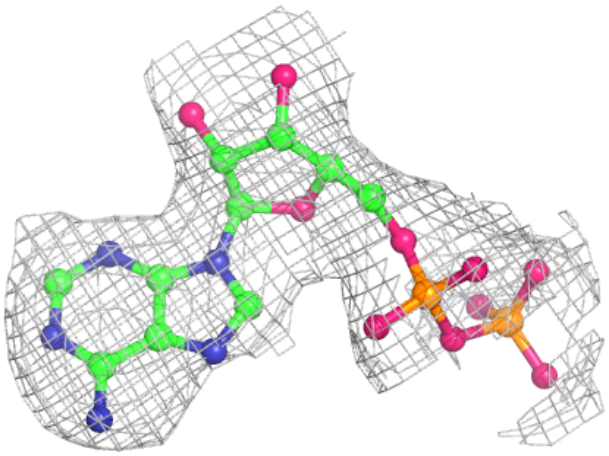
Electron density around FBP B 802:

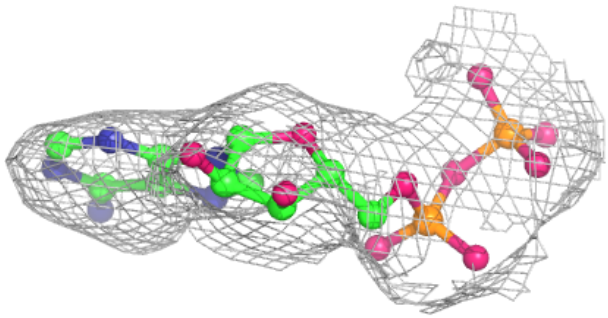
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

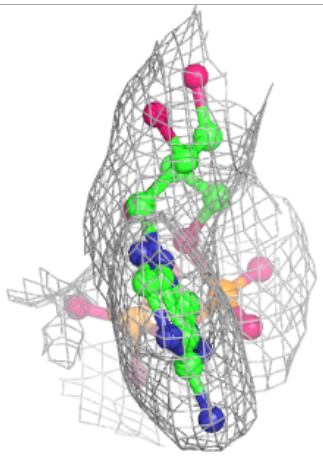


Electron density around ADP D 801:

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

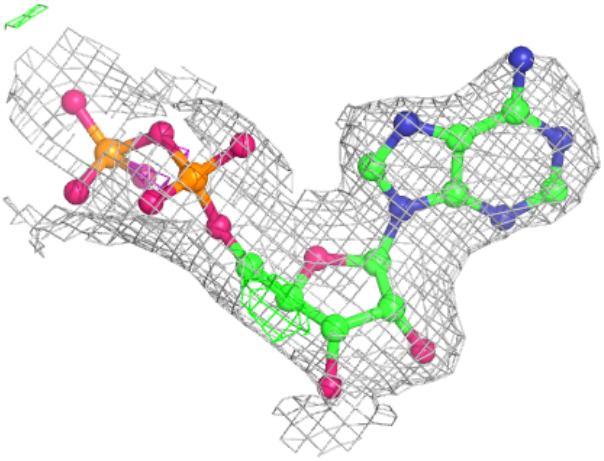


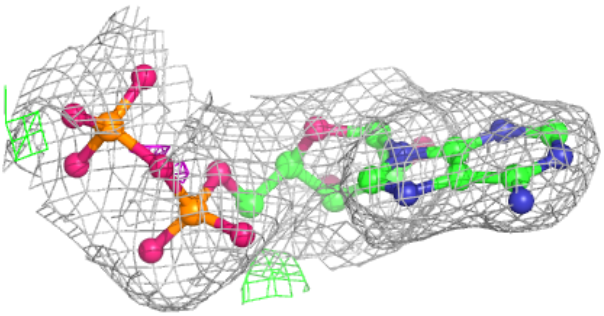


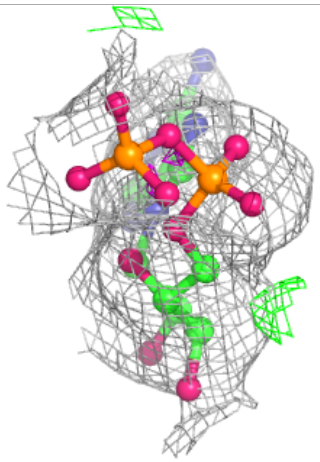


Electron density around ADP B 801:

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

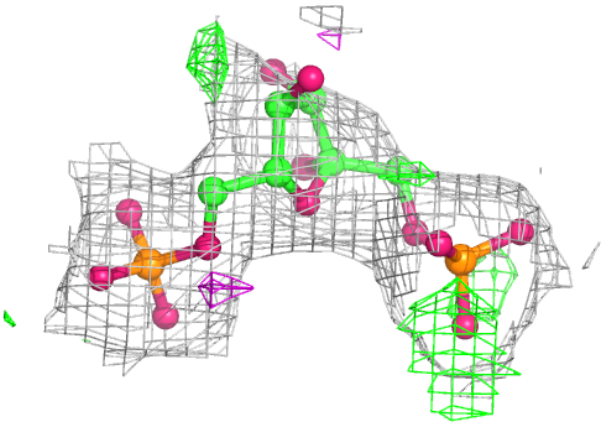


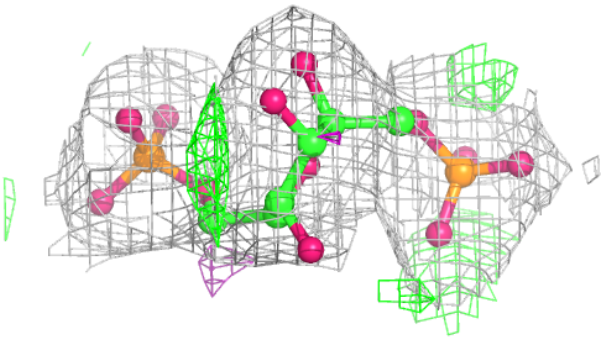


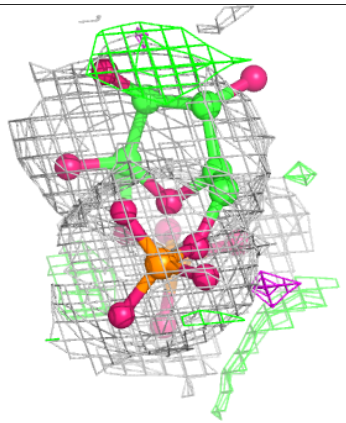


Electron density around FBP D 802:

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

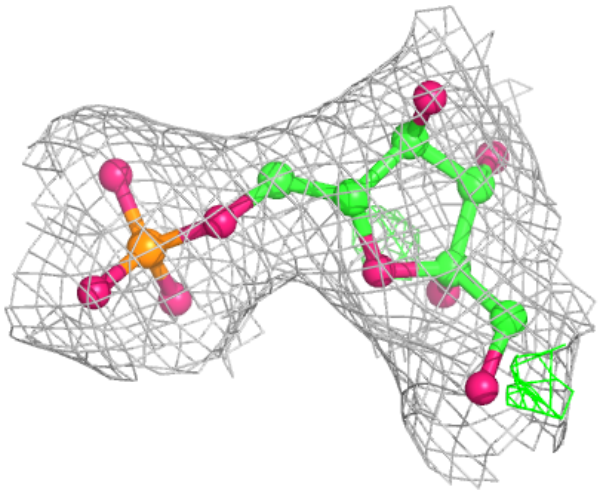


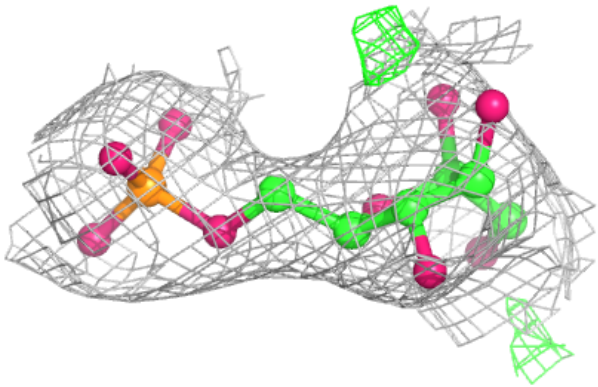


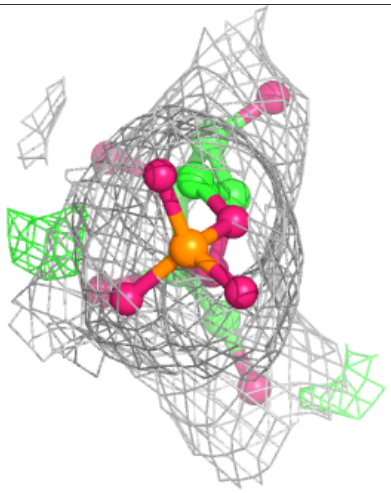


Electron density around F6P B 803:

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

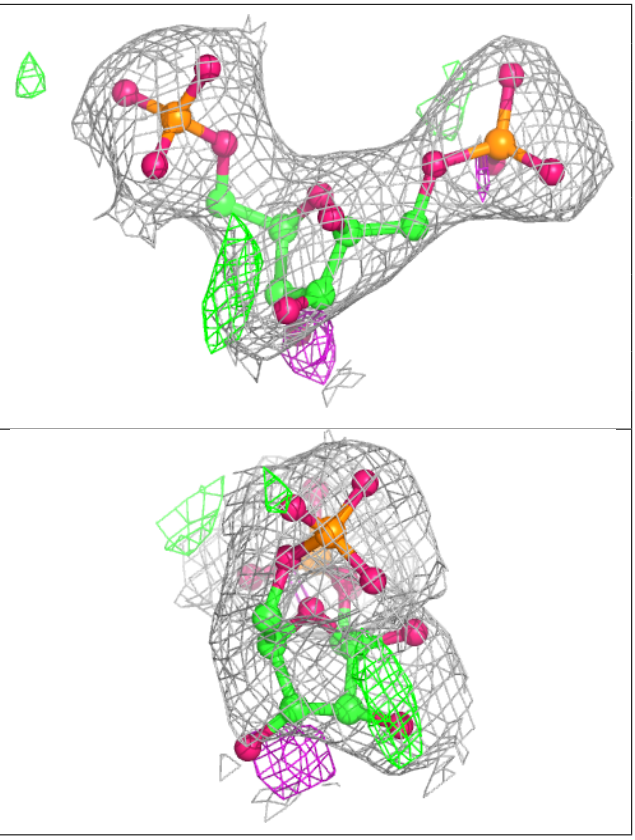


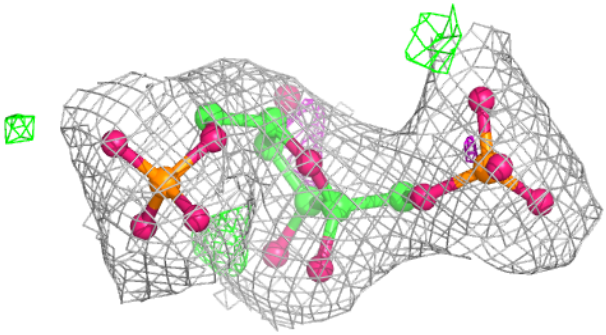




Electron density around FBP C 801:

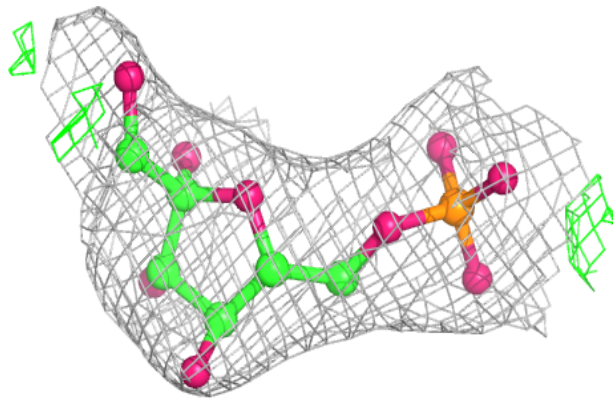
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

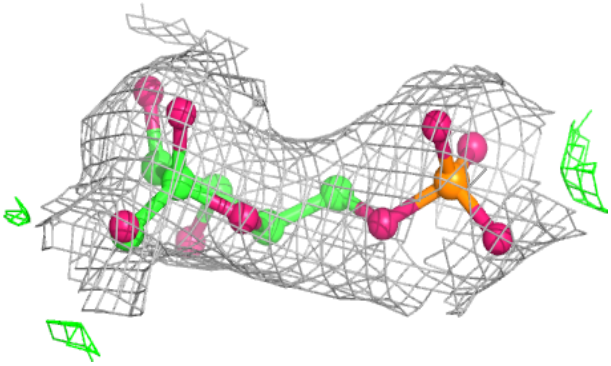


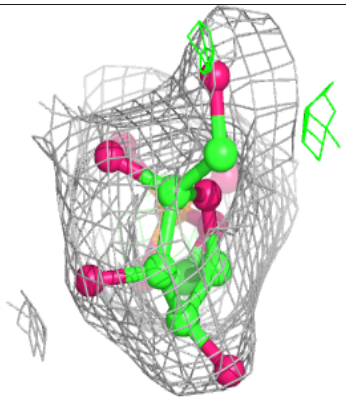


Electron density around F6P D 803:

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

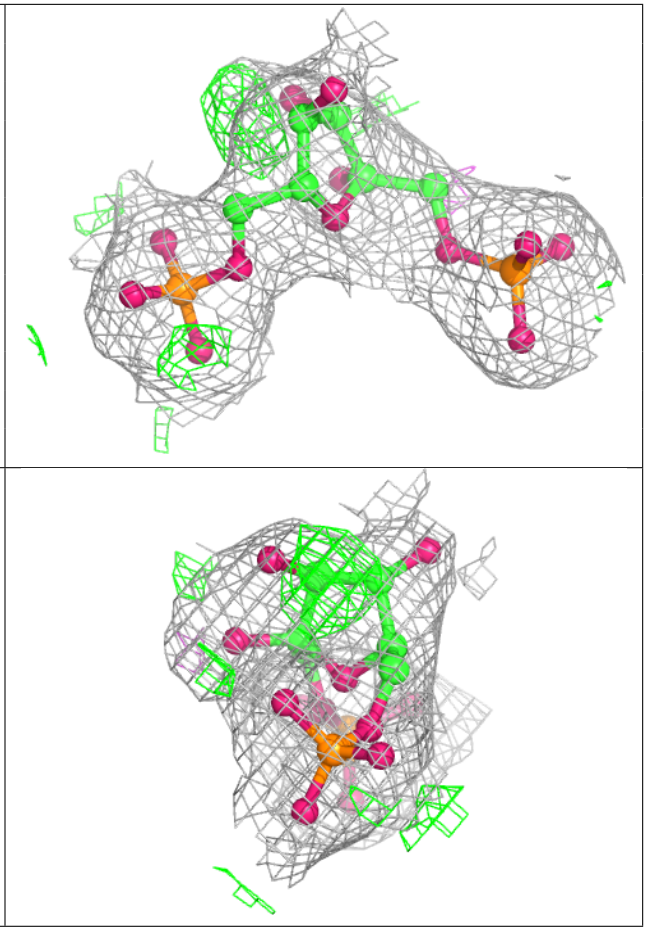






Electron density around FBP A 802:

$2mF_o$-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.