Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 06:32 AM EDT

PDB ID	:	4FXF
Title	:	Structure of M2 pyruvate kinase in complex with phenylalanine
Authors	:	Walkinshaw, M.D.; Morgan, H.P.
Deposited on	:	2012-07-03
Resolution	:	2.55 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:

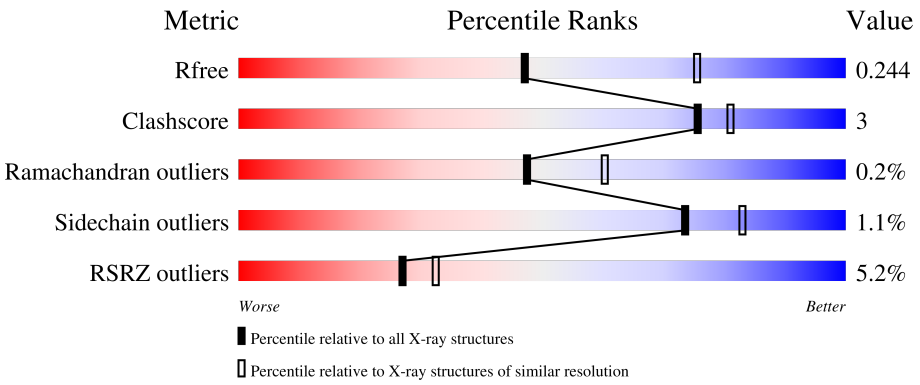
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	551	4% 82% 9% 9%
1	B	551	6% 85% 7% • 8%
1	C	551	2% 83% 8% 9%
1	D	551	7% 83% 8% 9%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15977 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 isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	501	3823	2403	678	719	23	0	0	0
1	D	502	3845	2417	683	721	24	0	1	0
1	C	500	3821	2403	678	718	22	0	0	0
1	B	506	3884	2443	690	727	24	0	1	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P14618
A	-18	GLY	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	HIS	-	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	SER	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	GLY	-	expression tag	UNP P14618
A	-6	LEU	-	expression tag	UNP P14618
A	-5	VAL	-	expression tag	UNP P14618
A	-4	PRO	-	expression tag	UNP P14618
A	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
A	0	HIS	-	expression tag	UNP P14618
A	379	ASN	HIS	SEE REMARK 999	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618
D	379	ASN	HIS	SEE REMARK 999	UNP P14618
C	-19	MET	-	expression tag	UNP P14618
C	-18	GLY	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	HIS	-	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	SER	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	GLY	-	expression tag	UNP P14618
C	-6	LEU	-	expression tag	UNP P14618
C	-5	VAL	-	expression tag	UNP P14618
C	-4	PRO	-	expression tag	UNP P14618
C	-3	ARG	-	expression tag	UNP P14618
C	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
C	0	HIS	-	expression tag	UNP P14618
C	379	ASN	HIS	SEE REMARK 999	UNP P14618

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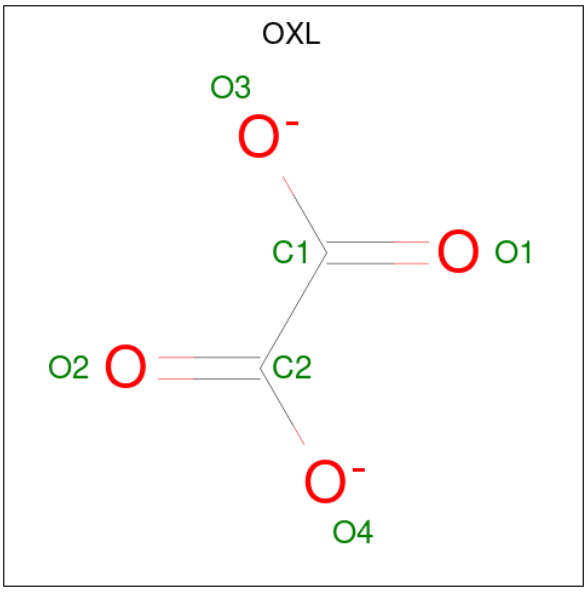
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	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	SER	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	GLY	-	expression tag	UNP P14618
B	-6	LEU	-	expression tag	UNP P14618
B	-5	VAL	-	expression tag	UNP P14618
B	-4	PRO	-	expression tag	UNP P14618
B	-3	ARG	-	expression tag	UNP P14618
B	-2	GLY	-	expression tag	UNP P14618
B	-1	SER	-	expression tag	UNP P14618
B	0	HIS	-	expression tag	UNP P14618
B	379	ASN	HIS	SEE REMARK 999	UNP P14618

- Molecule 2 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



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

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

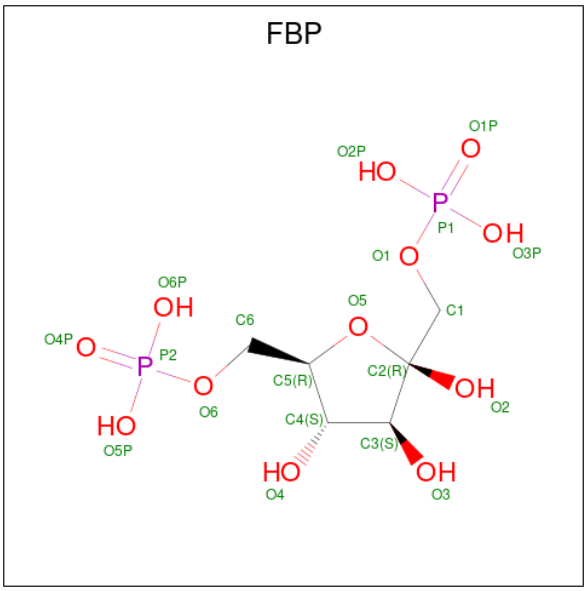
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

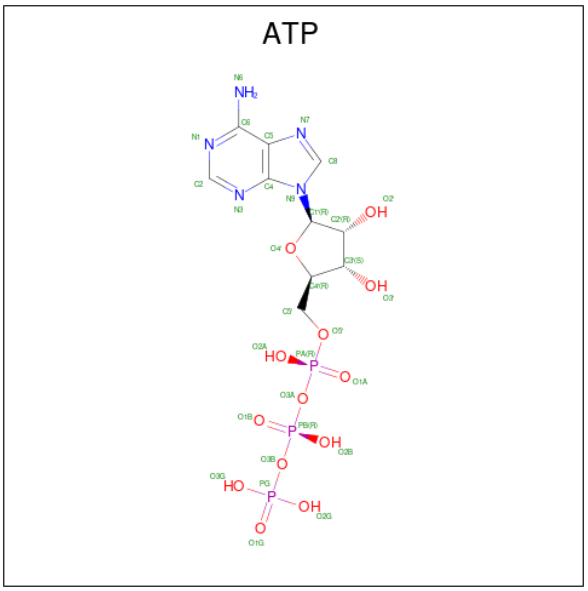
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
			Total	Mg		
4	D	2	2	2	0	0
			Total	Mg		
4	C	1	1	1	0	0
			Total	Mg		
4	B	2	2	2	0	0

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	D	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
6	B	1	31	10	5	13	3	0	0

- Molecule 7 is water.

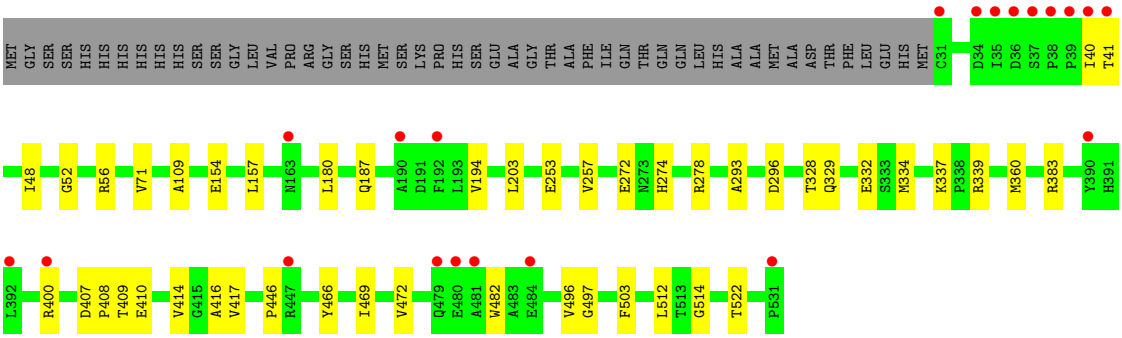
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	98	98	98	0	0
			Total	O		
7	D	80	80	80	0	0
			Total	O		
7	C	131	131	131	0	0
			Total	O		
7	B	119	119	119	0	0

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.

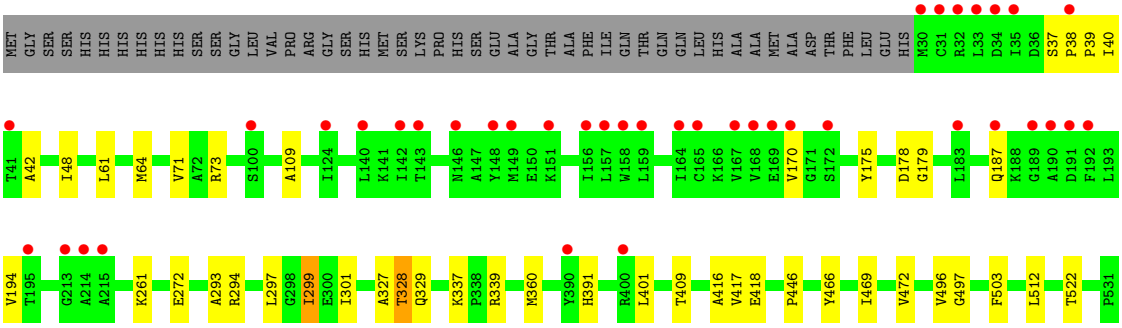
• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain A:



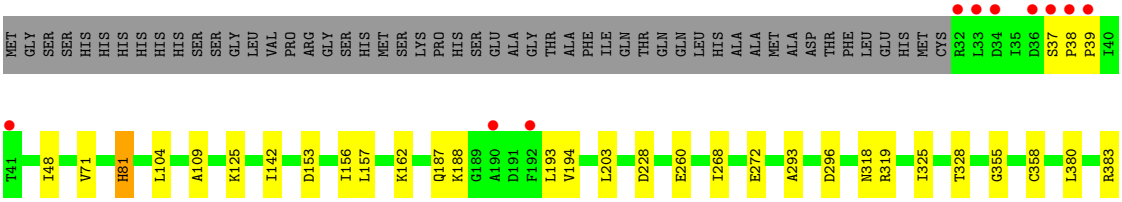
• Molecule 1: Pyruvate kinase isozymes M1/M2

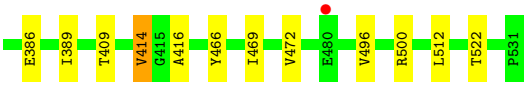
Chain D:



• Molecule 1: Pyruvate kinase isozymes M1/M2

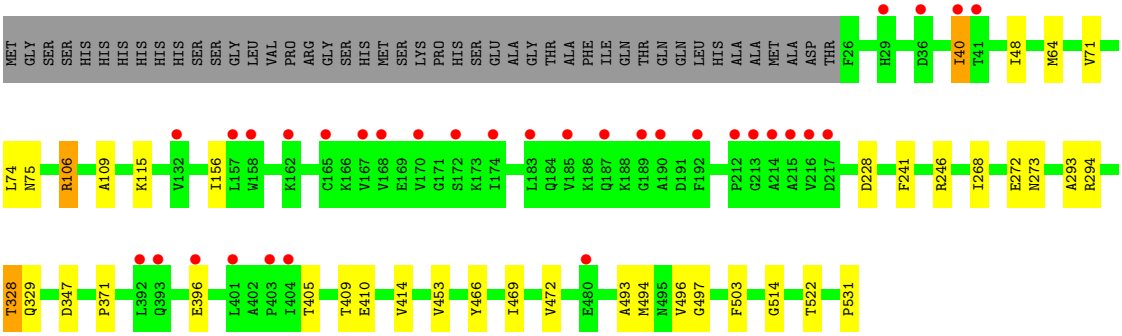
Chain C:





• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.60Å 139.35Å 111.28Å 90.00° 90.52° 90.00°	Depositor
Resolution (Å)	51.67 – 2.55 51.67 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.67-2.55) 98.1 (51.67-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.212 , 0.254 0.204 , 0.244	Depositor DCC
R_{free} test set	3978 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15977	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 3.29% 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: FBP, MG, OXL, K, ATP

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	0.31	0/3883	0.46	0/5245
1	B	0.31	0/3946	0.45	0/5328
1	C	0.31	0/3881	0.46	0/5241
1	D	0.31	0/3906	0.46	0/5274
All	All	0.31	0/15616	0.46	0/21088

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3823	0	3910	26	0
1	B	3884	0	3977	24	0
1	C	3821	0	3916	27	0
1	D	3845	0	3936	23	0
2	A	6	0	0	0	0
2	B	6	0	0	1	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	20	0	10	2	0
5	B	20	0	10	1	0
5	C	20	0	10	0	0
5	D	20	0	10	0	0
6	B	31	0	12	1	0
6	D	31	0	12	1	0
7	A	98	0	0	0	0
7	B	119	0	0	0	0
7	C	131	0	0	0	0
7	D	80	0	0	0	0
All	All	15977	0	15803	96	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 3.

All (96) 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:500:ARG:CG	1:C:500:ARG:HH11	2.00	0.74
1:A:329:GLN:HA	1:A:332:GLU:HG2	1.77	0.66
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.78	0.64
1:B:272:GLU:HG2	1:B:293:ALA:HB3	1.79	0.64
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.79	0.63
1:C:409:THR:HG23	1:C:522:THR:HB	1.81	0.63
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.81	0.62
1:B:472:VAL:HG11	1:B:496:VAL:HG21	1.81	0.62
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.82	0.62
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.84	0.60
1:A:187:GLN:HB2	1:A:194:VAL:HB	1.84	0.59
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.85	0.58
1:B:409:THR:HG23	1:B:522:THR:HB	1.87	0.57
1:C:500:ARG:HH11	1:C:500:ARG:HG3	1.70	0.57
1:B:410:GLU:O	1:B:414:VAL:HG23	2.04	0.57
1:D:418:GLU:HG3	1:C:414:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:GLN:HB2	1:C:194:VAL:HB	1.87	0.56
1:D:175:TYR:HB3	1:D:179:GLY:HA2	1.88	0.55
1:D:409:THR:HG23	1:D:522:THR:HB	1.89	0.54
1:A:400:ARG:HH22	1:B:396:GLU:HG3	1.73	0.54
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.90	0.53
1:C:104:LEU:HA	1:C:500:ARG:HH12	1.73	0.53
1:A:514:GLY:HA3	5:A:604:FBP:O3	2.08	0.53
1:C:125:LYS:HE3	1:C:153:ASP:HB3	1.90	0.53
1:C:380:LEU:HD23	1:C:383:ARG:HH12	1.73	0.53
1:A:339:ARG:NH2	1:D:179:GLY:O	2.41	0.53
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.91	0.53
1:D:187:GLN:HB2	1:D:194:VAL:HB	1.92	0.52
1:B:75:ASN:ND2	6:B:604:ATP:O3A	2.43	0.52
1:D:272:GLU:HB3	1:D:293:ALA:HB3	1.91	0.51
1:A:329:GLN:HG2	1:A:332:GLU:CG	2.41	0.51
1:D:294:ARG:HD3	1:D:327:ALA:O	2.10	0.51
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.94	0.50
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.93	0.49
1:D:40:ILE:HD12	1:D:42:ALA:HB3	1.94	0.49
1:C:500:ARG:CG	1:C:500:ARG:NH1	2.69	0.49
1:C:318:ASN:HD21	1:C:355:GLY:HA3	1.77	0.49
1:C:500:ARG:HH11	1:C:500:ARG:HG2	1.76	0.49
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.94	0.49
1:D:61:LEU:HA	1:D:64:MET:HG3	1.96	0.48
1:B:405:THR:HG21	1:B:410:GLU:HB3	1.96	0.47
1:A:180:LEU:HD22	1:D:337:LYS:HD2	1.96	0.47
1:A:410:GLU:O	1:A:414:VAL:HG23	2.15	0.47
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.97	0.47
1:C:500:ARG:HG3	1:C:500:ARG:NH1	2.29	0.47
1:B:40:ILE:H	1:B:40:ILE:HD13	1.80	0.46
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.98	0.46
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.98	0.46
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.98	0.46
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.46	0.46
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.51	0.46
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.98	0.46
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.98	0.46
1:C:272:GLU:HB2	1:C:296:ASP:HB2	1.97	0.45
1:A:253:GLU:O	1:A:257:VAL:HG23	2.16	0.45
1:A:40:ILE:CG2	1:A:41:THR:N	2.80	0.45
1:C:38:PRO:HA	1:C:39:PRO:HD3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLY:O	1:A:56:ARG:HB2	2.17	0.44
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.98	0.44
1:C:142:ILE:HB	1:C:193:LEU:HB2	1.99	0.44
1:A:272:GLU:HB3	1:A:293:ALA:HB3	1.98	0.44
1:C:272:GLU:HB3	1:C:293:ALA:HB3	2.00	0.44
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.53	0.44
1:B:514:GLY:HA3	5:B:606:FBP:O3	2.18	0.44
1:B:241:PHE:HD1	1:B:268:ILE:HB	1.83	0.43
1:C:386:GLU:HA	1:C:389:ILE:HD12	1.99	0.43
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.53	0.43
1:D:38:PRO:HA	1:D:39:PRO:HD3	1.87	0.43
1:A:274:HIS:CD2	1:A:278:ARG:HE	2.36	0.43
1:B:106:ARG:HH21	1:B:106:ARG:HB2	1.83	0.43
1:A:409:THR:HG23	1:A:522:THR:HB	2.01	0.43
1:D:466:TYR:HB2	1:D:469:ILE:HD12	2.00	0.43
1:B:246:ARG:HG2	1:B:273:ASN:HD21	1.83	0.42
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.02	0.42
1:C:268:ILE:HG21	1:C:325:ILE:HD12	2.02	0.42
1:A:407:ASP:HA	1:A:408:PRO:HD3	1.91	0.42
1:D:178:ASP:HA	1:D:299:ILE:HD11	2.01	0.42
1:B:115:LYS:HE2	1:B:228:ASP:OD2	2.20	0.42
1:B:294:ARG:NH2	1:B:347:ASP:OD1	2.43	0.41
1:A:482:TRP:HZ2	5:A:604:FBP:H12	1.85	0.41
1:D:48:ILE:HB	1:D:360:MET:HG3	2.01	0.41
1:B:64:MET:HE3	1:B:371:PRO:HB2	2.02	0.41
1:A:272:GLU:HB2	1:A:296:ASP:HB2	2.02	0.41
1:B:328:THR:HG22	1:B:329:GLN:HG3	2.02	0.41
1:A:48:ILE:HB	1:A:360:MET:HG3	2.02	0.41
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.02	0.41
1:A:417:VAL:HG13	1:A:446:PRO:HB3	2.02	0.41
1:C:81:HIS:HE1	1:C:228:ASP:OD1	2.04	0.41
1:B:293:ALA:HB1	2:B:601:OXL:C1	2.51	0.41
1:D:73:ARG:NH2	6:D:604:ATP:O1A	2.54	0.41
1:C:37:SER:HA	1:C:38:PRO:HD3	1.93	0.41
1:A:334:MET:HA	1:A:337:LYS:O	2.21	0.40
1:D:297:LEU:O	1:D:301:ILE:HG12	2.20	0.40
1:D:37:SER:HA	1:D:38:PRO:HD3	1.88	0.40
1:A:71:VAL:HG22	1:A:109:ALA:HB3	2.04	0.40
1:D:417:VAL:HG13	1:D:446:PRO:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/551 (91%)	486 (97%)	12 (2%)	1 (0%)	47	60
1	B	505/551 (92%)	496 (98%)	8 (2%)	1 (0%)	47	60
1	C	498/551 (90%)	489 (98%)	8 (2%)	1 (0%)	47	60
1	D	501/551 (91%)	489 (98%)	10 (2%)	2 (0%)	34	46
All	All	2003/2204 (91%)	1960 (98%)	38 (2%)	5 (0%)	47	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	328	THR
1	B	328	THR
1	A	328	THR
1	C	328	THR
1	D	170	VAL

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	411/453 (91%)	409 (100%)	2 (0%)	88	93
1	B	418/453 (92%)	414 (99%)	4 (1%)	76	84
1	C	411/453 (91%)	404 (98%)	7 (2%)	60	75
1	D	414/453 (91%)	408 (99%)	6 (1%)	67	79
All	All	1654/1812 (91%)	1635 (99%)	19 (1%)	73	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
1	A	383	ARG
1	D	261	LYS
1	D	299	ILE
1	D	339	ARG
1	D	391[A]	HIS
1	D	391[B]	HIS
1	D	401	LEU
1	C	81	HIS
1	C	156	ILE
1	C	162	LYS
1	C	188	LYS
1	C	260	GLU
1	C	319	ARG
1	C	414	VAL
1	B	40	ILE
1	B	74	LEU
1	B	106	ARG
1	B	156	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	274	HIS
1	A	458	GLN
1	A	495	ASN
1	C	227	GLN
1	C	318	ASN
1	C	458	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)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
5	FBP	C	604	-	18,20,20	0.93	1 (5%)	23,32,32	0.72	0
5	FBP	A	604	-	18,20,20	0.94	1 (5%)	23,32,32	0.68	0
5	FBP	D	606	-	18,20,20	0.92	1 (5%)	23,32,32	0.82	0
5	FBP	B	606	-	18,20,20	0.91	1 (5%)	23,32,32	0.74	0
6	ATP	B	604	3,4	26,33,33	0.99	1 (3%)	31,52,52	1.39	5 (16%)
6	ATP	D	604	3,4	26,33,33	1.01	2 (7%)	31,52,52	1.31	4 (12%)
2	OXL	C	601	4	5,5,5	1.34	0	6,6,6	1.05	0
2	OXL	A	601	4	5,5,5	1.24	0	6,6,6	1.18	0
2	OXL	D	601	4	5,5,5	1.36	0	6,6,6	0.94	0
2	OXL	B	601	4	5,5,5	1.33	0	6,6,6	0.96	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
5	FBP	C	604	-	-	2/13/32/32	0/1/1/1
5	FBP	A	604	-	-	2/13/32/32	0/1/1/1
5	FBP	D	606	-	-	5/13/32/32	0/1/1/1
5	FBP	B	606	-	-	8/13/32/32	0/1/1/1
6	ATP	B	604	3,4	-	8/18/38/38	0/3/3/3
6	ATP	D	604	3,4	-	7/18/38/38	0/3/3/3
2	OXL	C	601	4	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OXL	A	601	4	-	0/4/4/4	-
2	OXL	D	601	4	-	0/4/4/4	-
2	OXL	B	601	4	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	604	FBP	O2-C2	2.93	1.45	1.40
5	A	604	FBP	O2-C2	2.91	1.45	1.40
5	B	606	FBP	O2-C2	2.85	1.45	1.40
5	D	606	FBP	O2-C2	2.84	1.45	1.40
6	D	604	ATP	C5-C4	2.70	1.48	1.40
6	B	604	ATP	C5-C4	2.56	1.47	1.40
6	D	604	ATP	O4'-C1'	2.10	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	604	ATP	N3-C2-N1	-3.43	123.32	128.68
6	D	604	ATP	N3-C2-N1	-3.41	123.34	128.68
6	B	604	ATP	PB-O3B-PG	-2.95	122.72	132.83
6	B	604	ATP	PA-O3A-PB	-2.75	123.40	132.83
6	D	604	ATP	C3'-C2'-C1'	2.66	104.99	100.98
6	D	604	ATP	C4-C5-N7	-2.53	106.76	109.40
6	B	604	ATP	C4-C5-N7	-2.48	106.81	109.40
6	B	604	ATP	C3'-C2'-C1'	2.39	104.58	100.98
6	D	604	ATP	PB-O3B-PG	-2.29	124.96	132.83

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	FBP	C4-C5-C6-O6
5	D	606	FBP	C1-O1-P1-O3P
5	D	606	FBP	O1-C1-C2-C3
5	C	604	FBP	C4-C5-C6-O6
5	B	606	FBP	O1-C1-C2-O2
5	B	606	FBP	O1-C1-C2-C3
5	B	606	FBP	O1-C1-C2-O5
5	B	606	FBP	C4-C5-C6-O6
5	B	606	FBP	C6-O6-P2-O4P

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Mol	Chain	Res	Type	Atoms
5	B	606	FBP	C6-O6-P2-O6P
6	B	604	ATP	PB-O3B-PG-O2G
6	B	604	ATP	C5'-O5'-PA-O1A
6	B	604	ATP	C5'-O5'-PA-O2A
6	B	604	ATP	O4'-C4'-C5'-O5'
5	A	604	FBP	O5-C5-C6-O6
5	B	606	FBP	O5-C5-C6-O6
5	C	604	FBP	O5-C5-C6-O6
6	B	604	ATP	PB-O3A-PA-O5'
5	D	606	FBP	O5-C5-C6-O6
6	B	604	ATP	PB-O3B-PG-O3G
5	D	606	FBP	O1-C1-C2-O5
5	D	606	FBP	O1-C1-C2-O2
6	D	604	ATP	O4'-C4'-C5'-O5'
6	D	604	ATP	PA-O3A-PB-O1B
6	D	604	ATP	PB-O3A-PA-O1A
6	D	604	ATP	PB-O3A-PA-O2A
5	B	606	FBP	C6-O6-P2-O5P
6	D	604	ATP	PB-O3B-PG-O1G
6	B	604	ATP	PB-O3B-PG-O1G
6	B	604	ATP	C5'-O5'-PA-O3A
6	D	604	ATP	C3'-C4'-C5'-O5'
6	D	604	ATP	PA-O3A-PB-O2B

There are no ring outliers.

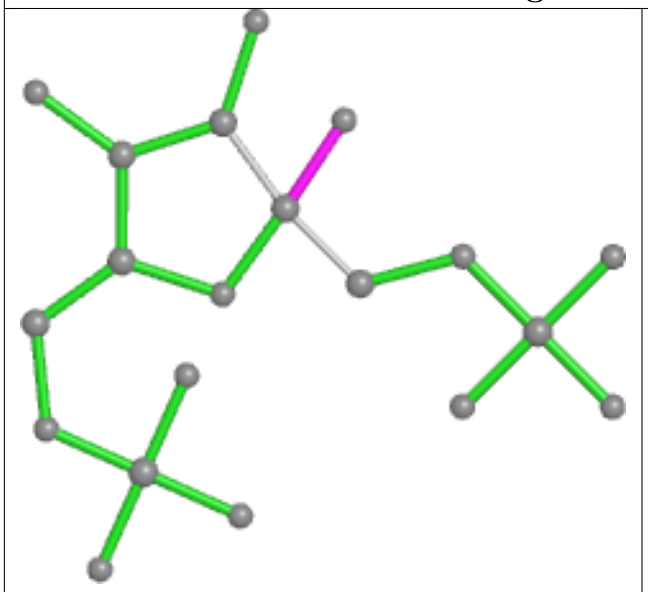
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	FBP	2	0
5	B	606	FBP	1	0
6	B	604	ATP	1	0
6	D	604	ATP	1	0
2	B	601	OXL	1	0

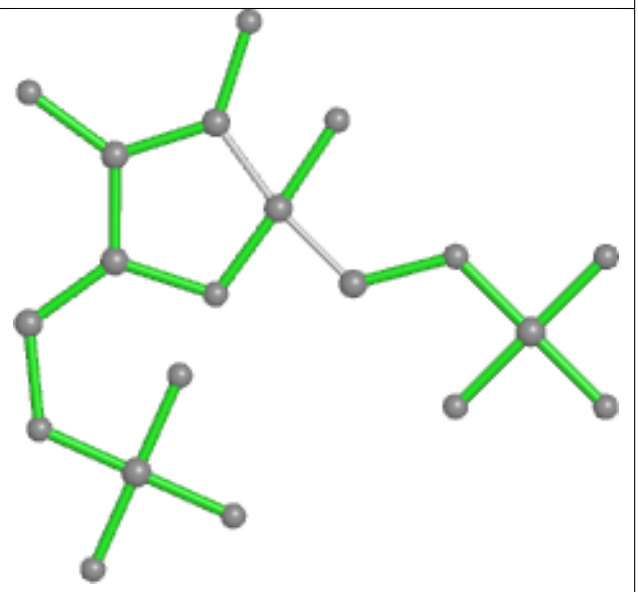
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

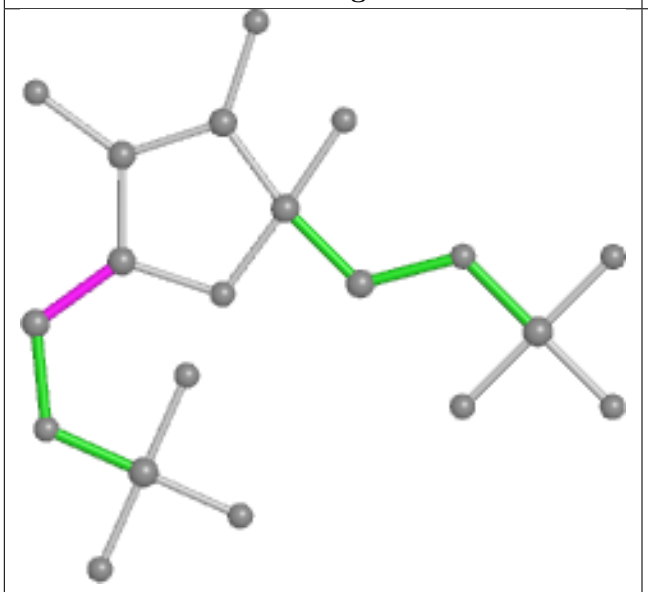
Ligand FBP C 604



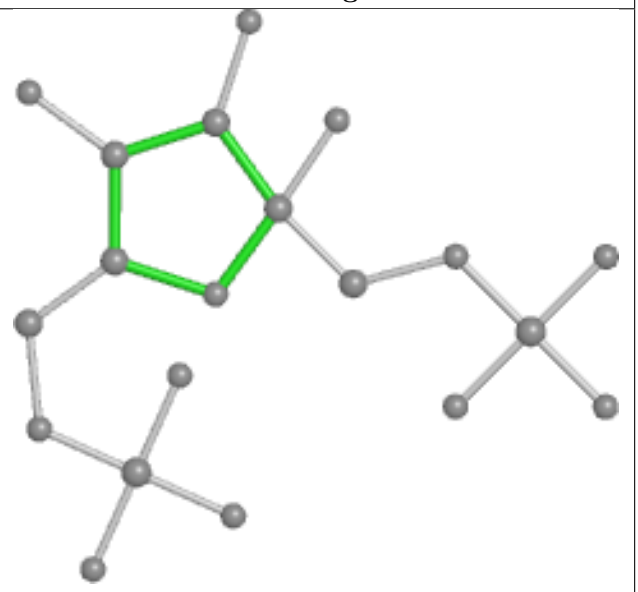
Bond lengths



Bond angles

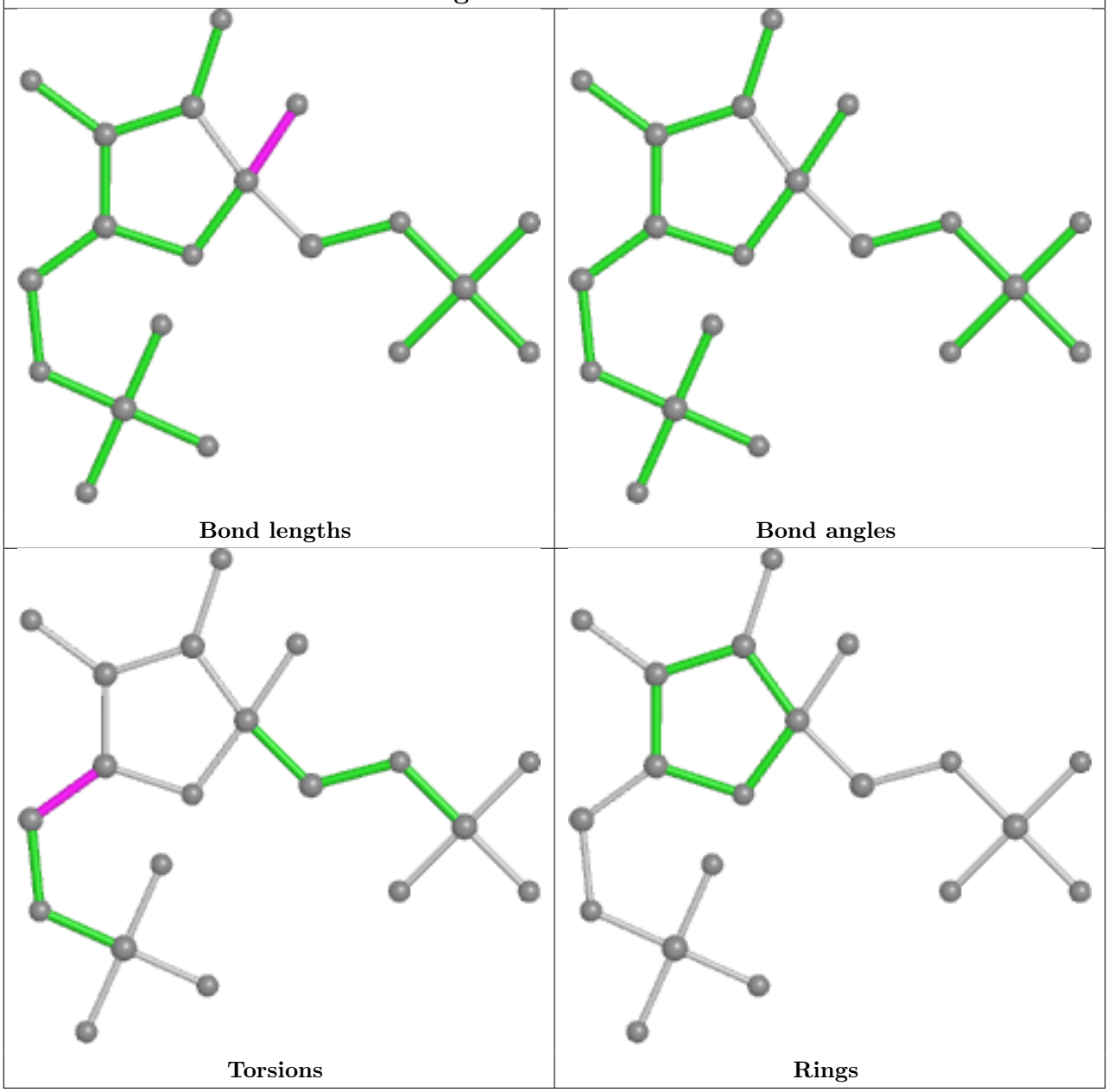


Torsions

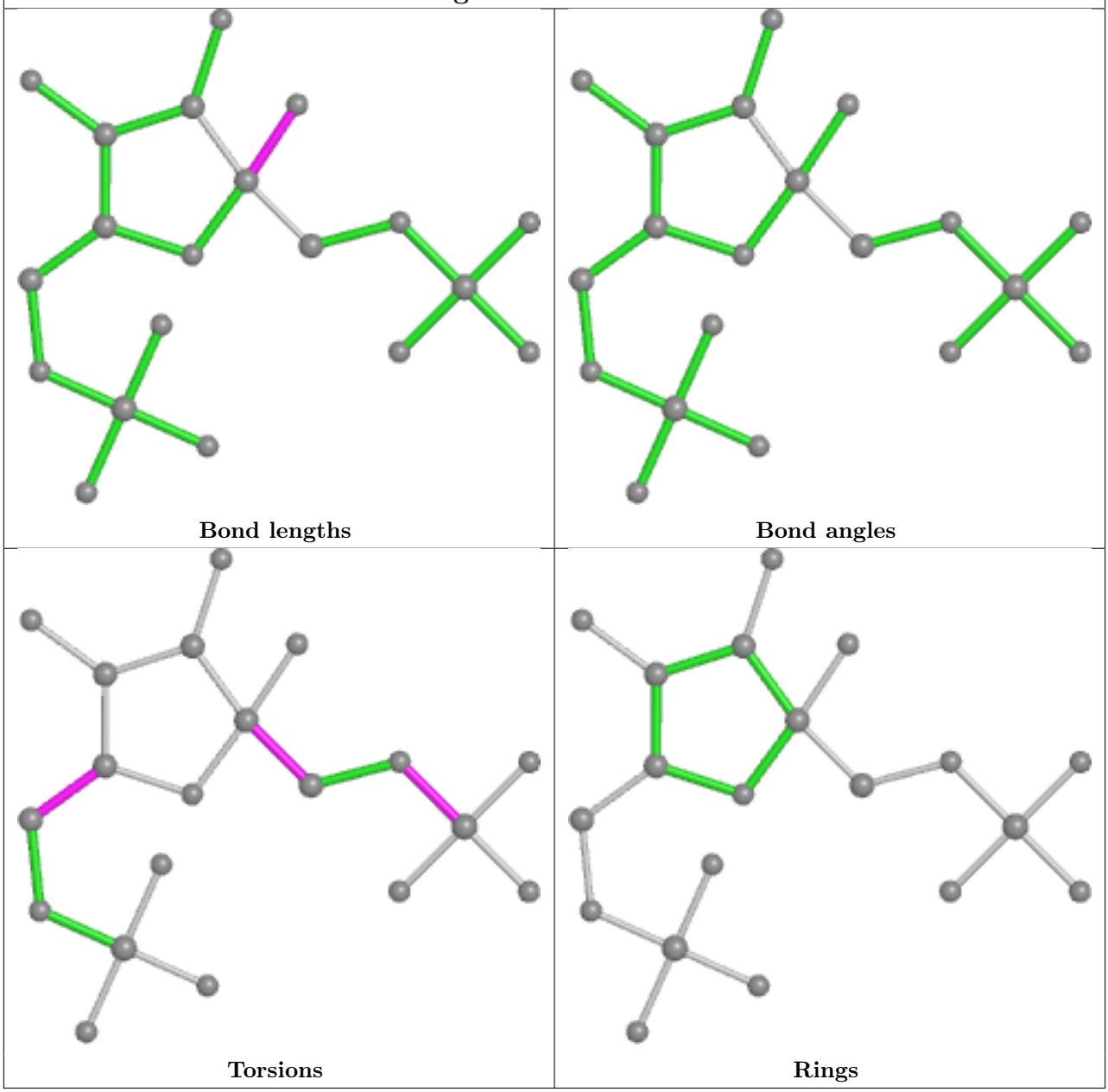


Rings

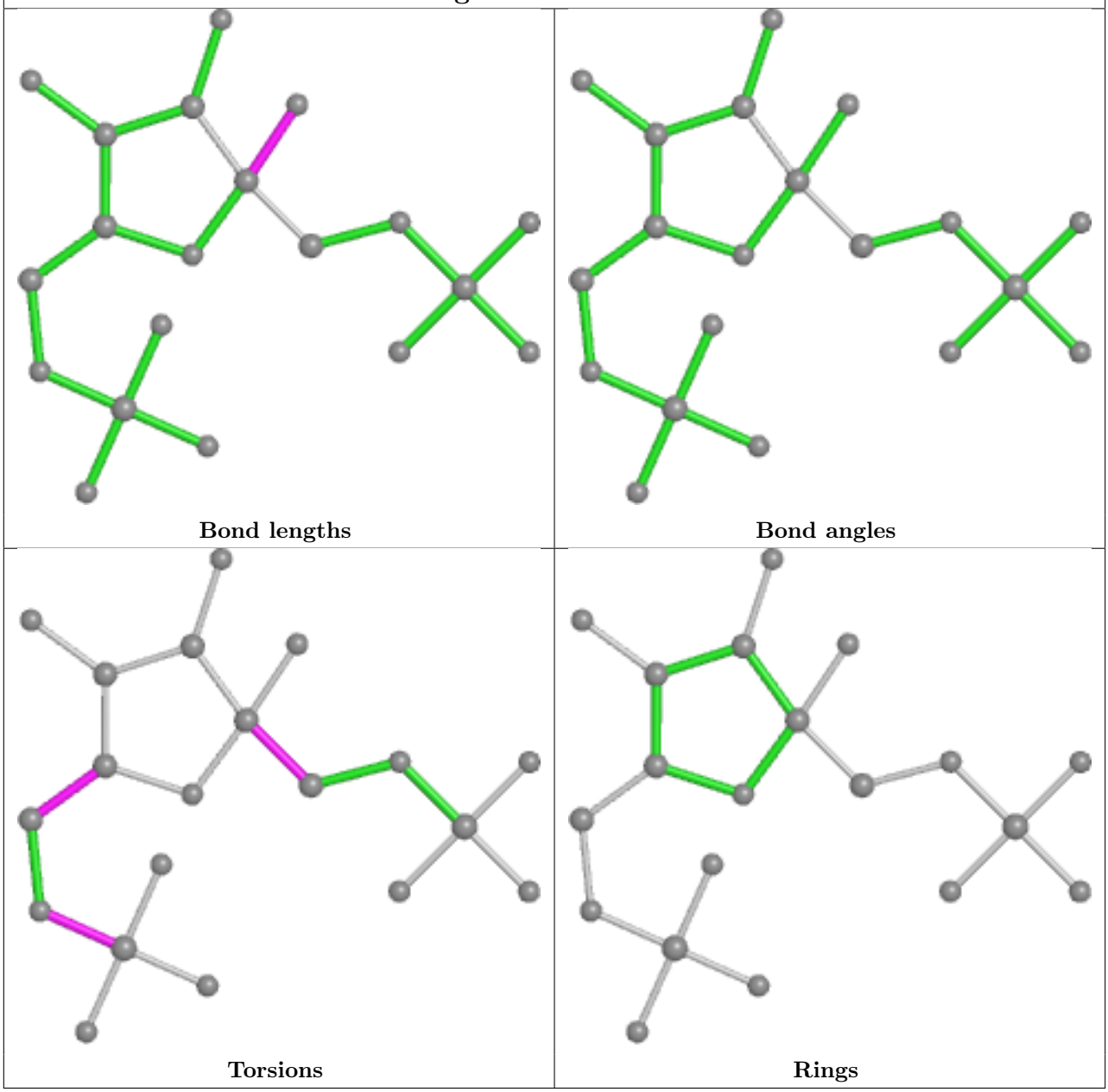
Ligand FBP A 604



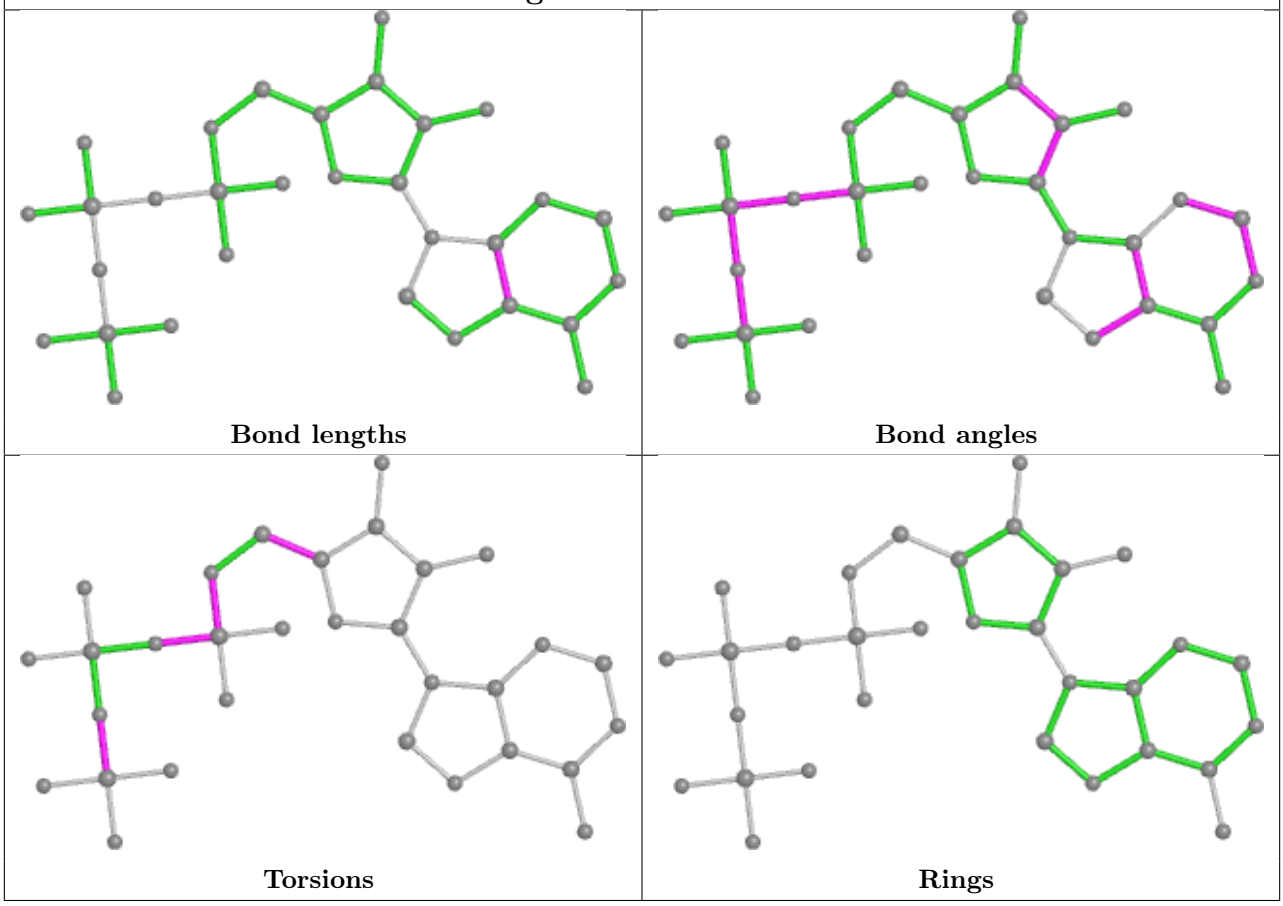
Ligand FBP D 606



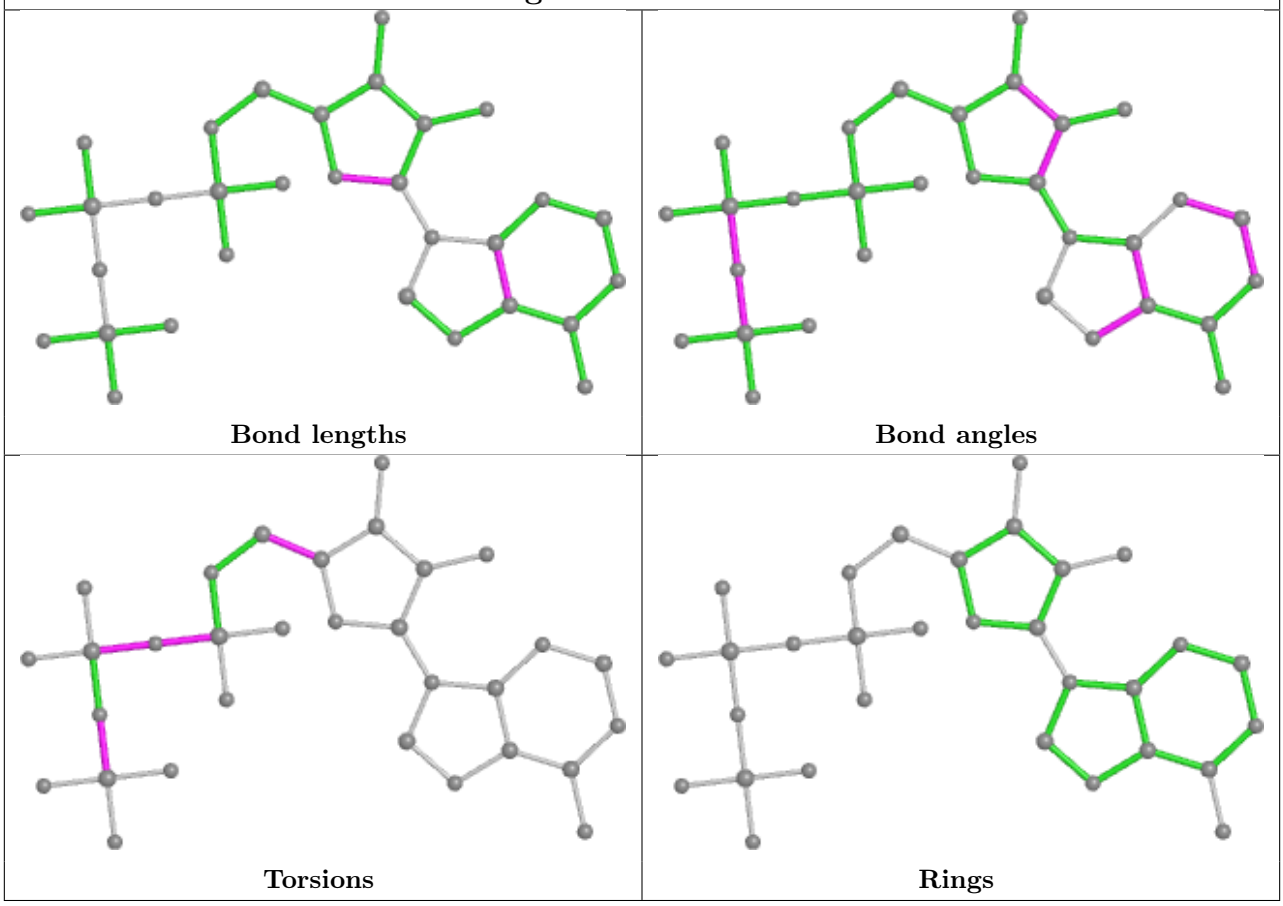
Ligand FBP B 606



Ligand ATP B 604



Ligand ATP D 604



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	501/551 (90%)	0.17	21 (4%)	36	42	29, 44, 71, 90	0
1	B	506/551 (91%)	0.34	33 (6%)	18	22	31, 47, 81, 90	0
1	C	500/551 (90%)	-0.03	11 (2%)	62	68	30, 41, 67, 86	0
1	D	502/551 (91%)	0.33	40 (7%)	12	15	30, 50, 87, 95	0
All	All	2009/2204 (91%)	0.20	105 (5%)	27	32	29, 45, 80, 95	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	8.5
1	D	148	TYR	5.6
1	B	213	GLY	5.5
1	C	38	PRO	5.2
1	D	33	LEU	5.2
1	D	192	PHE	4.9
1	A	37	SER	4.8
1	D	190	ALA	4.6
1	D	168	VAL	4.4
1	B	215	ALA	4.2
1	D	157	LEU	4.0
1	C	39	PRO	4.0
1	B	165	CYS	3.9
1	A	480	GLU	3.9
1	B	190	ALA	3.9
1	B	29	HIS	3.9
1	A	36	ASP	3.8
1	D	170	VAL	3.8
1	C	36	ASP	3.8
1	A	39	PRO	3.8
1	D	38	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	215	ALA	3.7
1	D	187	GLN	3.7
1	A	392	LEU	3.7
1	D	151	LYS	3.6
1	D	32	ARG	3.5
1	D	30	MET	3.5
1	D	149	MET	3.5
1	D	214	ALA	3.5
1	A	41	THR	3.4
1	D	31	CYS	3.4
1	C	37	SER	3.4
1	D	158	TRP	3.3
1	A	481	ALA	3.3
1	D	169	GLU	3.3
1	D	34	ASP	3.2
1	D	183	LEU	3.2
1	A	400	ARG	3.2
1	D	140	LEU	3.2
1	D	124	ILE	3.2
1	A	34	ASP	3.1
1	D	390	TYR	3.1
1	B	392	LEU	3.1
1	D	142	ILE	3.1
1	B	167	VAL	3.0
1	D	143	THR	2.9
1	B	216	VAL	2.9
1	B	214	ALA	2.9
1	D	165	CYS	2.9
1	B	168	VAL	2.9
1	D	156	ILE	2.9
1	D	195	THR	2.8
1	D	172	SER	2.8
1	D	164	ILE	2.8
1	A	190	ALA	2.8
1	B	401	LEU	2.8
1	C	190	ALA	2.7
1	B	480	GLU	2.7
1	D	159	LEU	2.7
1	B	192	PHE	2.7
1	D	213	GLY	2.7
1	D	189	GLY	2.6
1	A	31	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	174	ILE	2.6
1	B	393	GLN	2.6
1	C	32	ARG	2.6
1	B	217	ASP	2.6
1	D	400	ARG	2.6
1	D	41	THR	2.5
1	A	35	ILE	2.5
1	A	479	GLN	2.5
1	A	40	ILE	2.5
1	B	187	GLN	2.5
1	B	185	VAL	2.5
1	A	192	PHE	2.5
1	B	404	ILE	2.4
1	B	189	GLY	2.4
1	C	480	GLU	2.4
1	B	172	SER	2.4
1	A	531	PRO	2.4
1	B	157	LEU	2.4
1	B	212	PRO	2.4
1	D	35	ILE	2.4
1	B	36	ASP	2.3
1	C	34	ASP	2.3
1	B	396	GLU	2.3
1	D	146	ASN	2.3
1	C	192	PHE	2.3
1	B	40	ILE	2.3
1	A	163	ASN	2.2
1	D	191	ASP	2.2
1	B	170	VAL	2.2
1	B	403	PRO	2.2
1	D	100	SER	2.2
1	A	484	GLU	2.2
1	C	41	THR	2.1
1	B	41	THR	2.1
1	B	158	TRP	2.1
1	A	390	TYR	2.1
1	B	183	LEU	2.1
1	B	162	LYS	2.1
1	C	33	LEU	2.1
1	A	447	ARG	2.1
1	D	167	VAL	2.0
1	B	132	VAL	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)

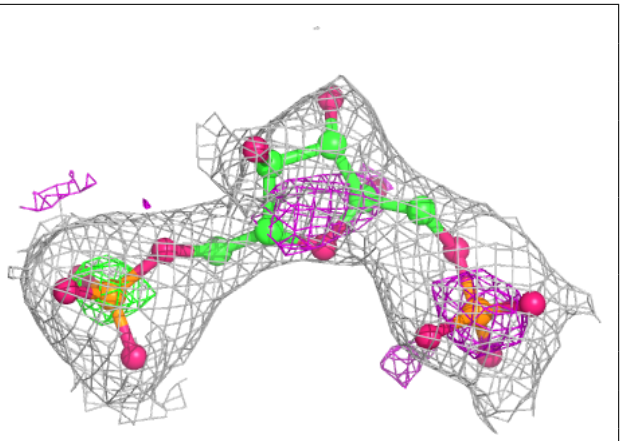
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

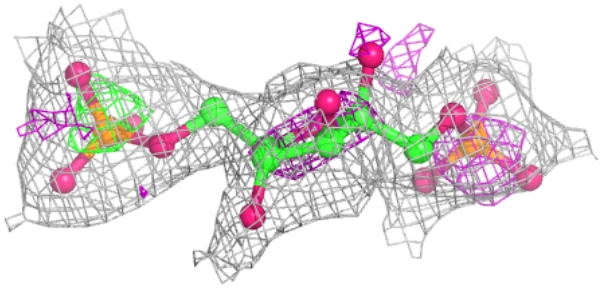
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FBP	D	606	20/20	0.80	0.28	74,79,82,82	0
4	MG	B	605	1/1	0.85	0.14	39,39,39,39	0
4	MG	D	605	1/1	0.85	0.08	70,70,70,70	0
5	FBP	A	604	20/20	0.88	0.18	56,61,64,64	0
5	FBP	B	606	20/20	0.89	0.16	67,71,73,73	0
4	MG	B	603	1/1	0.91	0.16	39,39,39,39	0
2	OXL	D	601	6/6	0.92	0.15	53,54,54,54	0
4	MG	A	603	1/1	0.92	0.14	32,32,32,32	0
4	MG	C	603	1/1	0.93	0.11	33,33,33,33	0
2	OXL	B	601	6/6	0.93	0.16	52,52,52,53	0
2	OXL	C	601	6/6	0.94	0.13	40,41,41,41	0
2	OXL	A	601	6/6	0.95	0.12	38,39,39,39	0
4	MG	D	603	1/1	0.96	0.23	56,56,56,56	0
3	K	C	602	1/1	0.96	0.08	36,36,36,36	0
6	ATP	D	604	31/31	0.96	0.12	50,51,53,53	0
6	ATP	B	604	31/31	0.96	0.15	45,48,50,50	0
3	K	D	602	1/1	0.97	0.08	40,40,40,40	0
3	K	B	602	1/1	0.97	0.08	39,39,39,39	0
5	FBP	C	604	20/20	0.97	0.11	38,41,45,45	0
3	K	A	602	1/1	0.99	0.06	38,38,38,38	0

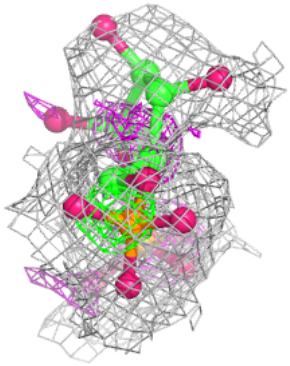
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP D 606:

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

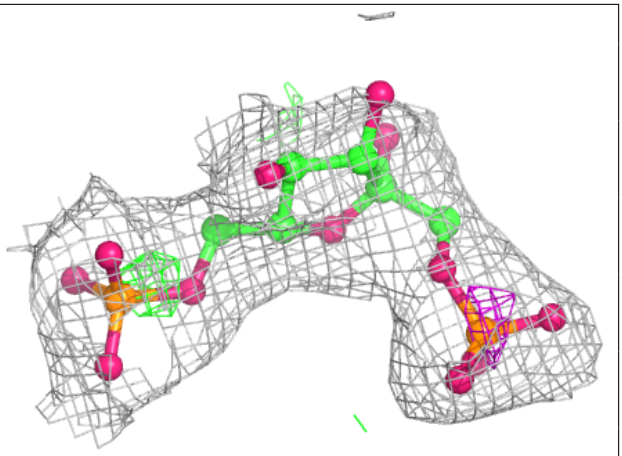


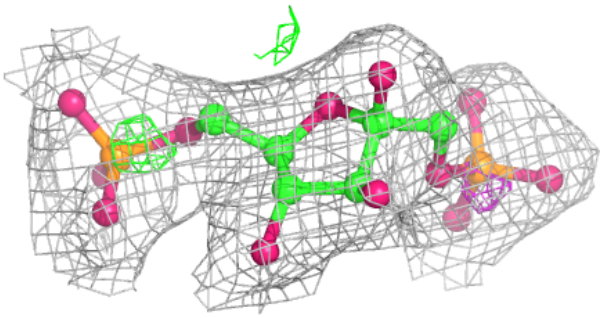


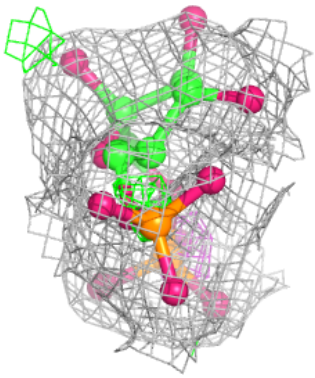


Electron density around FBP A 604:

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

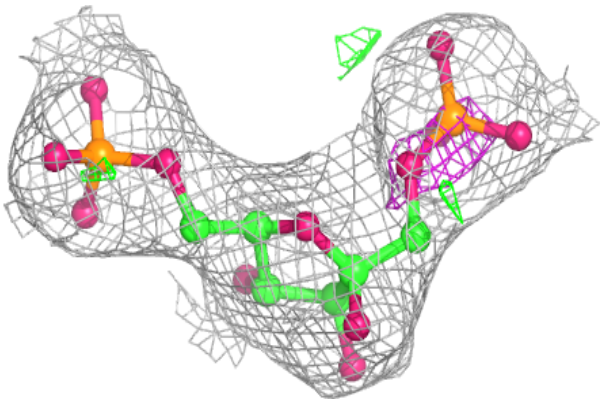


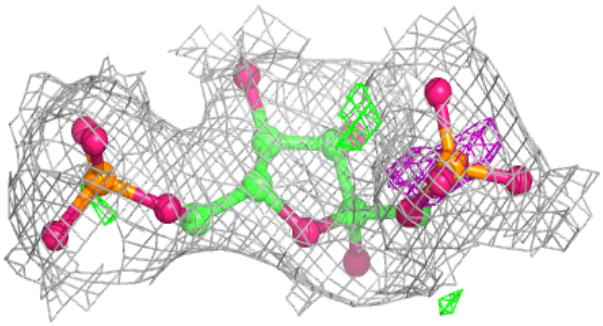


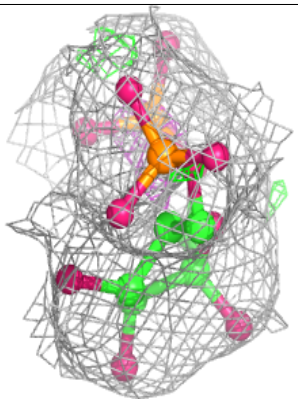


Electron density around FBP B 606:

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

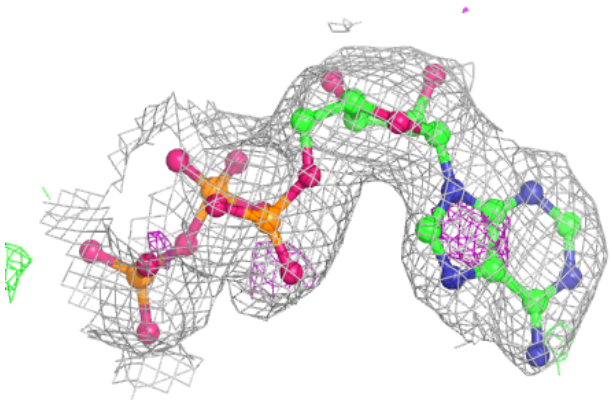


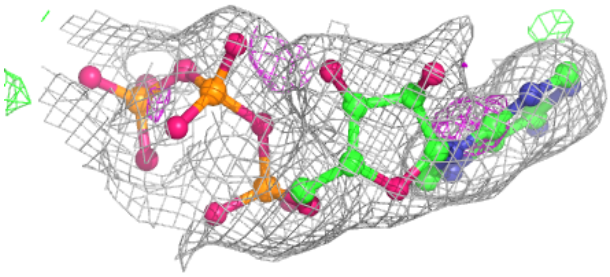


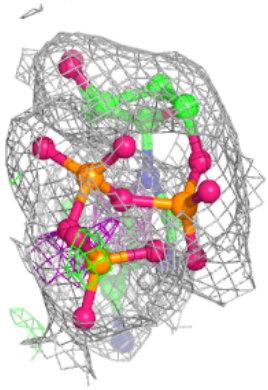


Electron density around ATP D 604:

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

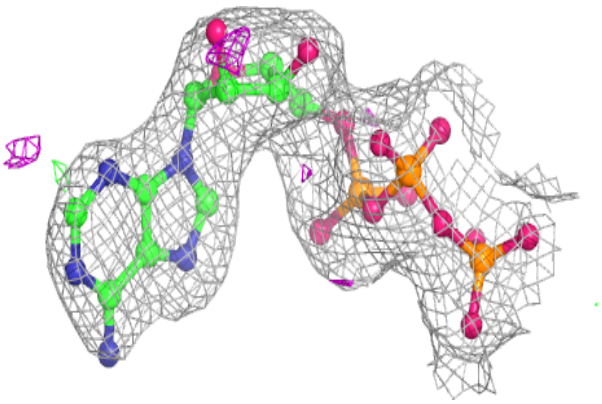


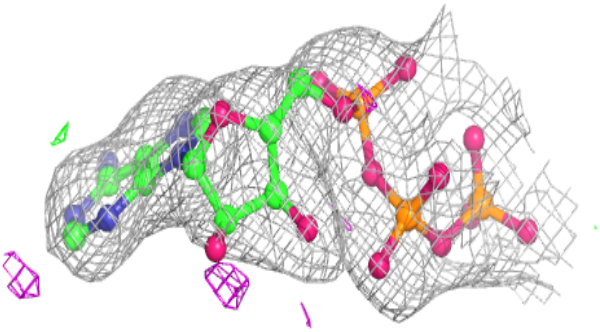


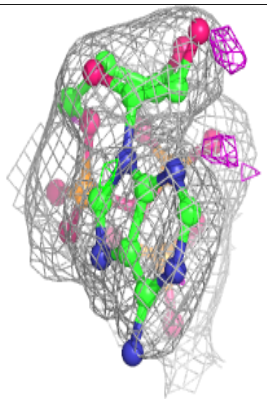


Electron density around ATP B 604:

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

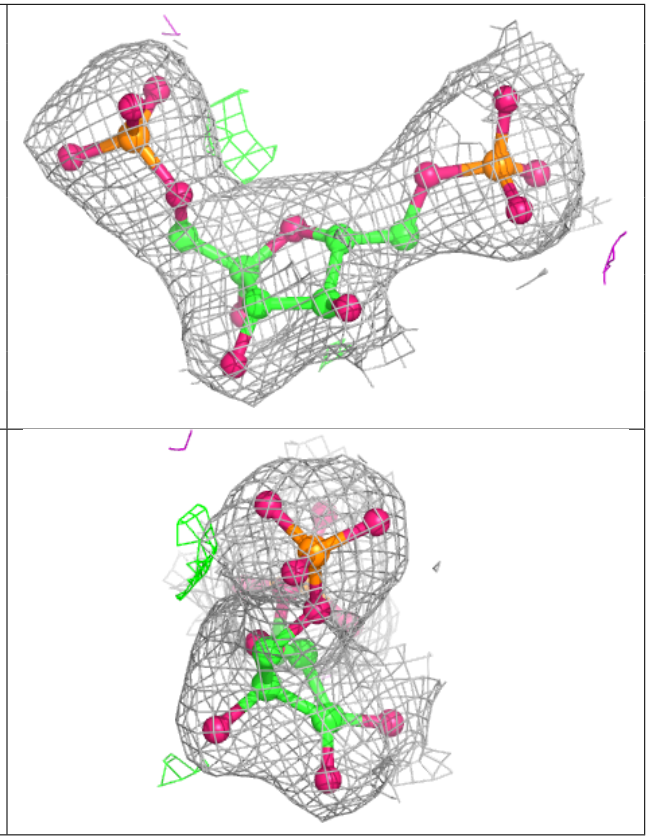






Electron density around FBP C 604:

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



6.5 Other polymers (i)

There are no such residues in this entry.