



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:27 PM UTC

PDB ID : 4RPP / pdb_00004rpp
Title : crystal structure of PKM2-K422R mutant bound with FBP
Authors : Wang, P.; Sun, C.; Zhu, T.; Xu, Y.
Deposited on : 2014-10-31
Resolution : 2.58 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

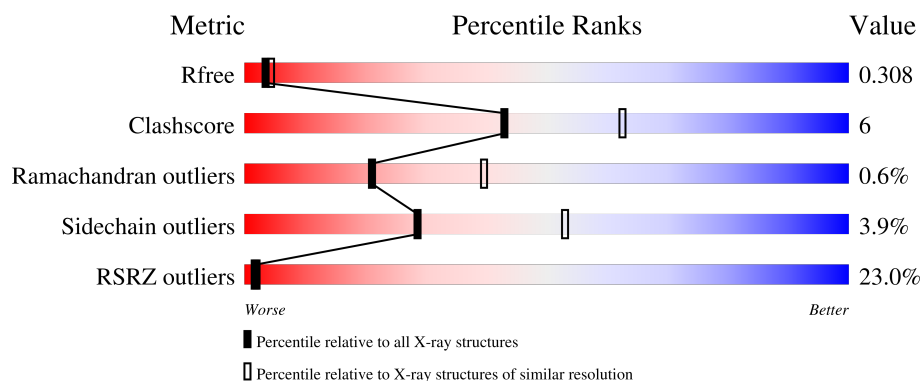
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	535	18% 62% 13% • 23%
1	B	535	19% 62% 13% • 24%
1	C	535	17% 63% 11% • 26%
1	D	535	16% 64% 12% • 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12596 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

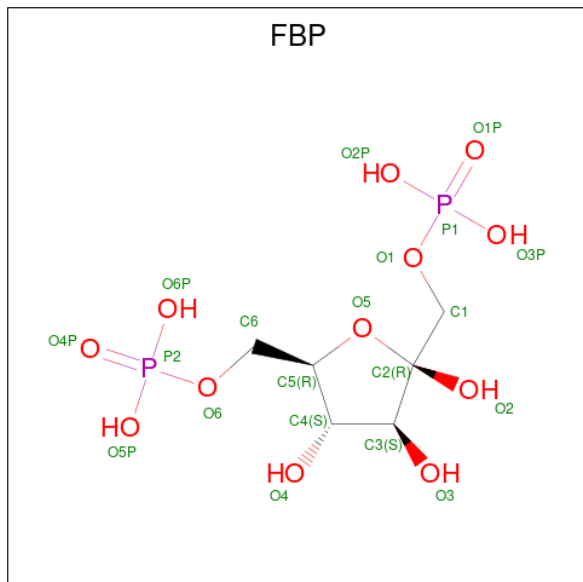
- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3153	1978	568	586	21			
1	B	408	Total	C	N	O	S	0	0	0
			3140	1970	568	581	21			
1	C	396	Total	C	N	O	S	0	0	0
			3050	1912	552	565	21			
1	D	408	Total	C	N	O	S	0	0	0
			3143	1973	568	581	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	expression tag	UNP P14618
A	-2	LEU	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
A	422	ARG	LYS	engineered mutation	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	LEU	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	422	ARG	LYS	engineered mutation	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	LEU	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
C	422	ARG	LYS	engineered mutation	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	LEU	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	422	ARG	LYS	engineered mutation	UNP P14618

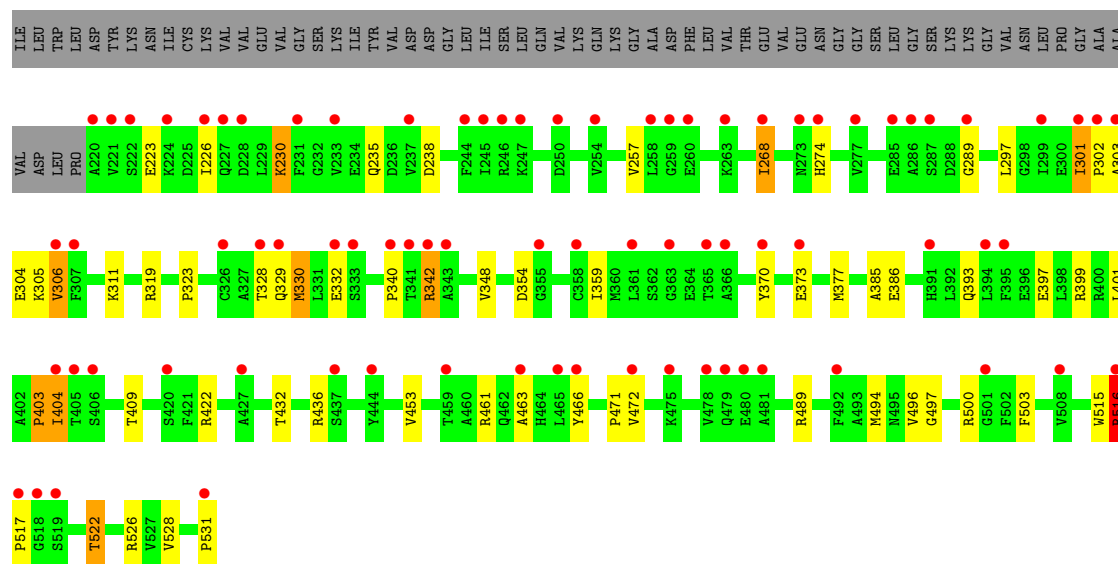
- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



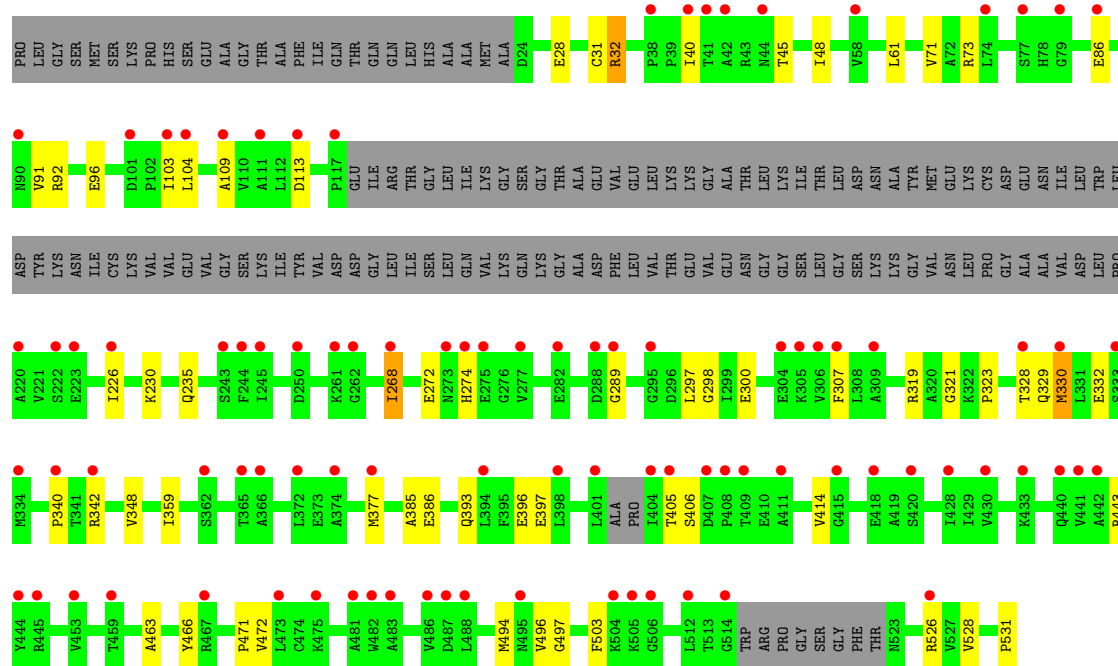
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is water.

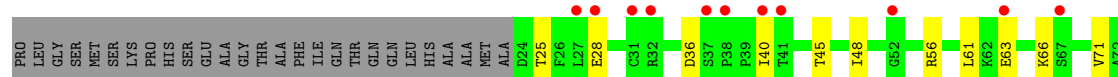
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	7	Total	O	0	0
			7	7		
3	C	8	Total	O	0	0
			8	8		
3	D	8	Total	O	0	0
			8	8		

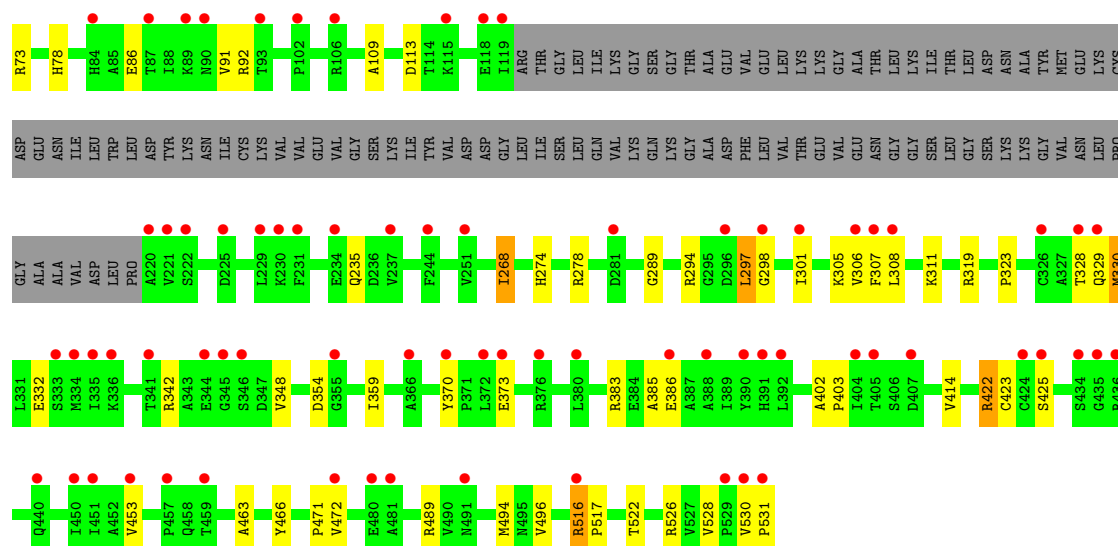


• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.67Å 152.55Å 97.68Å 90.00° 104.24° 90.00°	Depositor
Resolution (Å)	38.31 – 2.58 38.31 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.6 (38.31-2.58) 97.6 (38.31-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.274 , 0.308 0.282 , 0.308	Depositor DCC
R_{free} test set	3473 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12596	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: 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	0.32	0/3204	0.80	3/4330 (0.1%)
1	B	0.32	0/3194	0.81	7/4315 (0.2%)
1	C	0.29	0/3097	0.77	0/4178
1	D	0.29	0/3197	0.75	0/4319
All	All	0.31	0/12692	0.78	10/17142 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	VAL	CB-CA-C	-6.41	103.77	111.97
1	A	218	LEU	CA-C-N	-6.07	112.25	119.84
1	A	218	LEU	C-N-CA	-6.07	112.25	119.84
1	B	305	LYS	N-CA-C	5.42	119.95	113.23
1	A	343	ALA	N-CA-C	-5.34	105.57	111.71
1	B	301	ILE	CA-C-N	5.08	125.08	119.90
1	B	301	ILE	C-N-CA	5.08	125.08	119.90
1	B	516	ARG	CA-C-N	5.06	126.16	119.84
1	B	516	ARG	C-N-CA	5.06	126.16	119.84
1	B	342	ARG	CG-CD-NE	-5.02	100.95	112.00

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	3153	0	3214	53	0
1	B	3140	0	3191	57	0
1	C	3050	0	3109	36	0
1	D	3143	0	3197	41	0
2	A	20	0	10	1	0
2	B	20	0	10	2	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	1	0
All	All	12596	0	12751	157	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 6.

All (157) 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:306:VAL:HG11	1:B:342:ARG:HH22	1.37	0.88
1:A:342:ARG:NH2	1:B:302:PRO:O	2.06	0.88
1:B:56:ARG:NH2	1:B:83:TYR:O	2.17	0.75
1:A:494:MET:HG2	1:A:531:PRO:HD2	1.69	0.74
1:B:274:HIS:CE1	1:B:301:ILE:HG22	2.25	0.71
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.73	0.70
1:A:422:ARG:HG3	1:C:414:VAL:HG11	1.72	0.70
1:A:306:VAL:HG11	1:B:342:ARG:NH2	2.06	0.70
1:C:494:MET:HG2	1:C:531:PRO:HD2	1.74	0.69
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.75	0.68
1:B:301:ILE:HD11	1:B:306:VAL:HG22	1.76	0.67
1:A:298:GLY:HA3	1:B:342:ARG:NH1	2.10	0.67
1:A:342:ARG:NE	1:B:306:VAL:HB	2.11	0.66
1:A:342:ARG:CZ	1:B:306:VAL:H	2.08	0.66
1:C:298:GLY:HA3	1:D:342:ARG:NH2	2.10	0.66
1:B:399:ARG:HG2	1:D:422:ARG:HH22	1.61	0.66
1:A:342:ARG:NH2	1:B:306:VAL:H	1.94	0.66
1:A:342:ARG:HH12	1:B:304:GLU:C	2.04	0.65
1:A:294:ARG:HB3	1:B:342:ARG:HH21	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:THR:HG23	1:D:28:GLU:H	1.63	0.63
1:A:433:LYS:NZ	2:A:600:FBP:O3P	2.31	0.62
1:C:321:GLY:HA3	1:C:443:ARG:HD2	1.81	0.62
1:A:399:ARG:NH2	1:C:396:GLU:OE2	2.34	0.61
1:A:472:VAL:HG21	1:A:496:VAL:HG11	1.82	0.61
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.83	0.61
1:B:403:PRO:O	1:B:404:ILE:HG13	2.01	0.61
1:C:342:ARG:HH12	1:D:306:VAL:HG21	1.66	0.61
1:D:92:ARG:NH1	1:D:235:GLN:O	2.31	0.60
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.85	0.59
1:B:522:THR:HG22	2:B:600:FBP:H4	1.85	0.59
1:D:383:ARG:NH2	3:D:706:HOH:O	2.34	0.58
1:C:92:ARG:NH1	1:C:235:GLN:O	2.31	0.57
1:A:103:ILE:O	1:A:500:ARG:NH2	2.38	0.57
1:B:496:VAL:HG13	1:B:500:ARG:NH1	2.20	0.57
1:B:73:ARG:NH1	1:B:113:ASP:OD2	2.38	0.56
1:A:233:VAL:HG11	1:A:261:LYS:HB3	1.88	0.55
1:C:28:GLU:O	1:C:32:ARG:HG2	2.06	0.55
1:B:329:GLN:HA	1:B:332:GLU:HG2	1.88	0.54
1:B:56:ARG:NH2	1:B:87:THR:OG1	2.40	0.54
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.89	0.54
1:D:73:ARG:NH1	1:D:113:ASP:OD2	2.41	0.54
1:A:445:ARG:HD2	1:A:467:ARG:HH21	1.73	0.53
1:C:342:ARG:CD	1:D:294:ARG:HB3	2.39	0.53
1:A:342:ARG:O	1:A:346:SER:N	2.29	0.53
1:A:294:ARG:HB3	1:B:342:ARG:NH2	2.24	0.53
1:D:274:HIS:CD2	1:D:301:ILE:HG22	2.44	0.53
1:C:31:CYS:HB3	1:D:319:ARG:HH21	1.74	0.53
1:C:73:ARG:NH1	1:C:113:ASP:OD2	2.41	0.53
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.91	0.53
1:D:329:GLN:HA	1:D:332:GLU:HG2	1.91	0.52
1:A:298:GLY:HA3	1:B:342:ARG:HH12	1.74	0.52
1:B:393:GLN:O	1:B:397:GLU:HG3	2.09	0.52
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.44	0.52
1:A:31:CYS:HB3	1:B:319:ARG:HH21	1.73	0.52
1:C:342:ARG:HH22	1:D:298:GLY:HA3	1.75	0.52
1:B:422:ARG:HG3	1:D:414:VAL:HG11	1.93	0.51
1:A:243:SER:HA	1:A:270:LYS:HD3	1.92	0.51
1:A:330:MET:HG3	1:A:348:VAL:HG22	1.92	0.51
1:A:342:ARG:CD	1:B:306:VAL:HB	2.41	0.51
1:A:472:VAL:HG11	1:A:496:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.92	0.51
1:D:40:ILE:O	1:D:40:ILE:HG22	2.11	0.51
1:C:385:ALA:HA	1:D:307:PHE:HZ	1.76	0.51
1:D:330:MET:HG3	1:D:348:VAL:HG22	1.93	0.51
1:B:24:ASP:OD1	1:B:24:ASP:N	2.43	0.50
1:C:329:GLN:HA	1:C:332:GLU:HG2	1.93	0.50
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.95	0.49
1:A:496:VAL:HG13	1:A:500:ARG:NH1	2.27	0.49
1:A:493:ALA:HA	1:A:496:VAL:HB	1.95	0.49
1:D:61:LEU:HD13	1:D:91:VAL:HA	1.95	0.49
1:C:342:ARG:NH1	1:D:306:VAL:HG21	2.28	0.48
1:D:516:ARG:NE	1:D:517:PRO:O	2.41	0.48
1:D:274:HIS:O	1:D:278:ARG:HG3	2.13	0.47
1:A:405:THR:O	1:A:406:SER:OG	2.15	0.47
1:A:307:PHE:HZ	1:B:385:ALA:HA	1.78	0.47
1:B:302:PRO:C	1:B:304:GLU:H	2.22	0.47
1:C:272:GLU:O	1:C:300:GLU:HG3	2.14	0.47
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.97	0.47
1:C:319:ARG:O	1:C:443:ARG:NH1	2.35	0.47
1:C:393:GLN:O	1:C:397:GLU:HG3	2.15	0.47
1:B:496:VAL:HG13	1:B:500:ARG:HH11	1.79	0.46
1:D:311:LYS:NZ	1:D:354:ASP:OD1	2.48	0.46
1:C:307:PHE:HZ	1:D:385:ALA:HA	1.80	0.46
1:A:61:LEU:HD13	1:A:91:VAL:HA	1.96	0.46
1:B:432:THR:OG1	2:B:600:FBP:O5P	2.30	0.46
1:C:61:LEU:HD13	1:C:91:VAL:HA	1.98	0.46
1:B:56:ARG:HH22	1:B:83:TYR:C	2.19	0.46
1:D:63:GLU:HA	1:D:66:LYS:HE3	1.97	0.46
1:A:211:LEU:HD13	1:A:299:ILE:HG21	1.98	0.46
1:C:268:ILE:HD13	1:C:289:GLY:HA3	1.98	0.46
1:A:319:ARG:HH21	1:B:31:CYS:HB3	1.80	0.45
1:A:405:THR:HG21	1:A:410:GLU:HG2	1.99	0.45
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.97	0.45
1:B:453:VAL:HG11	1:B:489:ARG:HB3	1.98	0.45
1:B:463:ALA:HB3	1:B:471:PRO:HB3	1.98	0.45
1:A:56:ARG:NH2	1:A:86:GLU:HB3	2.32	0.45
1:A:268:ILE:HD13	1:A:289:GLY:HA3	1.99	0.45
1:A:329:GLN:HA	1:A:332:GLU:HG2	1.98	0.45
1:A:274:HIS:CE1	1:A:301:ILE:HG22	2.51	0.45
1:A:437:SER:OG	1:A:522:THR:HG21	2.16	0.45
1:A:453:VAL:HG11	1:A:489:ARG:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:O	1:A:342:ARG:HG2	2.17	0.45
1:B:61:LEU:HD13	1:B:91:VAL:HA	1.98	0.45
1:B:268:ILE:HD13	1:B:289:GLY:HA3	1.99	0.45
1:C:319:ARG:C	1:C:443:ARG:HH12	2.23	0.45
1:C:472:VAL:HG21	1:C:496:VAL:HG11	1.98	0.44
1:A:73:ARG:NH1	1:A:113:ASP:OD2	2.50	0.44
1:C:298:GLY:HA3	1:D:342:ARG:HH21	1.82	0.44
1:B:92:ARG:NH1	1:B:235:GLN:O	2.40	0.44
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.99	0.44
1:D:297:LEU:O	1:D:301:ILE:HG12	2.18	0.44
1:D:402:ALA:HA	1:D:403:PRO:HD3	1.87	0.44
1:D:472:VAL:HG21	1:D:496:VAL:HG11	1.99	0.44
1:B:223:GLU:HA	1:B:226:ILE:HD12	2.00	0.43
1:A:92:ARG:NH1	1:A:235:GLN:O	2.40	0.43
1:A:311:LYS:NZ	1:A:354:ASP:OD1	2.51	0.43
1:B:409:THR:HG23	1:B:522:THR:OG1	2.18	0.43
1:C:323:PRO:HD3	1:C:466:TYR:CE2	2.54	0.43
1:C:330:MET:HG3	1:C:348:VAL:HG22	2.00	0.43
1:D:323:PRO:HD3	1:D:466:TYR:CE2	2.54	0.43
1:D:423:CYS:SG	1:D:425:SER:OG	2.77	0.43
1:B:230:LYS:HE3	1:B:257:VAL:O	2.19	0.43
1:A:423:CYS:SG	1:A:425:SER:OG	2.77	0.43
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.89	0.43
1:B:515:TRP:CZ3	1:B:516:ARG:HG3	2.54	0.42
1:C:274:HIS:CE1	1:D:36:ASP:OD1	2.72	0.42
1:A:418:GLU:O	1:A:422:ARG:HG2	2.20	0.42
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.55	0.42
1:C:463:ALA:HB3	1:C:471:PRO:HB3	2.02	0.42
1:C:226:ILE:HG22	1:C:230:LYS:NZ	2.35	0.42
1:B:311:LYS:NZ	1:B:354:ASP:OD1	2.52	0.42
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.55	0.42
1:D:274:HIS:NE2	1:D:301:ILE:HG22	2.34	0.42
1:D:453:VAL:HG11	1:D:489:ARG:HB3	2.02	0.42
1:A:298:GLY:CA	1:B:342:ARG:HH12	2.33	0.42
1:B:370:TYR:HB3	1:B:373:GLU:HB2	2.01	0.41
1:A:514:GLY:CA	1:A:522:THR:HA	2.50	0.41
1:C:40:ILE:HG22	1:C:40:ILE:O	2.21	0.41
1:B:238:ASP:CG	1:B:461:ARG:HE	2.28	0.41
1:A:55:SER:HA	1:A:60:THR:HG21	2.03	0.41
1:B:436:ARG:HE	1:B:436:ARG:HB2	1.67	0.41
1:C:92:ARG:O	1:C:96:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HG3	1:B:348:VAL:HG22	2.01	0.41
1:D:463:ALA:HB3	1:D:471:PRO:HB3	2.03	0.41
1:A:323:PRO:HD3	1:A:466:TYR:CE2	2.55	0.41
1:D:268:ILE:HD13	1:D:289:GLY:HA3	2.03	0.41
1:D:494:MET:HG3	1:D:530:VAL:HG13	2.02	0.41
1:B:302:PRO:O	1:B:304:GLU:N	2.53	0.40
1:D:48:ILE:HG12	1:D:71:VAL:HB	2.03	0.40
1:A:392:LEU:HA	1:A:392:LEU:HD13	1.83	0.40
1:B:40:ILE:O	1:B:40:ILE:HG22	2.22	0.40
1:B:103:ILE:O	1:B:500:ARG:NH1	2.48	0.40
1:B:323:PRO:HD3	1:B:466:TYR:CE2	2.56	0.40
1:D:305:LYS:O	1:D:308:LEU:HB2	2.21	0.40
1:C:103:ILE:HG23	1:C:104:LEU:HG	2.03	0.40
1:D:56:ARG:NH2	1:D:86:GLU:HB3	2.37	0.40
1:D:370:TYR:HB3	1:D:373:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/535 (76%)	393 (97%)	10 (2%)	2 (0%)	24	44
1	B	404/535 (76%)	391 (97%)	8 (2%)	5 (1%)	10	22
1	C	388/535 (72%)	380 (98%)	6 (2%)	2 (0%)	24	44
1	D	404/535 (76%)	397 (98%)	6 (2%)	1 (0%)	43	63
All	All	1601/2140 (75%)	1561 (98%)	30 (2%)	10 (1%)	21	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	404	ILE
1	B	303	ALA
1	B	403	PRO
1	C	406	SER
1	A	212	PRO
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	D	328	THR
1	B	517	PRO

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	339/439 (77%)	323 (95%)	16 (5%)	23	46
1	B	336/439 (76%)	323 (96%)	13 (4%)	28	53
1	C	328/439 (75%)	317 (97%)	11 (3%)	32	58
1	D	337/439 (77%)	325 (96%)	12 (4%)	31	56
All	All	1340/1756 (76%)	1288 (96%)	52 (4%)	28	53

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	59	GLU
1	A	217	ASP
1	A	268	ILE
1	A	274	HIS
1	A	297	LEU
1	A	330	MET
1	A	359	ILE
1	A	386	GLU
1	A	392	LEU
1	A	399	ARG
1	A	496	VAL

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Mol	Chain	Res	Type
1	A	508	VAL
1	A	522	THR
1	A	526	ARG
1	A	528	VAL
1	B	24	ASP
1	B	45	THR
1	B	59	GLU
1	B	230	LYS
1	B	268	ILE
1	B	297	LEU
1	B	330	MET
1	B	359	ILE
1	B	386	GLU
1	B	516	ARG
1	B	522	THR
1	B	526	ARG
1	B	528	VAL
1	C	32	ARG
1	C	45	THR
1	C	86	GLU
1	C	268	ILE
1	C	297	LEU
1	C	330	MET
1	C	359	ILE
1	C	386	GLU
1	C	405	THR
1	C	526	ARG
1	C	528	VAL
1	D	45	THR
1	D	78	HIS
1	D	268	ILE
1	D	297	LEU
1	D	330	MET
1	D	359	ILE
1	D	386	GLU
1	D	422	ARG
1	D	516	ARG
1	D	522	THR
1	D	526	ARG
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	235	GLN
1	B	44	ASN
1	B	78	HIS
1	B	235	GLN
1	B	439	HIS
1	B	464	HIS
1	C	29	HIS
1	C	44	ASN
1	C	227	GLN
1	C	235	GLN
1	C	391	HIS
1	D	29	HIS
1	D	44	ASN
1	D	235	GLN
1	D	350	ASN
1	D	379	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	FBP	A	600	-	18,20,20	0.93	1 (5%)	21,32,32	0.66	0
2	FBP	D	600	-	18,20,20	0.93	1 (5%)	21,32,32	0.69	0
2	FBP	C	600	-	18,20,20	0.94	1 (5%)	21,32,32	0.67	0
2	FBP	B	600	-	18,20,20	0.93	1 (5%)	21,32,32	0.70	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
2	FBP	A	600	-	-	8/13/32/32	0/1/1/1
2	FBP	D	600	-	-	5/13/32/32	0/1/1/1
2	FBP	C	600	-	-	2/13/32/32	0/1/1/1
2	FBP	B	600	-	-	4/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FBP	O2-C2	2.76	1.45	1.40
2	D	600	FBP	O2-C2	2.74	1.45	1.40
2	C	600	FBP	O2-C2	2.73	1.45	1.40
2	B	600	FBP	O2-C2	2.72	1.45	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FBP	C1-O1-P1-O2P
2	A	600	FBP	C1-O1-P1-O3P
2	A	600	FBP	O1-C1-C2-O2
2	A	600	FBP	O1-C1-C2-C3
2	A	600	FBP	O1-C1-C2-O5
2	A	600	FBP	O5-C5-C6-O6
2	B	600	FBP	O1-C1-C2-O2
2	B	600	FBP	O1-C1-C2-O5
2	D	600	FBP	C6-O6-P2-O4P
2	A	600	FBP	C4-C5-C6-O6

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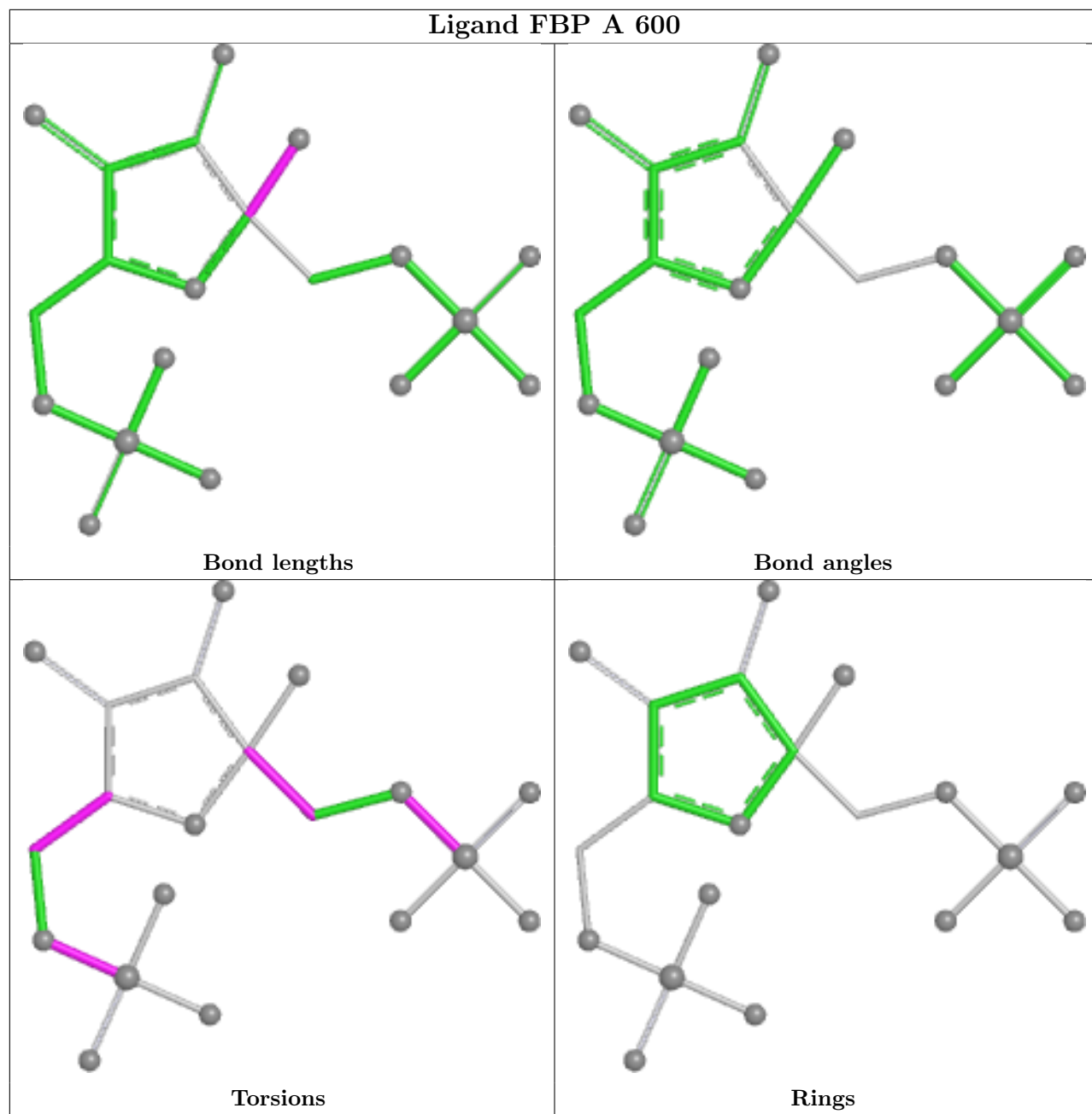
Mol	Chain	Res	Type	Atoms
2	B	600	FBP	C4-C5-C6-O6
2	C	600	FBP	C4-C5-C6-O6
2	D	600	FBP	C4-C5-C6-O6
2	B	600	FBP	O5-C5-C6-O6
2	C	600	FBP	O5-C5-C6-O6
2	D	600	FBP	O5-C5-C6-O6
2	A	600	FBP	C6-O6-P2-O5P
2	D	600	FBP	C1-O1-P1-O1P
2	D	600	FBP	C6-O6-P2-O6P

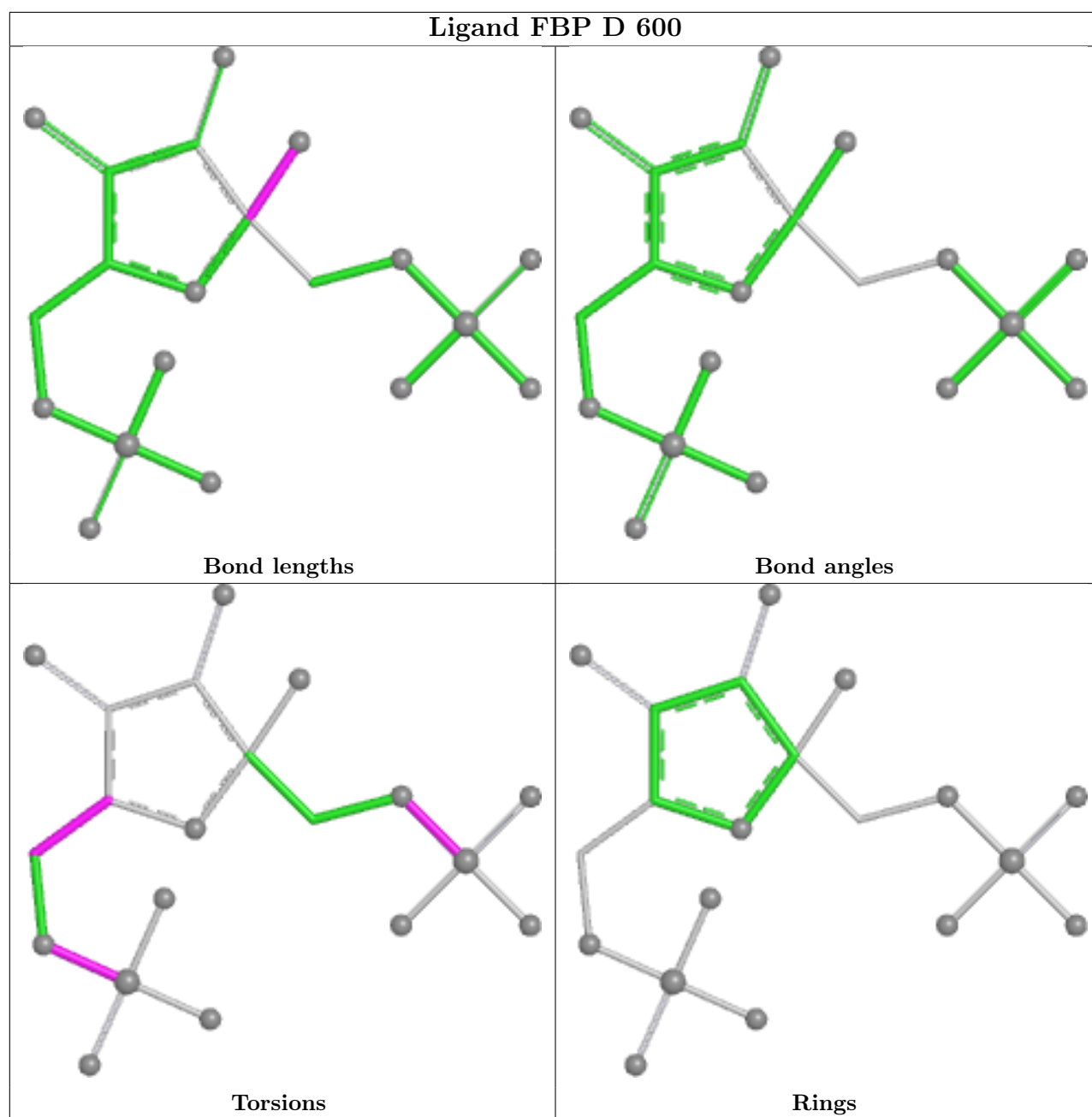
There are no ring outliers.

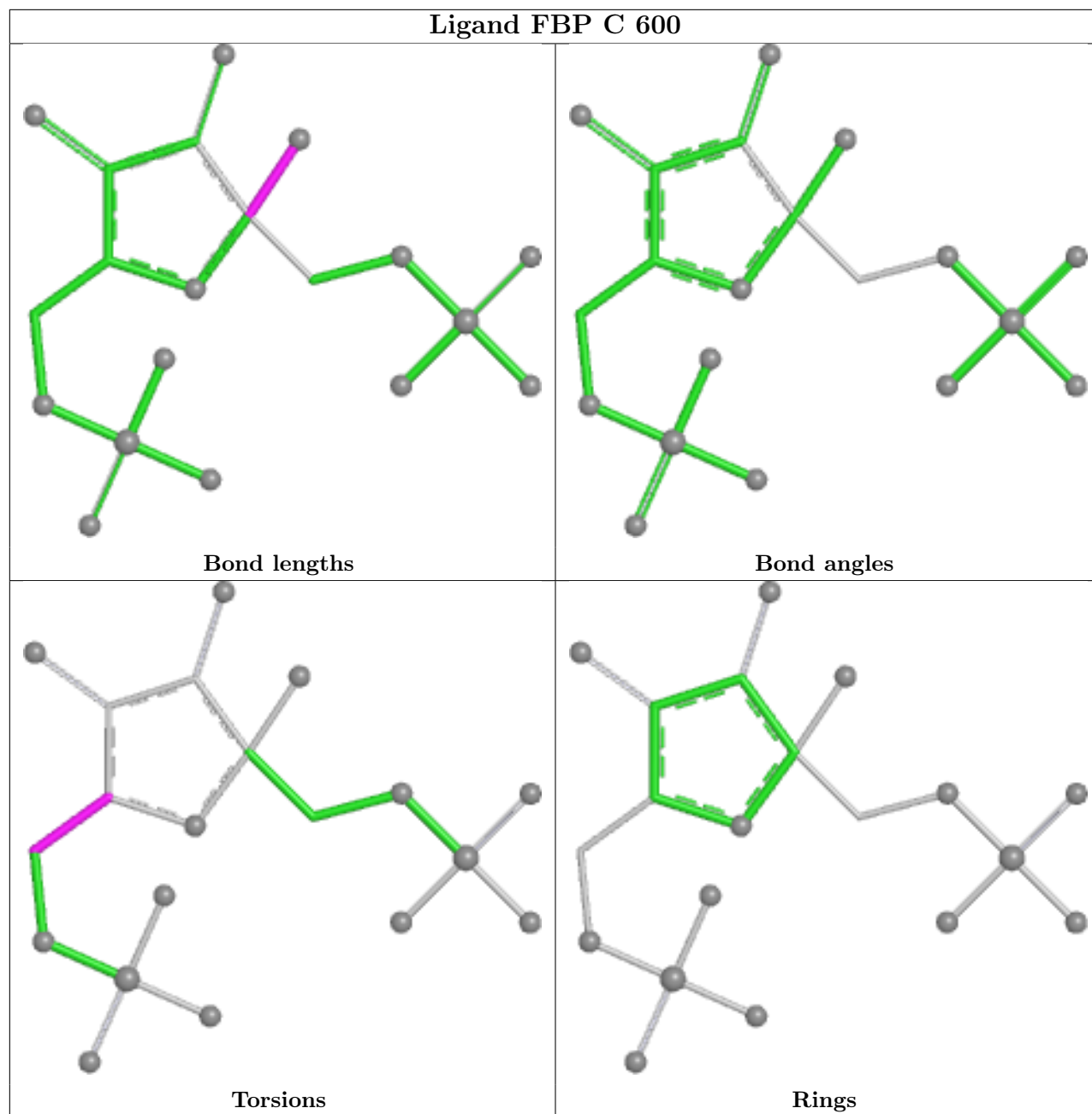
2 monomers are involved in 3 short contacts:

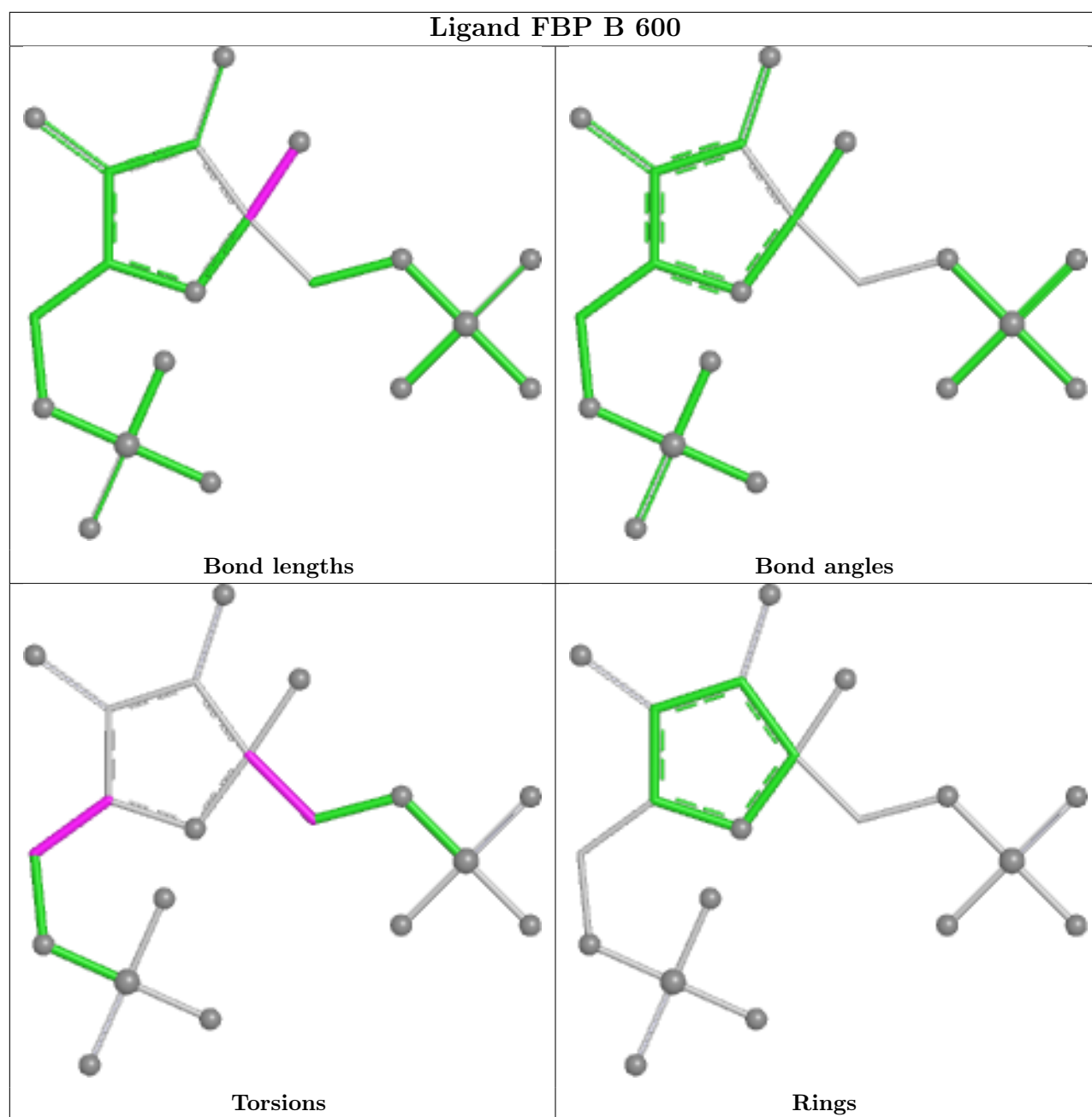
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FBP	1	0
2	B	600	FBP	2	0

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









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	411/535 (76%)	1.39	97 (23%) 2 1	47, 80, 131, 203	0
1	B	408/535 (76%)	1.50	101 (24%) 2 1	55, 88, 134, 167	0
1	C	396/535 (74%)	1.48	92 (23%) 2 1	68, 95, 130, 167	0
1	D	408/535 (76%)	1.29	84 (20%) 2 2	50, 82, 121, 155	0
All	All	1623/2140 (75%)	1.41	374 (23%) 2 2	47, 87, 129, 203	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	ALA	7.2
1	C	220	ALA	6.4
1	B	306	VAL	6.0
1	B	228	ASP	5.8
1	B	37	SER	5.7
1	B	259	GLY	5.3
1	B	303	ALA	5.2
1	A	53	PRO	5.1
1	D	405	THR	5.0
1	B	404	ILE	5.0
1	C	304	GLU	5.0
1	C	401	LEU	4.9
1	D	335	ILE	4.9
1	D	307	PHE	4.8
1	B	405	THR	4.8
1	A	500	ARG	4.8
1	B	220	ALA	4.7
1	C	394	LEU	4.7
1	B	102	PRO	4.6
1	B	250	ASP	4.5
1	D	328	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	117	PRO	4.4
1	B	333	SER	4.2
1	C	41	THR	4.2
1	B	302	PRO	4.2
1	A	375	VAL	4.2
1	B	406	SER	4.2
1	C	117	PRO	4.2
1	A	100	SER	4.1
1	D	106	ARG	4.1
1	D	392	LEU	4.1
1	B	244	PHE	4.1
1	C	262	GLY	4.0
1	A	527	VAL	4.0
1	B	326	CYS	4.0
1	D	90	ASN	4.0
1	A	220	ALA	3.9
1	A	366	ALA	3.9
1	A	210	ASN	3.9
1	D	345	GLY	3.9
1	B	342	ARG	3.9
1	A	482	TRP	3.8
1	C	482	TRP	3.8
1	D	390	TYR	3.8
1	A	342	ARG	3.8
1	B	365	THR	3.8
1	A	377	MET	3.8
1	A	405	THR	3.8
1	A	488	LEU	3.8
1	D	40	ILE	3.7
1	B	274	HIS	3.7
1	B	394	LEU	3.7
1	C	42	ALA	3.6
1	C	411	ALA	3.6
1	A	392	LEU	3.6
1	A	212	PRO	3.6
1	A	343	ALA	3.6
1	D	221	VAL	3.6
1	B	286	ALA	3.6
1	B	517	PRO	3.6
1	B	260	GLU	3.5
1	B	437	SER	3.5
1	A	221	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	531	PRO	3.5
1	D	119	ILE	3.5
1	D	244	PHE	3.5
1	C	250	ASP	3.5
1	C	405	THR	3.4
1	B	258	LEU	3.4
1	D	372	LEU	3.4
1	B	83	TYR	3.4
1	A	106	ARG	3.4
1	A	219	PRO	3.4
1	B	358	CYS	3.4
1	A	217	ASP	3.4
1	A	522	THR	3.4
1	A	299	ILE	3.4
1	B	363	GLY	3.3
1	C	487	ASP	3.3
1	D	491	ASN	3.3
1	D	472	VAL	3.3
1	A	295	GLY	3.3
1	A	483	ALA	3.3
1	A	491	ASN	3.3
1	A	372	LEU	3.3
1	A	111	ALA	3.3
1	B	366	ALA	3.3
1	C	244	PHE	3.3
1	A	373	GLU	3.3
1	C	243	SER	3.2
1	A	415	GLY	3.2
1	B	32	ARG	3.2
1	B	53	PRO	3.2
1	C	473	LEU	3.2
1	B	247	LYS	3.2
1	A	226	ILE	3.2
1	D	37	SER	3.2
1	A	45	THR	3.2
1	B	391	HIS	3.1
1	B	245	ILE	3.1
1	C	40	ILE	3.1
1	D	93	THR	3.1
1	D	436	ARG	3.1
1	A	422	ARG	3.1
1	C	486	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	3.1
1	A	341	THR	3.1
1	D	301	ILE	3.1
1	C	334	MET	3.1
1	A	328	THR	3.0
1	C	340	PRO	3.0
1	C	342	ARG	3.0
1	C	415	GLY	3.0
1	A	393	GLN	3.0
1	A	25	THR	3.0
1	D	84	HIS	3.0
1	C	512	LEU	3.0
1	D	326	CYS	3.0
1	B	40	ILE	3.0
1	B	58	VAL	3.0
1	B	518	GLY	3.0
1	B	268	ILE	3.0
1	B	481	ALA	3.0
1	A	514	GLY	3.0
1	A	40	ILE	2.9
1	C	274	HIS	2.9
1	B	231	PHE	2.9
1	A	326	CYS	2.9
1	C	295	GLY	2.9
1	D	234	GLU	2.9
1	B	341	THR	2.9
1	C	374	ALA	2.9
1	A	52	GLY	2.9
1	B	519	SER	2.9
1	D	404	ILE	2.9
1	D	530	VAL	2.9
1	A	87	THR	2.9
1	B	101	ASP	2.9
1	C	362	SER	2.9
1	B	277	VAL	2.9
1	C	309	ALA	2.9
1	C	483	ALA	2.9
1	A	396	GLU	2.9
1	D	63	GLU	2.9
1	D	386	GLU	2.9
1	C	245	ILE	2.8
1	D	28	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	370	TYR	2.8
1	C	433	LYS	2.8
1	B	237	VAL	2.8
1	D	237	VAL	2.8
1	C	444	TYR	2.8
1	A	467	ARG	2.8
1	C	288	ASP	2.8
1	B	98	PHE	2.8
1	B	427	ALA	2.7
1	D	281	ASP	2.7
1	D	27	LEU	2.7
1	B	343	ALA	2.7
1	B	516	ARG	2.7
1	A	119	ILE	2.7
1	C	428	ILE	2.7
1	A	414	VAL	2.7
1	B	475	LYS	2.7
1	C	481	ALA	2.7
1	D	32	ARG	2.7
1	A	38	PRO	2.7
1	A	456	ASN	2.7
1	D	115	LYS	2.7
1	C	74	LEU	2.7
1	D	225	ASP	2.6
1	D	31	CYS	2.6
1	B	289	GLY	2.6
1	A	331	LEU	2.6
1	B	63	GLU	2.6
1	C	58	VAL	2.6
1	C	277	VAL	2.6
1	D	251	VAL	2.6
1	A	376	ARG	2.6
1	C	408	PRO	2.6
1	B	307	PHE	2.6
1	A	394	LEU	2.6
1	B	221	VAL	2.6
1	D	366	ALA	2.6
1	D	376	ARG	2.6
1	B	478	VAL	2.6
1	D	333	SER	2.6
1	C	261	LYS	2.6
1	C	306	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	430	VAL	2.5
1	A	506	GLY	2.5
1	A	401	LEU	2.5
1	A	503	PHE	2.5
1	B	395	PHE	2.5
1	C	372	LEU	2.5
1	A	58	VAL	2.5
1	A	430	VAL	2.5
1	D	391	HIS	2.5
1	A	485	ASP	2.5
1	C	407	ASP	2.5
1	C	377	MET	2.5
1	D	38	PRO	2.5
1	A	300	GLU	2.5
1	C	275	GLU	2.5
1	C	404	ILE	2.5
1	D	41	THR	2.5
1	D	434	SER	2.5
1	B	466	TYR	2.4
1	A	211	LEU	2.4
1	B	112	LEU	2.4
1	D	231	PHE	2.4
1	A	455	ARG	2.4
1	B	254	VAL	2.4
1	C	273	ASN	2.4
1	D	388	ALA	2.4
1	D	87	THR	2.4
1	D	459	THR	2.4
1	B	373	GLU	2.4
1	C	505	LYS	2.4
1	C	506	GLY	2.4
1	A	296	ASP	2.4
1	B	28	GLU	2.4
1	C	333	SER	2.4
1	D	336	LYS	2.4
1	B	355	GLY	2.4
1	C	459	THR	2.4
1	D	355	GLY	2.4
1	C	307	PHE	2.4
1	A	528	VAL	2.4
1	C	495	ASN	2.4
1	D	373	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	480	GLU	2.4
1	D	341	THR	2.3
1	C	103	ILE	2.3
1	C	488	LEU	2.3
1	A	216	VAL	2.3
1	B	41	THR	2.3
1	A	227	GLN	2.3
1	B	492	PHE	2.3
1	D	89	LYS	2.3
1	D	453	VAL	2.3
1	D	481	ALA	2.3
1	D	450	ILE	2.3
1	A	26	PHE	2.3
1	B	463	ALA	2.3
1	C	38	PRO	2.3
1	D	102	PRO	2.3
1	C	328	THR	2.3
1	A	213	GLY	2.3
1	D	346	SER	2.3
1	D	308	LEU	2.3
1	D	334	MET	2.3
1	A	281	ASP	2.3
1	A	529	PRO	2.3
1	B	340	PRO	2.3
1	B	444	TYR	2.3
1	C	109	ALA	2.2
1	B	227	GLN	2.2
1	C	440	GLN	2.2
1	B	465	LEU	2.2
1	C	222	SER	2.2
1	D	380	LEU	2.2
1	D	407	ASP	2.2
1	A	28	GLU	2.2
1	C	282	GLU	2.2
1	A	278	ARG	2.2
1	A	472	VAL	2.2
1	A	486	VAL	2.2
1	D	529	PRO	2.2
1	A	448	ALA	2.2
1	A	501	GLY	2.2
1	C	514	GLY	2.2
1	A	381	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	222	SER	2.2
1	C	268	ILE	2.2
1	D	222	SER	2.2
1	D	451	ILE	2.2
1	D	296	ASP	2.2
1	A	480	GLU	2.2
1	C	86	GLU	2.2
1	B	246	ARG	2.2
1	C	526	ARG	2.2
1	B	233	VAL	2.2
1	C	441	VAL	2.2
1	B	328	THR	2.2
1	B	370	TYR	2.2
1	B	459	THR	2.2
1	D	298	GLY	2.2
1	B	299	ILE	2.2
1	A	333	SER	2.2
1	C	420	SER	2.2
1	C	101	ASP	2.2
1	C	223	GLU	2.2
1	C	467	ARG	2.2
1	C	44	ASN	2.2
1	C	409	THR	2.2
1	D	229	LEU	2.2
1	A	307	PHE	2.2
1	B	263	LYS	2.2
1	B	472	VAL	2.1
1	D	306	VAL	2.1
1	C	90	ASN	2.1
1	D	329	GLN	2.1
1	B	501	GLY	2.1
1	C	289	GLY	2.1
1	D	52	GLY	2.1
1	C	113	ASP	2.1
1	D	531	PRO	2.1
1	D	440	GLN	2.1
1	A	94	ALA	2.1
1	C	111	ALA	2.1
1	A	454	THR	2.1
1	A	447	ARG	2.1
1	D	118	GLU	2.1
1	B	420	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	458	GLN	2.1
1	B	329	GLN	2.1
1	C	442	ALA	2.1
1	A	273	ASN	2.1
1	A	365	THR	2.1
1	B	79	GLY	2.1
1	B	114	THR	2.1
1	B	106	ARG	2.1
1	A	253	GLU	2.1
1	A	301	ILE	2.1
1	B	332	GLU	2.1
1	A	370	TYR	2.1
1	C	305	LYS	2.1
1	C	475	LYS	2.1
1	C	504	LYS	2.1
1	C	77	SER	2.1
1	D	425	SER	2.1
1	A	274	HIS	2.1
1	B	479	GLN	2.1
1	B	71	VAL	2.1
1	C	366	ALA	2.1
1	B	90	ASN	2.1
1	B	273	ASN	2.1
1	B	56	ARG	2.1
1	B	361	LEU	2.1
1	C	418	GLU	2.1
1	D	344	GLU	2.1
1	B	301	ILE	2.1
1	C	226	ILE	2.1
1	A	62	LYS	2.1
1	B	224	LYS	2.1
1	A	478	VAL	2.0
1	B	508	VAL	2.0
1	C	453	VAL	2.0
1	C	445	ARG	2.0
1	D	516	ARG	2.0
1	C	398	LEU	2.0
1	A	386	GLU	2.0
1	B	118	GLU	2.0
1	B	480	GLU	2.0
1	B	226	ILE	2.0
1	D	230	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	36	ASP	2.0
1	A	30	MET	2.0
1	A	406	SER	2.0
1	D	67	SER	2.0
1	D	424	CYS	2.0
1	A	218	LEU	2.0
1	A	481	ALA	2.0
1	A	484	GLU	2.0
1	B	285	GLU	2.0
1	C	104	LEU	2.0
1	C	79	GLY	2.0
1	D	435	GLY	2.0
1	A	450	ILE	2.0
1	C	365	THR	2.0
1	C	330	MET	2.0
1	D	457	PRO	2.0
1	B	287	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

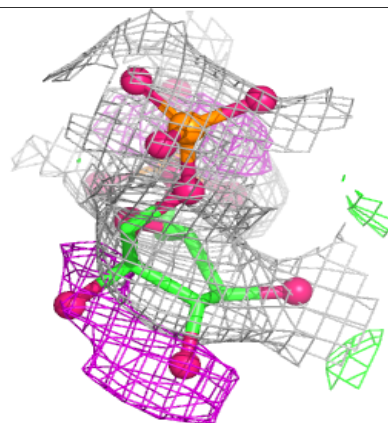
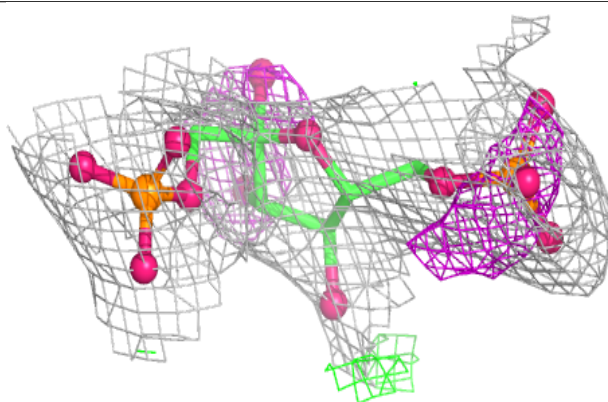
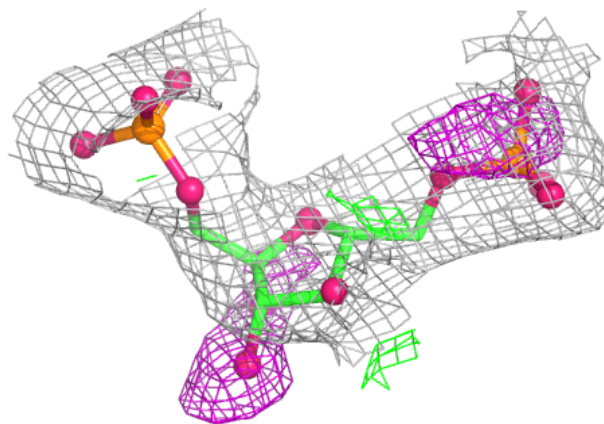
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	C	600	20/20	0.81	0.14	78,86,103,112	0
2	FBP	A	600	20/20	0.89	0.12	70,90,100,102	0
2	FBP	B	600	20/20	0.91	0.15	59,74,94,99	0
2	FBP	D	600	20/20	0.93	0.12	54,66,83,89	0

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.

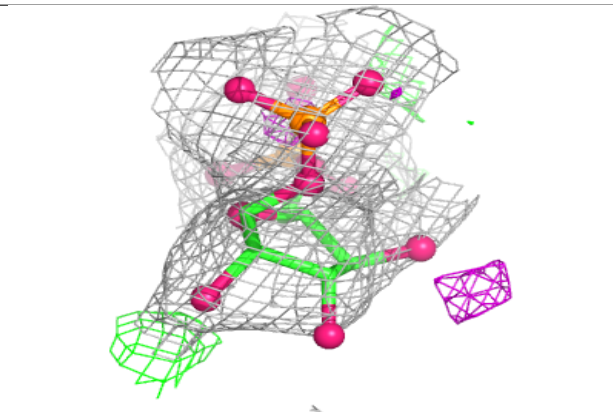
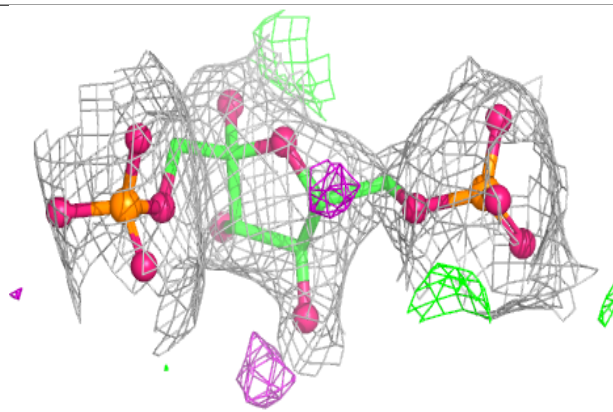
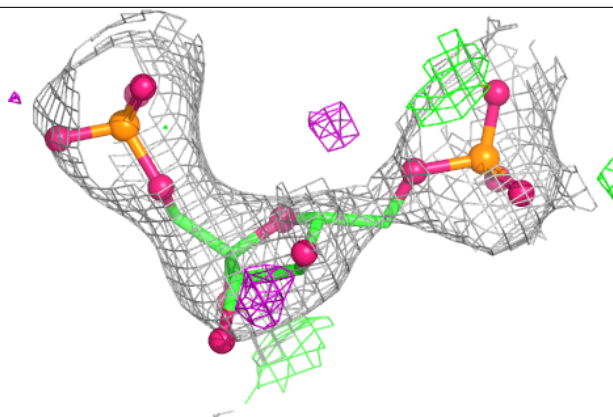
Electron density around FBP C 600:

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

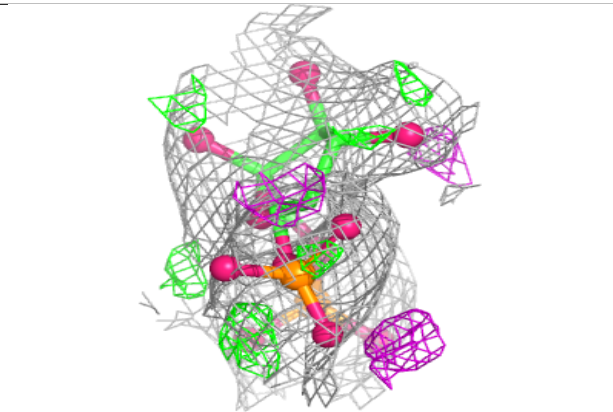
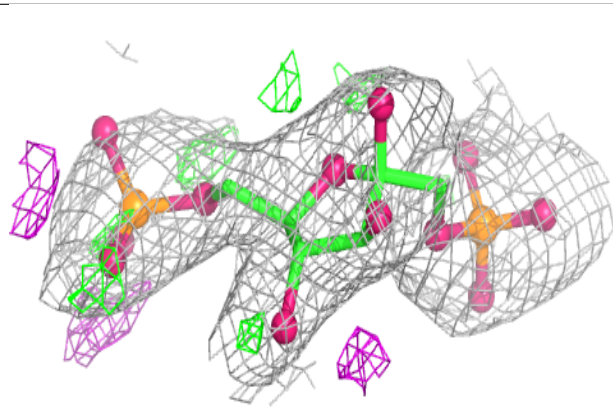
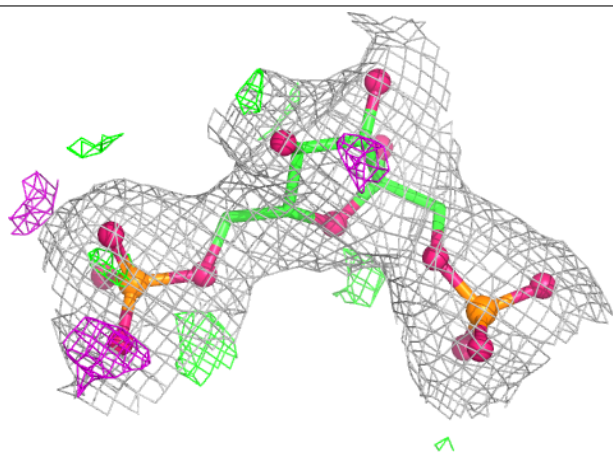


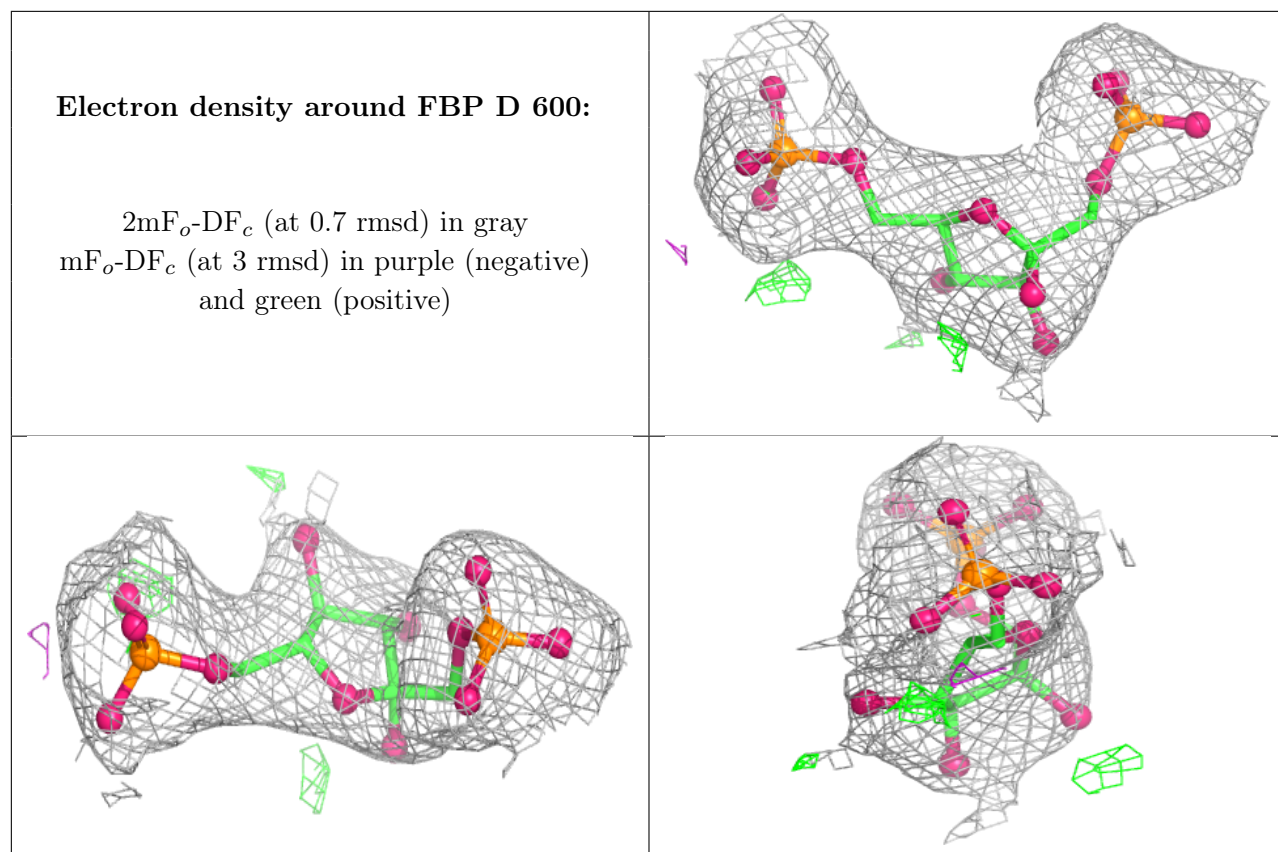
Electron density around FBP A 600:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.