



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:11 AM BST

PDB ID : 4B2D
Title : human PKM2 with L-serine and FBP bound.
Authors : Chaneton, B.; Hillmann, P.; Zheng, L.; Martin, A.C.L.; Maddocks, O.D.K.; Chokkathukalam, A.; Coyle, J.E.; Jankevics, A.; Holding, F.P.; Vousden, K.H.; Frezza, C.; O'Reilly, M.; Gottlieb, E.
Deposited on : 2012-07-13
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

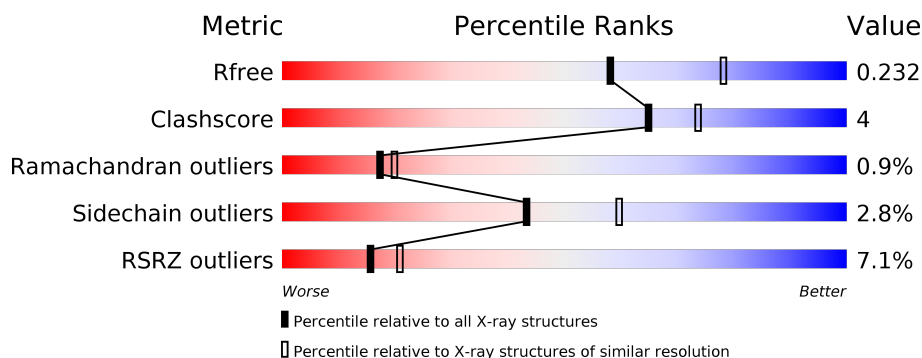
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	548	<div> <div>11%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
1	B	548	<div> <div>11%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	C	548	<div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
2	D	548	<div> <div>14%</div> <div>81%</div> <div>12%</div> <div>5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16980 atoms, of which 28 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
1	A	518	Total	C	N	O	S	0	0	0
			3906	2453	695	733	25			
1	B	514	Total	C	N	O	S	0	1	0
			3872	2436	691	721	24			
1	C	518	Total	C	N	O	S	0	0	0
			3907	2460	695	728	24			

There are 54 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is a protein called PYRUVATE KINASE ISOZYMES M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	518	Total	C	N	O	S	0	0	0
			3914	2462	692	735	25			

There are 19 discrepancies between the modelled and reference sequences:

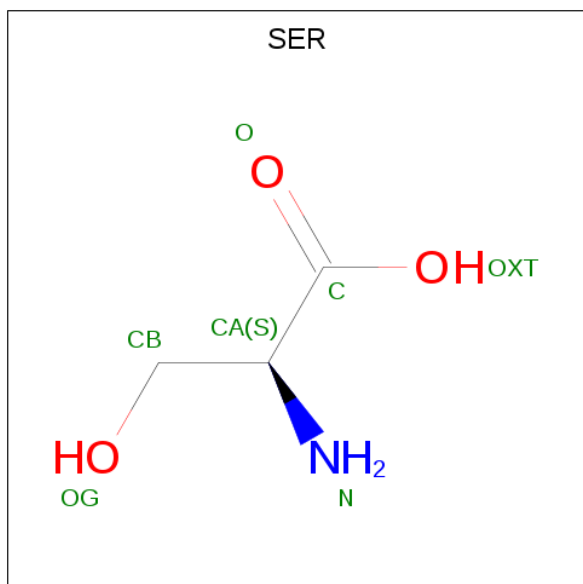
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	expression tag	UNP P14618
D	-14	SER	-	expression tag	UNP P14618
D	-13	SER	-	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	HIS	-	expression tag	UNP P14618
D	-8	HIS	-	expression tag	UNP P14618
D	-7	HIS	-	expression tag	UNP P14618
D	-6	SER	-	expression tag	UNP P14618
D	-5	SER	-	expression tag	UNP P14618
D	-4	GLY	-	expression tag	UNP P14618
D	-3	LEU	-	expression tag	UNP P14618
D	-2	VAL	-	expression tag	UNP P14618
D	-1	PRO	-	expression tag	UNP P14618
D	0	ARG	-	expression tag	UNP P14618
D	1	GLY	-	expression tag	UNP P14618
D	142	LEU	ILE	conflict	UNP P14618

- Molecule 3 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



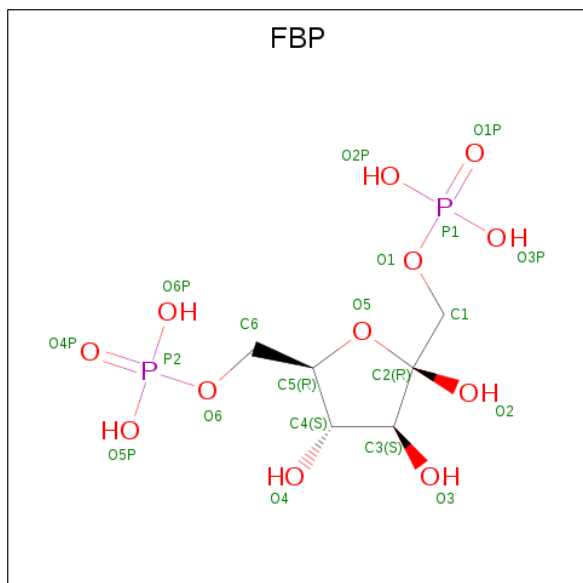
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			14	3	7	1	3		
3	B	1	Total	C	H	N	O	0	0
			14	3	7	1	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	0	0
			14	3	7	1	3		
3	D	1	Total	C	H	N	O	0	0
			14	3	7	1	3		

- Molecule 4 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
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

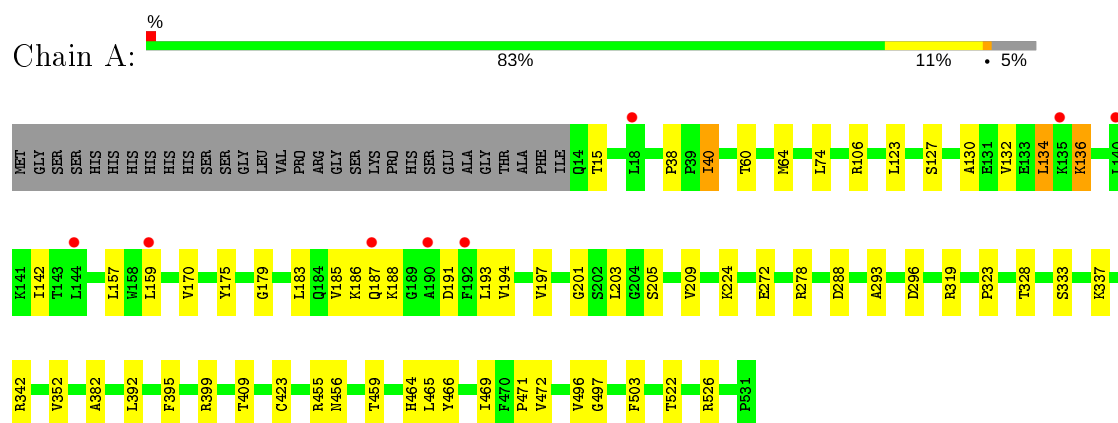
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	395	Total 395	O 395	0	0
6	B	270	Total 270	O 270	0	0
6	C	327	Total 327	O 327	0	0
6	D	251	Total 251	O 251	0	0

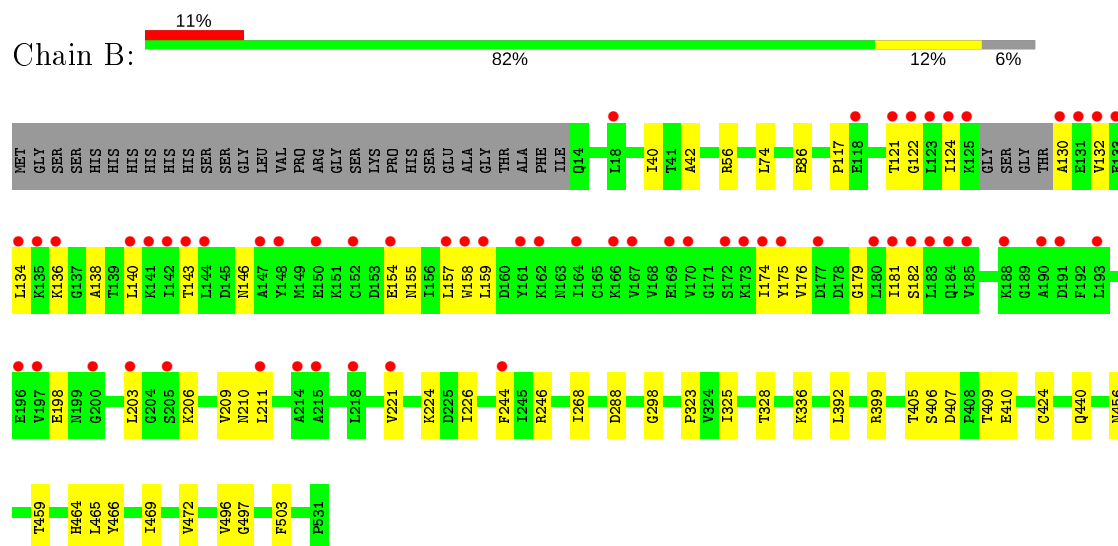
3 Residue-property plots [i](#)

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.

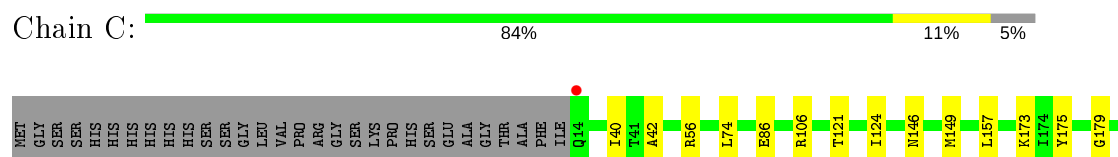
• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2

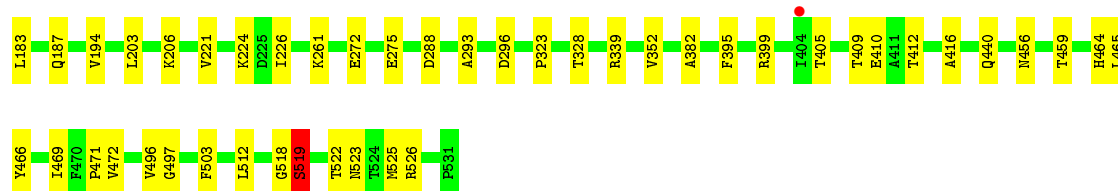


• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2

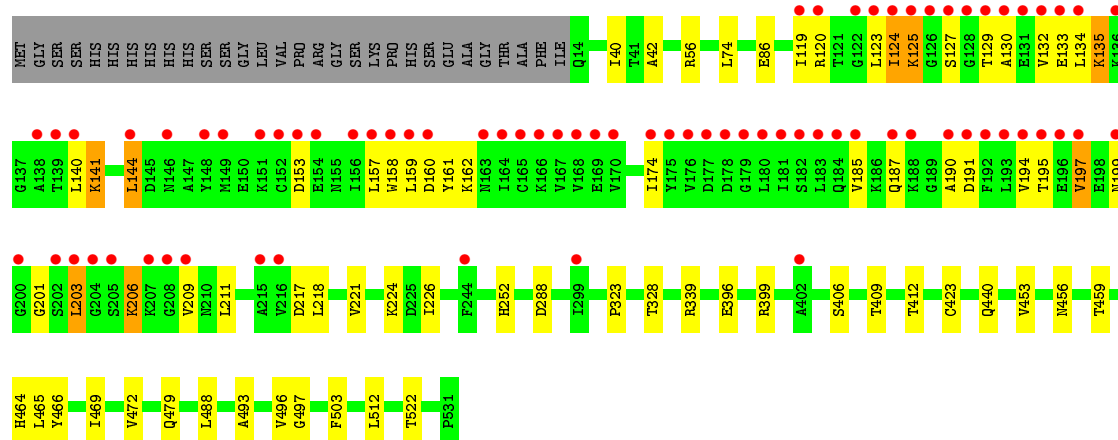
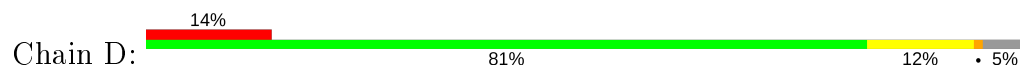


• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2





• Molecule 2: PYRUVATE KINASE ISOZYMES M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.61Å 151.10Å 91.79Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	78.85 – 2.30 78.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (78.85-2.30) 97.9 (78.85-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.173 , 0.226 0.179 , 0.232	Depositor DCC
R_{free} test set	4702 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16980	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.60	0/3970	0.65	0/5370
1	B	0.59	0/3937	0.65	0/5326
1	C	0.56	0/3971	0.63	0/5370
2	D	0.55	0/3978	0.66	0/5379
All	All	0.57	0/15856	0.65	0/21445

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	3906	0	3924	34	0
1	B	3872	0	3889	34	0
1	C	3907	0	3944	31	0
2	D	3914	0	3946	37	0
3	A	7	7	4	1	0
3	B	7	7	4	1	0
3	C	7	7	4	1	0
3	D	7	7	4	1	0
4	A	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	0	10	0	0
4	C	20	0	10	0	0
4	D	20	0	10	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	395	0	0	1	0
6	B	270	0	0	5	0
6	C	327	0	0	1	0
6	D	251	0	0	2	0
All	All	16952	28	15759	129	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 4.

All (129) 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:187:GLN:HB2	1:A:194:VAL:HB	1.58	0.85
1:C:518:GLY:O	1:C:519:SER:HB2	1.79	0.80
2:D:134:LEU:HA	2:D:135:LYS:HB2	1.65	0.76
1:A:106:ARG:NH2	1:A:471:PRO:O	2.18	0.75
1:C:464:HIS:HD1	3:C:1532:SER:N	1.88	0.71
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.71	0.70
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.74	0.70
1:C:410:GLU:HG2	1:C:440:GLN:HE21	1.57	0.69
1:C:187:GLN:HB3	1:C:194:VAL:HB	1.74	0.67
2:D:140:LEU:HD13	2:D:197:VAL:HG21	1.79	0.65
1:B:410:GLU:HG3	1:B:440:GLN:HE21	1.60	0.65
2:D:464:HIS:HD1	3:D:1532:SER:N	1.96	0.64
1:B:440:GLN:HG2	6:B:2211:HOH:O	1.98	0.63
1:C:146:ASN:O	1:C:149:MET:HB2	1.99	0.62
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.82	0.61
2:D:124:ILE:HD13	2:D:130:ALA:HB3	1.83	0.60
1:B:336:LYS:HG2	6:B:2186:HOH:O	2.01	0.59
2:D:56:ARG:NH2	2:D:86:GLU:HB3	2.19	0.58
1:A:319:ARG:HD2	6:B:2016:HOH:O	2.03	0.58
1:B:122:GLY:HA3	6:B:2097:HOH:O	2.03	0.57
1:B:121:THR:HB	1:B:157:LEU:HD11	1.86	0.57
1:A:142:ILE:HA	1:A:157:LEU:O	2.04	0.57
1:B:464:HIS:HD1	3:B:1532:SER:N	2.02	0.56
1:B:134:LEU:CD1	1:B:181:ILE:HG12	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.86	0.56
1:B:175:TYR:HB2	1:B:210:ASN:HB2	1.88	0.56
2:D:174:ILE:HG23	2:D:209:VAL:HG22	1.87	0.56
2:D:125:LYS:HA	2:D:129:THR:HG22	1.88	0.55
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.88	0.54
2:D:141:LYS:HB2	2:D:195:THR:HG21	1.89	0.54
2:D:409:THR:HG23	2:D:522:THR:HB	1.89	0.54
1:B:56:ARG:NH2	1:B:86:GLU:HB3	2.21	0.54
2:D:412:THR:HG22	2:D:512:LEU:HD22	1.90	0.54
2:D:409:THR:HG21	2:D:440:GLN:HE22	1.73	0.53
1:B:410:GLU:HG2	6:B:2229:HOH:O	2.07	0.53
2:D:174:ILE:HD12	2:D:185:VAL:HG21	1.91	0.53
2:D:409:THR:CG2	2:D:440:GLN:NE2	2.72	0.53
2:D:466:TYR:HB2	2:D:469:ILE:HD12	1.91	0.52
2:D:472:VAL:HG11	2:D:496:VAL:HG11	1.92	0.52
1:C:395:PHE:CE2	1:C:399:ARG:HD2	2.45	0.52
1:C:412:THR:HG22	1:C:512:LEU:HD22	1.92	0.52
1:B:288:ASP:O	1:B:323:PRO:HD2	2.10	0.52
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.92	0.51
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.92	0.51
2:D:409:THR:CG2	2:D:440:GLN:HE22	2.23	0.51
1:B:399:ARG:HH12	2:D:399:ARG:CD	2.23	0.51
1:A:132:VAL:HG23	1:A:203:LEU:HB3	1.92	0.50
1:A:423:CYS:HA	1:C:405:THR:O	2.11	0.50
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.46	0.50
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.47	0.50
1:C:121:THR:O	1:C:206:LYS:HA	2.12	0.49
1:A:123:LEU:HA	1:A:205:SER:HB3	1.93	0.49
2:D:120:ARG:HD2	2:D:206:LYS:HB3	1.94	0.49
2:D:288:ASP:O	2:D:323:PRO:HD2	2.12	0.49
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.94	0.49
1:C:352:VAL:HG21	1:C:382:ALA:HA	1.95	0.49
1:A:409:THR:HG23	1:A:522:THR:HB	1.94	0.48
1:A:342:ARG:HE	1:B:298:GLY:HA3	1.78	0.48
1:A:60:THR:O	1:A:64:MET:HG2	2.14	0.48
2:D:497:GLY:HA3	2:D:503:PHE:CZ	2.48	0.48
1:B:182:SER:HB3	1:B:198:GLU:HB2	1.96	0.48
1:C:272:GLU:HB3	1:C:293:ALA:HB3	1.95	0.48
1:A:288:ASP:O	1:A:323:PRO:HD2	2.13	0.47
1:A:395:PHE:CE2	1:A:399:ARG:HD2	2.48	0.47
1:B:134:LEU:HD13	1:B:181:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG22	1:A:38:PRO:HG2	1.95	0.47
1:C:409:THR:HG23	1:C:522:THR:HB	1.97	0.47
1:B:399:ARG:HH21	2:D:396:GLU:HG2	1.79	0.47
1:B:132:VAL:HG22	1:B:203:LEU:HB3	1.97	0.47
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.96	0.47
2:D:144:LEU:HD12	2:D:187:GLN:HE22	1.80	0.47
1:A:464:HIS:HD1	3:A:1532:SER:N	2.13	0.46
1:C:323:PRO:HB3	1:C:465:LEU:O	2.15	0.46
2:D:323:PRO:HB3	2:D:465:LEU:O	2.14	0.46
1:A:456:ASN:HB3	1:A:459:THR:HB	1.98	0.46
1:A:455:ARG:HD2	6:A:2359:HOH:O	2.16	0.46
1:B:176:VAL:HB	1:B:181:ILE:HB	1.98	0.46
2:D:134:LEU:HA	2:D:135:LYS:CB	2.40	0.46
2:D:479:GLN:HG2	2:D:488:LEU:HD22	1.97	0.46
1:A:159:LEU:HD22	1:A:209:VAL:HG21	1.97	0.45
2:D:409:THR:HG22	2:D:440:GLN:NE2	2.31	0.45
1:C:288:ASP:O	1:C:323:PRO:HD2	2.17	0.45
2:D:453:VAL:CG2	2:D:493:ALA:HB2	2.47	0.45
2:D:40:ILE:HD12	2:D:42:ALA:HB3	1.98	0.45
1:A:272:GLU:HB3	1:A:293:ALA:HB3	1.98	0.45
1:B:159:LEU:HD11	1:B:209:VAL:HG21	1.99	0.45
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.99	0.45
2:D:132:VAL:O	2:D:134:LEU:N	2.49	0.45
1:A:188:LYS:HA	1:A:193:LEU:HD23	1.99	0.44
2:D:339:ARG:NH1	6:D:2171:HOH:O	2.49	0.44
1:B:405:THR:O	2:D:423:CYS:HA	2.17	0.44
2:D:456:ASN:HB3	2:D:459:THR:HB	1.98	0.44
1:B:323:PRO:HB3	1:B:465:LEU:O	2.17	0.44
1:A:136:LYS:H	1:A:136:LYS:HD3	1.83	0.44
1:C:272:GLU:HB2	1:C:296:ASP:HB2	1.98	0.44
1:A:526:ARG:HA	1:C:523:ASN:O	2.17	0.44
1:A:127:SER:HB3	1:A:130:ALA:HB2	1.99	0.44
1:B:268:ILE:HG21	1:B:325:ILE:HD12	2.00	0.44
1:C:221:VAL:HG12	1:C:226:ILE:HG13	1.99	0.44
1:C:106:ARG:NH2	1:C:471:PRO:O	2.38	0.44
1:C:526:ARG:HD3	6:C:2320:HOH:O	2.18	0.43
1:C:124:ILE:HD11	1:C:203:LEU:HG	2.00	0.43
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.53	0.43
1:A:323:PRO:HB3	1:A:465:LEU:O	2.19	0.43
1:B:456:ASN:HB3	1:B:459:THR:HB	2.01	0.43
1:A:134:LEU:HB2	1:A:201:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ILE:HG12	1:B:211:LEU:HD22	2.01	0.43
1:C:40:ILE:HD12	1:C:42:ALA:HB3	2.01	0.43
1:B:122:GLY:O	1:B:206:LYS:N	2.51	0.43
1:A:272:GLU:HB2	1:A:296:ASP:HB2	2.01	0.43
1:B:117:PRO:HG3	1:B:246:ARG:NH2	2.34	0.43
1:C:56:ARG:NH2	1:C:86:GLU:HB2	2.34	0.43
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.00	0.42
1:A:134:LEU:HD22	1:A:203:LEU:HB2	2.01	0.42
1:B:407:ASP:OD1	1:B:409[B]:THR:OG1	2.23	0.42
1:B:40:ILE:HD12	1:B:42:ALA:HB3	2.02	0.42
1:C:456:ASN:HB3	1:C:459:THR:HB	2.01	0.42
2:D:161:TYR:CD1	2:D:218:LEU:HD21	2.54	0.42
2:D:119:ILE:HG12	2:D:161:TYR:HB3	2.01	0.42
2:D:221:VAL:HG12	2:D:226:ILE:HG13	2.01	0.42
1:B:124:ILE:HG21	1:B:130:ALA:HA	2.02	0.41
1:A:352:VAL:HG21	1:A:382:ALA:HA	2.03	0.41
2:D:129:THR:OG1	2:D:203:LEU:HB3	2.21	0.41
1:A:183:LEU:HD23	1:A:197:VAL:HA	2.03	0.40
1:A:399:ARG:HH12	1:C:399:ARG:CZ	2.33	0.40
2:D:252:HIS:HE1	6:D:2127:HOH:O	2.04	0.40
1:A:333:SER:HB2	1:A:337:LYS:HE3	2.04	0.40
1:C:173:LYS:HA	1:C:183:LEU:O	2.22	0.40
1:B:221:VAL:HG12	1:B:226:ILE:HG13	2.03	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	516/548 (94%)	499 (97%)	14 (3%)	3 (1%)	25 31
1	B	511/548 (93%)	489 (96%)	16 (3%)	6 (1%)	13 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	516/548 (94%)	502 (97%)	12 (2%)	2 (0%)	34	42
2	D	516/548 (94%)	461 (89%)	47 (9%)	8 (2%)	9	9
All	All	2059/2192 (94%)	1951 (95%)	89 (4%)	19 (1%)	17	20

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	B	138	ALA
1	C	519	SER
1	B	154	GLU
2	D	135	LYS
1	A	328	THR
1	B	155	ASN
2	D	162	LYS
2	D	190	ALA
2	D	206	LYS
2	D	328	THR
1	B	136	LYS
1	B	328	THR
1	C	328	THR
2	D	133	GLU
1	A	185	VAL
1	B	146	ASN
2	D	127	SER
2	D	201	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/450 (91%)	399 (98%)	10 (2%)	49	66
1	B	402/450 (89%)	393 (98%)	9 (2%)	52	69
1	C	408/450 (91%)	401 (98%)	7 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	411/450 (91%)	391 (95%)	20 (5%)	25	35
All	All	1630/1800 (91%)	1584 (97%)	46 (3%)	43	60

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	74	LEU
1	A	134	LEU
1	A	136	LYS
1	A	170	VAL
1	A	186	LYS
1	A	191	ASP
1	A	224	LYS
1	A	278	ARG
1	A	392	LEU
1	B	74	LEU
1	B	140	LEU
1	B	143	THR
1	B	158	TRP
1	B	224	LYS
1	B	244	PHE
1	B	392	LEU
1	B	406	SER
1	B	424	CYS
1	C	74	LEU
1	C	224	LYS
1	C	261	LYS
1	C	275	GLU
1	C	339	ARG
1	C	519	SER
1	C	525	MET
2	D	74	LEU
2	D	123	LEU
2	D	124	ILE
2	D	125	LYS
2	D	141	LYS
2	D	144	LEU
2	D	153	ASP
2	D	157	LEU
2	D	158	TRP
2	D	159	LEU

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Mol	Chain	Res	Type
2	D	160	ASP
2	D	191	ASP
2	D	194	VAL
2	D	197	VAL
2	D	199	ASN
2	D	203	LEU
2	D	211	LEU
2	D	217	ASP
2	D	224	LYS
2	D	406	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	274	HIS
1	B	440	GLN
1	C	199	ASN
1	C	440	GLN
2	D	187	GLN
2	D	199	ASN
2	D	440	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
4	FBP	B	600	-	18,20,20	1.06	2 (11%)	23,32,32	0.76	0
4	FBP	C	600	-	18,20,20	0.89	1 (5%)	23,32,32	0.73	0
4	FBP	A	600	-	18,20,20	0.85	0	23,32,32	0.73	0
4	FBP	D	600	-	18,20,20	0.75	0	23,32,32	0.73	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	FBP	B	600	-	-	2/13/32/32	0/1/1/1
4	FBP	C	600	-	-	2/13/32/32	0/1/1/1
4	FBP	A	600	-	-	2/13/32/32	0/1/1/1
4	FBP	D	600	-	-	2/13/32/32	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	FBP	O5-C2	3.12	1.48	1.43
4	C	600	FBP	O5-C2	2.68	1.47	1.43
4	B	600	FBP	O2-C2	2.28	1.44	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	600	FBP	C4-C5-C6-O6
4	C	600	FBP	C4-C5-C6-O6
4	A	600	FBP	C4-C5-C6-O6
4	D	600	FBP	C4-C5-C6-O6

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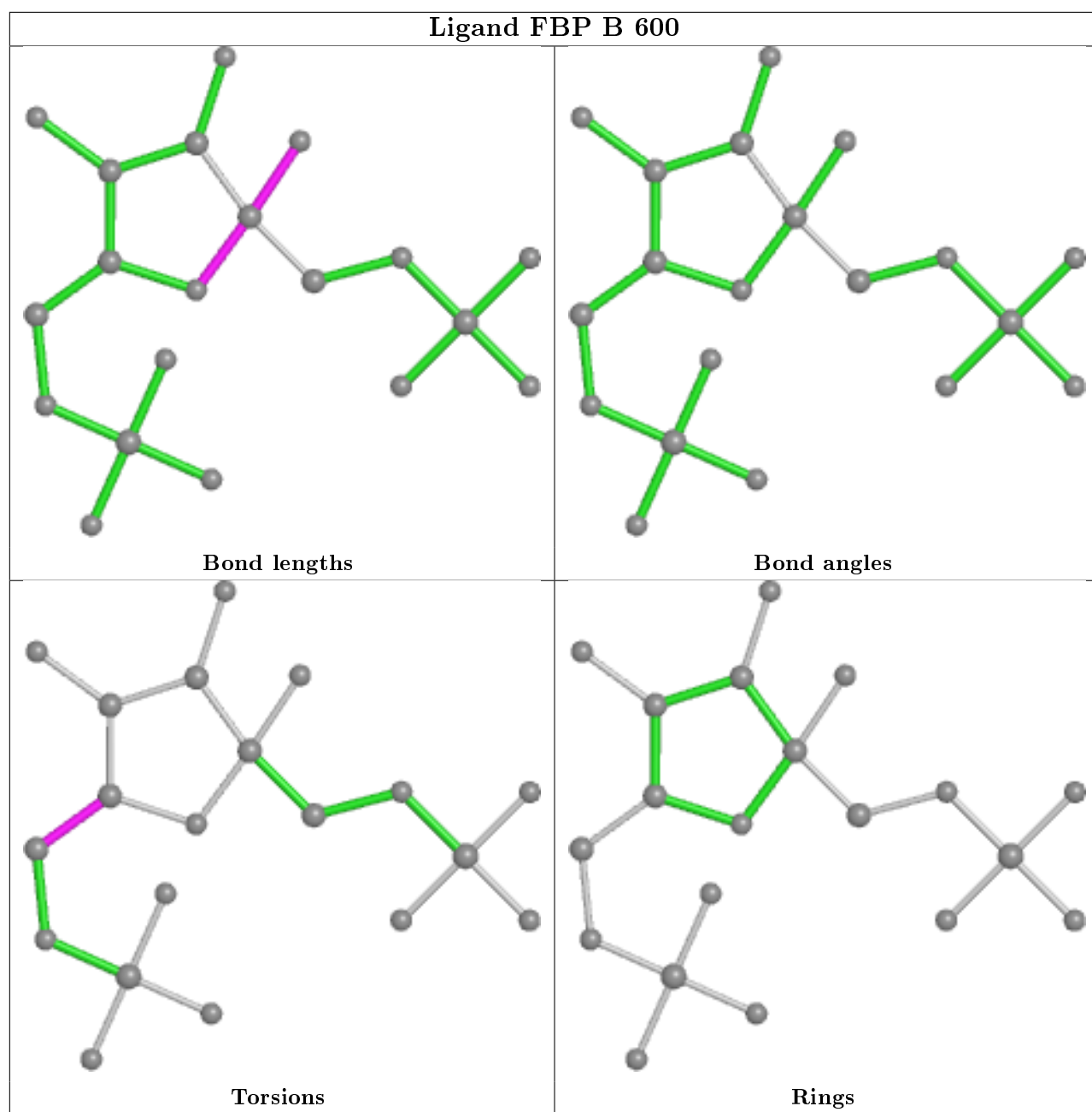
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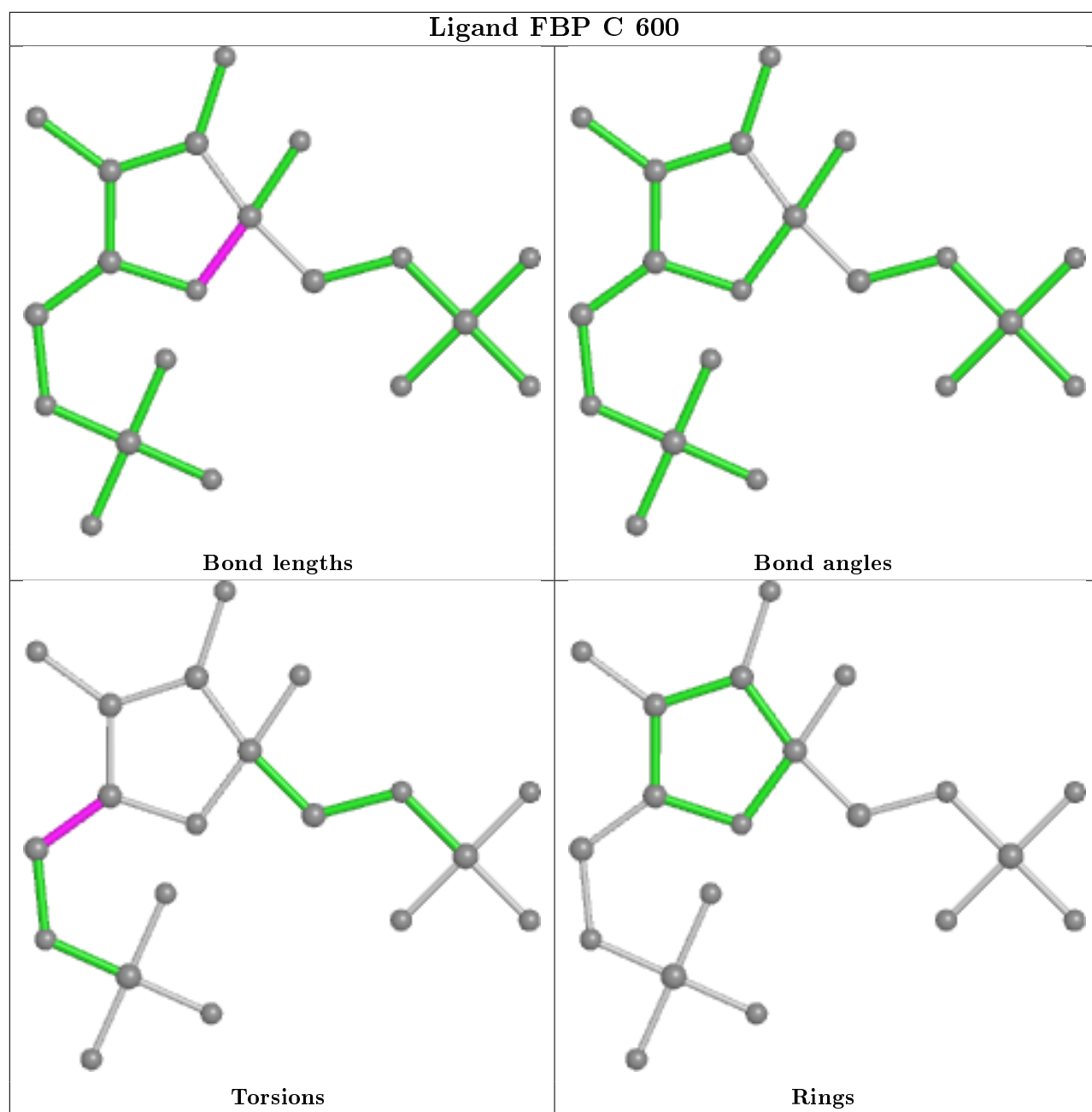
Mol	Chain	Res	Type	Atoms
4	C	600	FBP	O5-C5-C6-O6
4	B	600	FBP	O5-C5-C6-O6
4	D	600	FBP	O5-C5-C6-O6
4	A	600	FBP	O5-C5-C6-O6

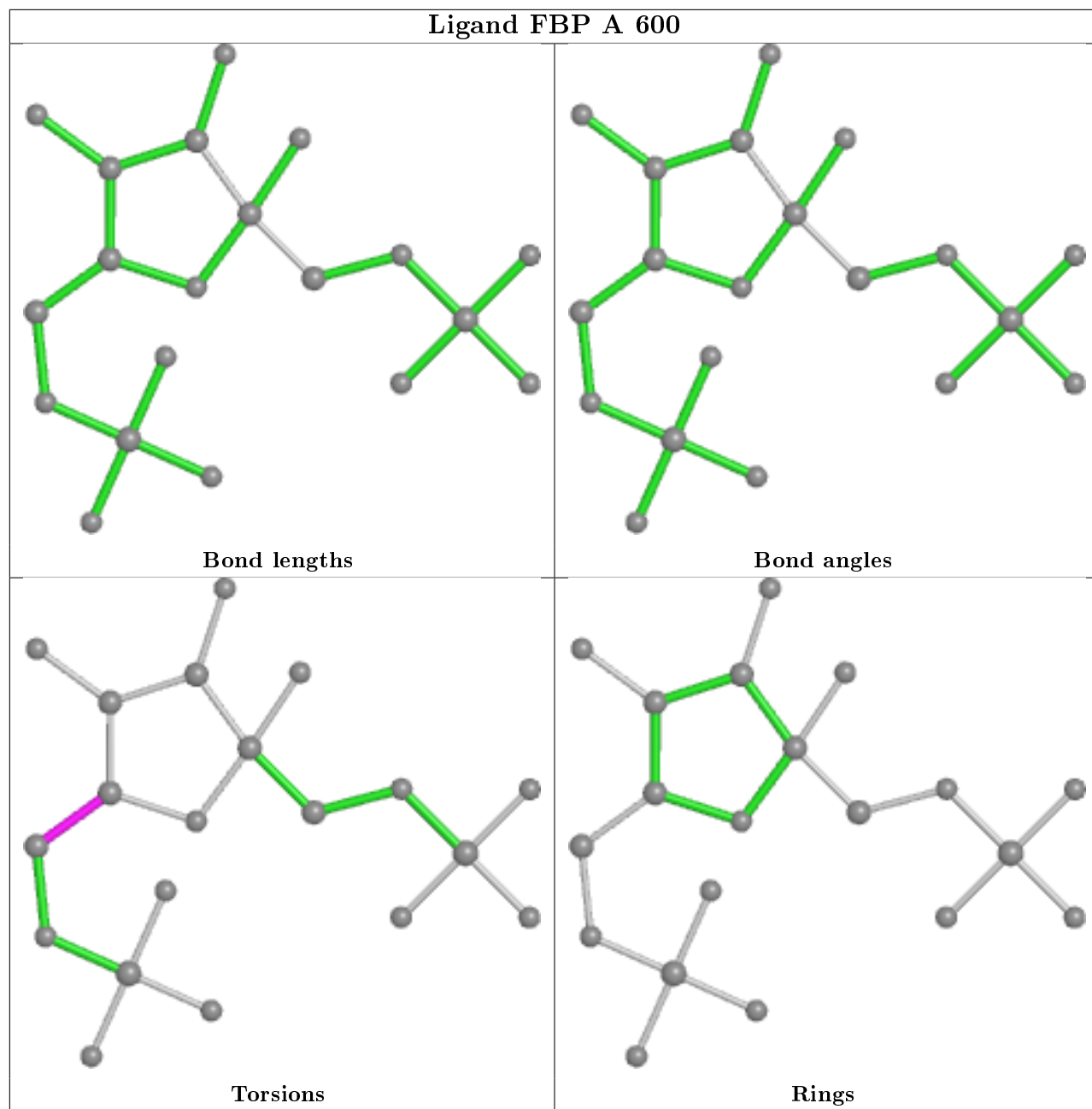
There are no ring outliers.

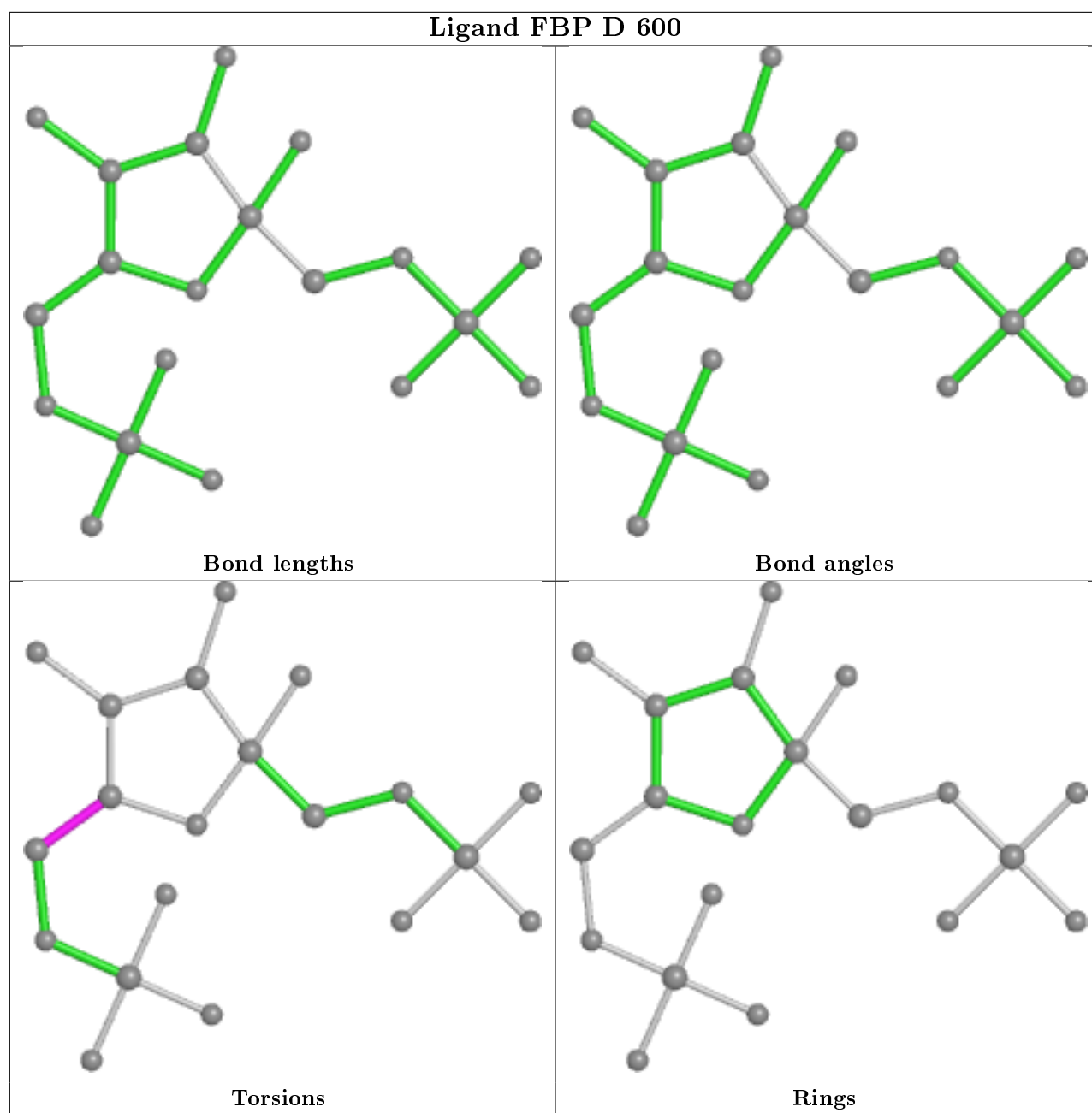
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	518/548 (94%)	-0.09	8 (1%) 73 79	33, 45, 83, 110	0
1	B	514/548 (93%)	0.35	60 (11%) 4 6	34, 50, 145, 173	0
1	C	518/548 (94%)	-0.17	2 (0%) 92 95	37, 47, 66, 90	0
2	D	518/548 (94%)	0.75	76 (14%) 2 3	39, 54, 161, 173	0
All	All	2068/2192 (94%)	0.21	146 (7%) 16 21	33, 50, 140, 173	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	194	VAL	16.3
2	D	192	PHE	13.7
2	D	193	LEU	12.2
2	D	152	CYS	10.8
1	B	147	ALA	9.9
2	D	140	LEU	9.6
2	D	180	LEU	9.4
2	D	204	GLY	9.4
2	D	157	LEU	8.3
2	D	123	LEU	7.9
2	D	190	ALA	7.9
2	D	167	VAL	7.7
2	D	153	ASP	7.3
1	B	132	VAL	7.3
2	D	185	VAL	7.3
2	D	144	LEU	7.2
2	D	197	VAL	7.1
2	D	132	VAL	7.1
1	B	124	ILE	7.0
2	D	196	GLU	6.8
2	D	128	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
2	D	139	THR	6.5
2	D	203	LEU	6.4
2	D	126	GLY	6.4
2	D	129	THR	6.2
2	D	151	LYS	6.2
2	D	177	ASP	6.2
1	B	135	LYS	6.1
1	B	134	LEU	5.8
2	D	154	GLU	5.8
2	D	130	ALA	5.7
1	B	140	LEU	5.7
1	B	185	VAL	5.7
1	B	193	LEU	5.5
2	D	138	ALA	5.4
2	D	205	SER	5.3
2	D	215	ALA	5.2
1	B	130	ALA	5.1
1	B	167	VAL	5.1
1	B	170	VAL	5.1
2	D	125	LYS	5.1
2	D	199	ASN	5.1
2	D	191	ASP	4.9
2	D	164	ILE	4.9
1	B	142	ILE	4.8
1	B	122	GLY	4.8
2	D	174	ILE	4.8
2	D	209	VAL	4.7
2	D	120	ARG	4.6
2	D	181	ILE	4.6
1	B	123	LEU	4.6
1	B	150	GLU	4.5
2	D	216	VAL	4.5
2	D	160	ASP	4.4
1	B	183	LEU	4.3
2	D	208	GLY	4.3
1	B	181	ILE	4.3
1	B	133	GLU	4.2
1	B	141	LYS	4.2
2	D	159	LEU	4.1
2	D	148	TYR	4.1
2	D	202	SER	4.1
2	D	179	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	D	124	ILE	3.9
2	D	163	ASN	3.9
1	B	125	LYS	3.9
1	B	143	THR	3.9
1	B	158	TRP	3.8
1	A	190	ALA	3.8
2	D	176	VAL	3.7
1	B	214	ALA	3.6
2	D	146	ASN	3.6
1	B	152	CYS	3.5
1	B	157	LEU	3.5
2	D	122	GLY	3.5
1	B	159	LEU	3.5
1	B	203	LEU	3.5
2	D	158	TRP	3.5
1	A	144	LEU	3.5
1	B	200	GLY	3.5
2	D	207	LYS	3.5
1	B	215	ALA	3.5
1	B	164	ILE	3.4
1	A	192	PHE	3.4
2	D	188	LYS	3.4
1	B	197	VAL	3.3
2	D	169	GLU	3.3
2	D	195	THR	3.2
2	D	200	GLY	3.2
1	B	161	TYR	3.1
2	D	168	VAL	3.1
2	D	166	LYS	3.1
2	D	244	PHE	3.0
2	D	183	LEU	2.9
1	B	184	GLN	2.9
1	B	148	TYR	2.9
2	D	127	SER	2.9
2	D	175	TYR	2.9
1	A	18	LEU	2.9
1	B	211	LEU	2.9
2	D	184	GLN	2.8
1	B	144	LEU	2.8
1	B	180	LEU	2.8
1	B	131	GLU	2.7
1	B	166	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	218	LEU	2.7
2	D	178	ASP	2.6
2	D	136	LYS	2.6
1	B	191	ASP	2.6
2	D	182	SER	2.6
2	D	299	ILE	2.6
1	B	172	SER	2.6
2	D	149	MET	2.6
2	D	402	ALA	2.5
1	C	14	GLN	2.5
1	B	121	THR	2.5
1	B	173	LYS	2.4
1	A	135	LYS	2.4
1	C	404	ILE	2.4
2	D	134	LEU	2.4
2	D	131	GLU	2.4
2	D	119	ILE	2.3
1	B	177	ASP	2.3
2	D	165	CYS	2.3
2	D	133	GLU	2.3
1	B	169	GLU	2.3
1	B	221	VAL	2.3
1	B	205	SER	2.3
2	D	187	GLN	2.2
1	B	196	GLU	2.2
1	B	182	SER	2.2
1	B	174	ILE	2.2
1	A	187	GLN	2.2
1	B	18	LEU	2.2
1	B	154	GLU	2.2
1	B	190	ALA	2.2
1	B	136	LYS	2.2
1	B	188	LYS	2.2
1	A	140	LEU	2.2
2	D	170	VAL	2.2
1	B	162	LYS	2.1
2	D	156	ILE	2.1
1	B	244	PHE	2.1
1	B	118	GLU	2.1
1	B	175	TYR	2.1
1	A	159	LEU	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](#)

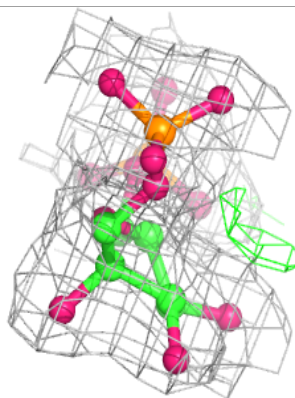
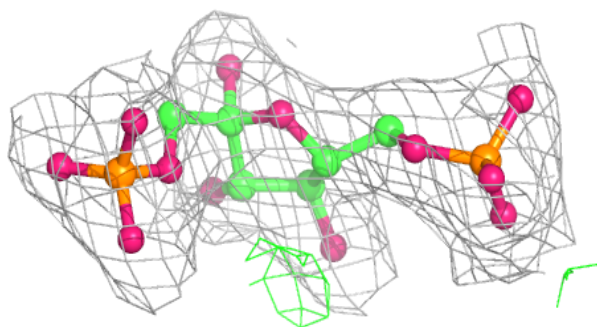
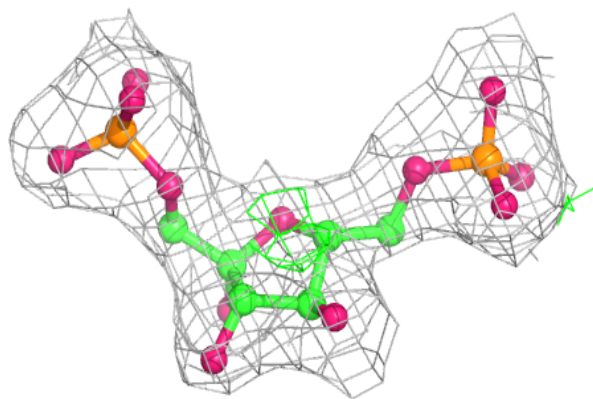
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	C	700	1/1	0.55	0.19	52,52,52,52	0
5	MG	A	700	1/1	0.90	0.27	53,53,53,53	0
3	SER	D	1532	7/7	0.94	0.17	36,45,47,47	14
3	SER	A	1532	7/7	0.97	0.11	26,36,43,43	14
3	SER	C	1532	7/7	0.98	0.15	27,36,44,44	0
4	FBP	C	600	20/20	0.98	0.11	38,44,47,48	0
3	SER	B	1532	7/7	0.98	0.11	39,41,43,44	0
4	FBP	A	600	20/20	0.99	0.10	35,40,48,48	0
4	FBP	B	600	20/20	0.99	0.09	33,38,45,45	0
4	FBP	D	600	20/20	0.99	0.10	41,46,49,49	0

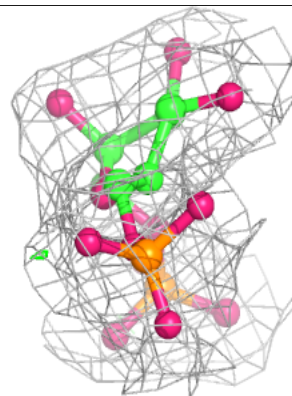
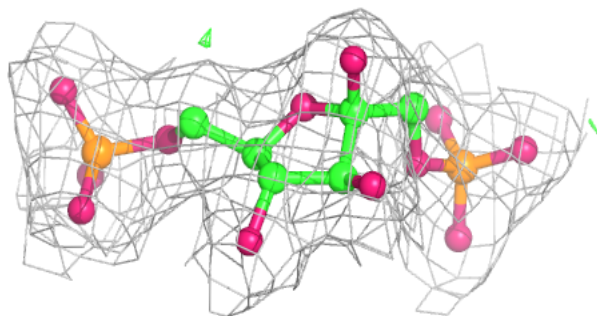
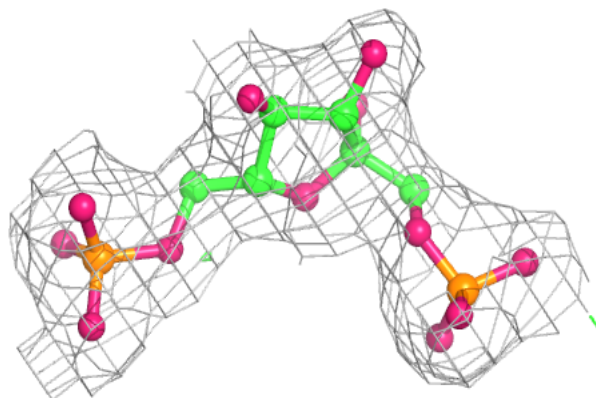
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP C 600:

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

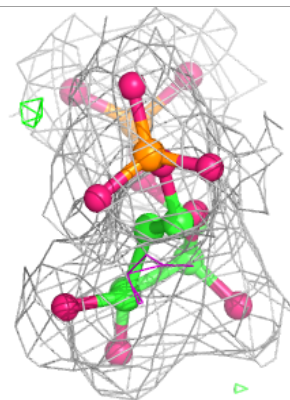
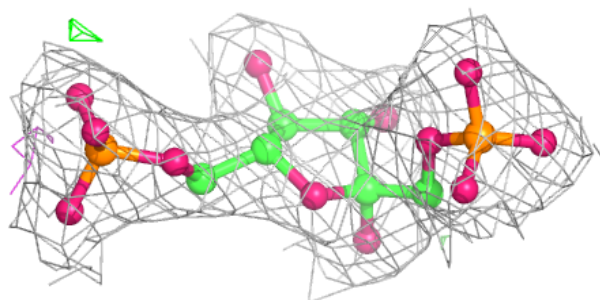
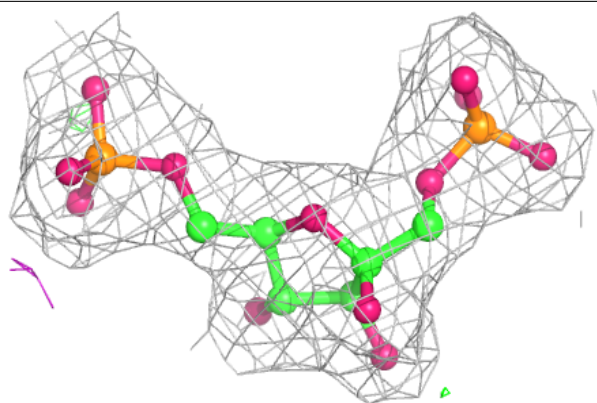
**Electron density around FBP A 600:**

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

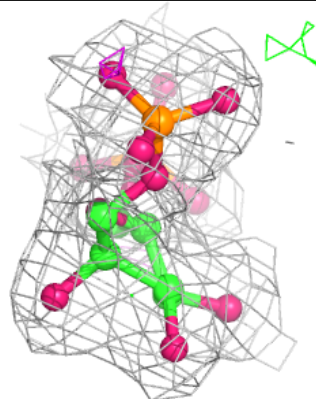
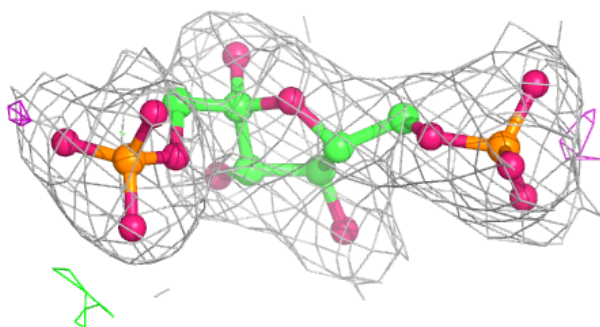
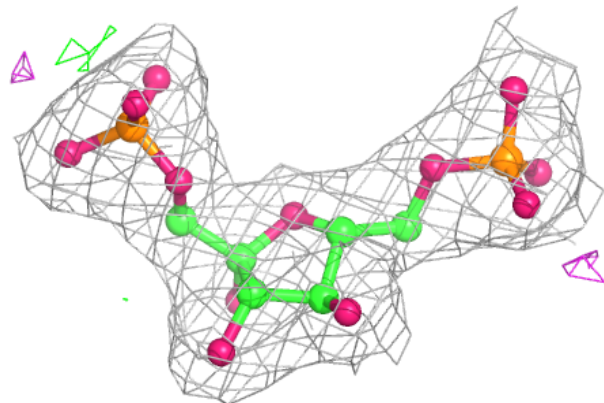


Electron density around FBP B 600:

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

**Electron density around FBP D 600:**

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



6.5 Other polymers

There are no such residues in this entry.