



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:14 AM UTC

PDB ID : 5X0I / pdb_00005x0i
Title : Crystal structure of PKM2 R399E mutant complexed with FBP and serine
Authors : Wang, W.C.; Chen, T.J.
Deposited on : 2017-01-20
Resolution : 2.64 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

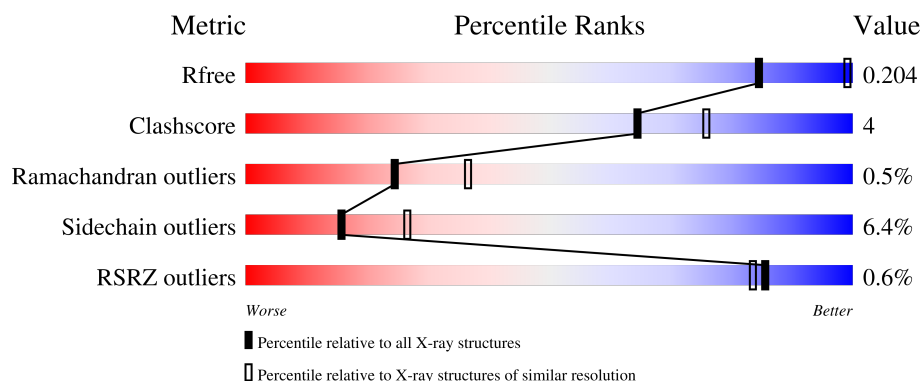
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	551	
1	B	551	
1	C	551	
1	D	551	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PYR	D	603	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16023 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	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			
1	B	515	Total	C	N	O	S	0	0	0
			3949	2484	698	742	25			
1	C	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			
1	D	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			

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	399	GLU	ARG	engineered mutation	UNP P14618

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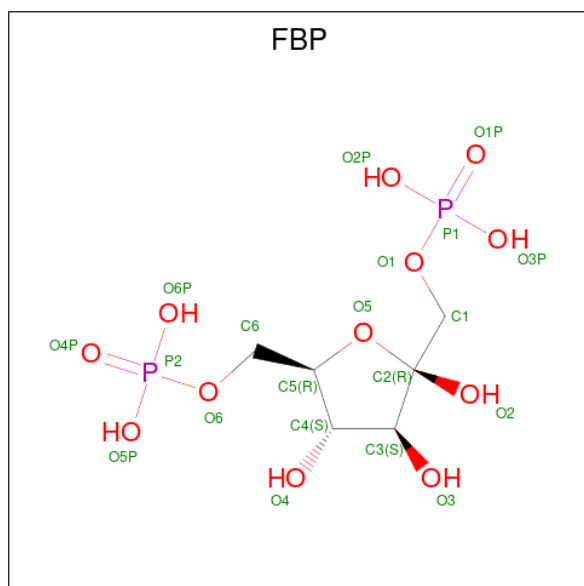
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	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	399	GLU	ARG	engineered mutation	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	399	GLU	ARG	engineered mutation	UNP P14618

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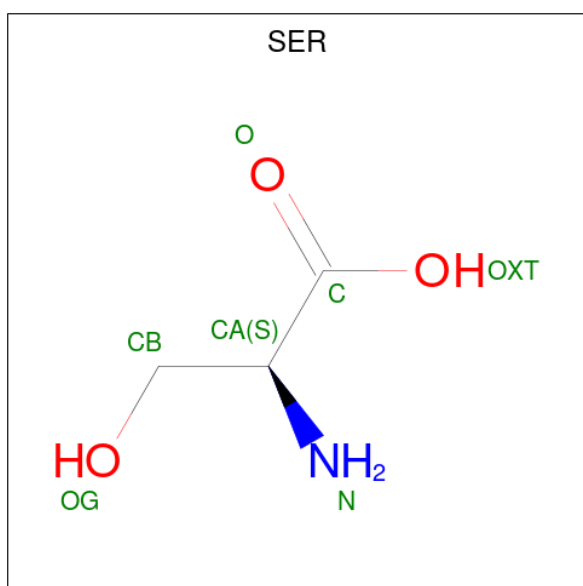
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	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	399	GLU	ARG	engineered mutation	UNP P14618

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



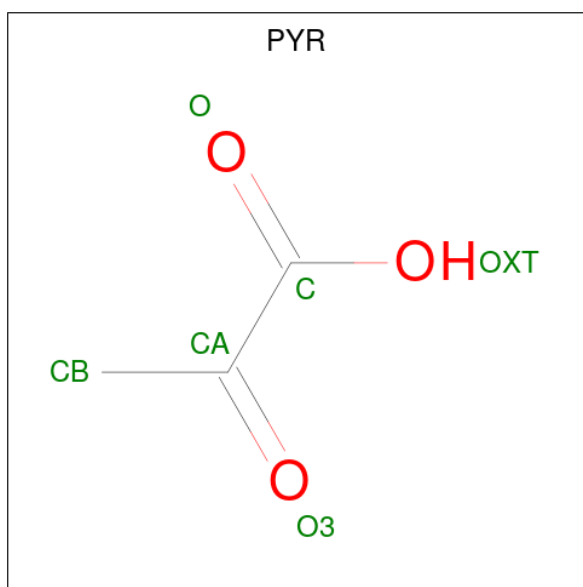
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



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

- Molecule 4 is PYRUVIC ACID (CCD ID: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		

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

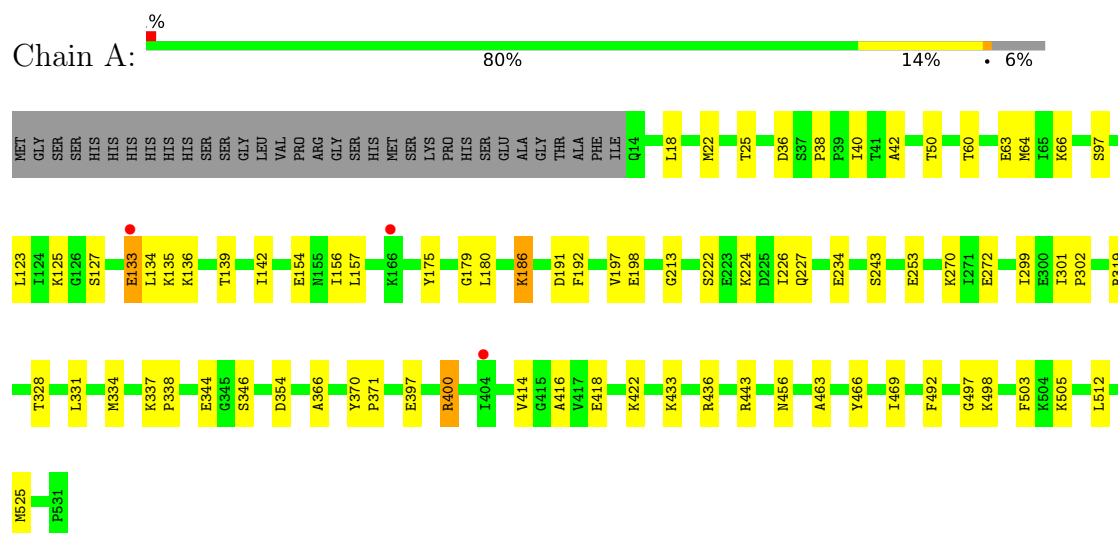
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	13	Total O 13 13	0	0
7	B	13	Total O 13 13	0	0
7	C	9	Total O 9 9	0	0
7	D	10	Total O 10 10	0	0

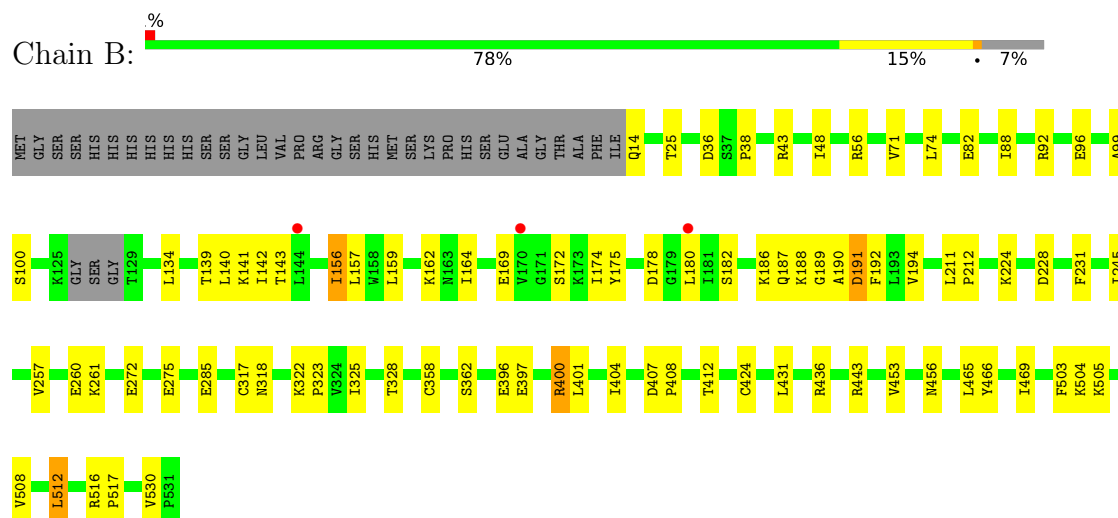
3 Residue-property plots [i](#)

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

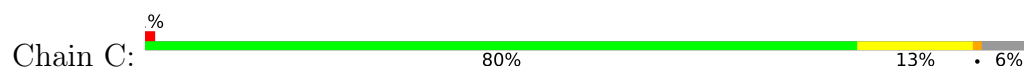
• Molecule 1: Pyruvate kinase PKM

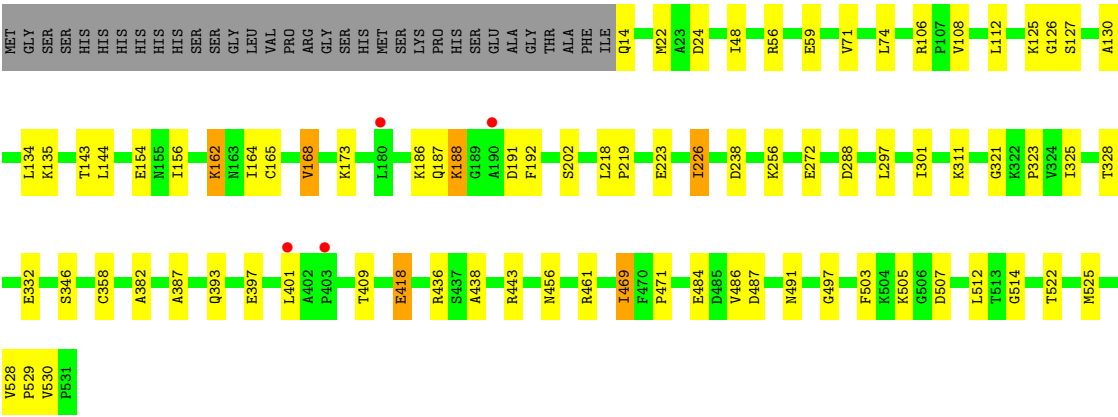


• Molecule 1: Pyruvate kinase PKM

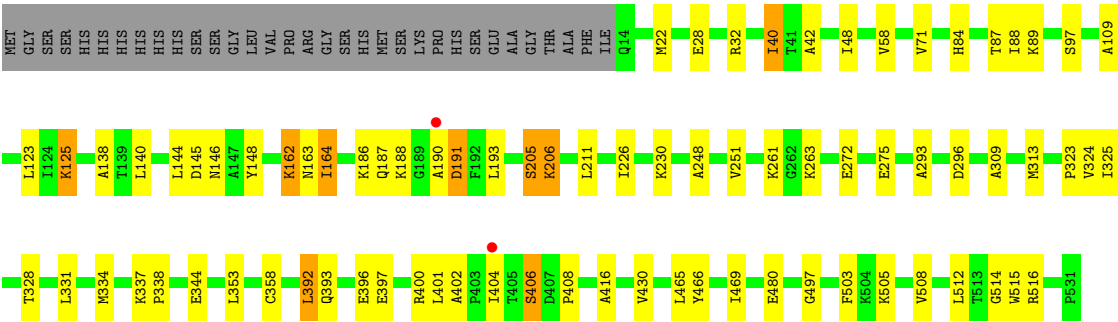
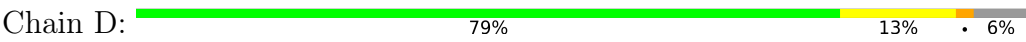


• Molecule 1: Pyruvate kinase PKM





● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.60Å 137.88Å 149.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.64 30.00 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.64) 99.9 (30.00-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.180 , 0.218 0.186 , 0.204	Depositor DCC
R_{free} test set	3616 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 18.5	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	0.95	EDS
Total number of atoms	16023	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.21	4/4027 (0.1%)	0.97	3/5439 (0.1%)
1	B	1.18	6/4012 (0.1%)	0.94	0/5418
1	C	1.12	4/4027 (0.1%)	0.94	2/5439 (0.0%)
1	D	1.12	0/4027	0.94	3/5439 (0.1%)
All	All	1.16	14/16093 (0.1%)	0.95	8/21735 (0.0%)

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

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	SER	CA-C	8.73	1.56	1.52
1	B	318	ASN	C-O	-7.74	1.15	1.24
1	C	226	ILE	CA-CB	6.50	1.62	1.54
1	B	257	VAL	C-O	-5.79	1.17	1.24
1	C	387	ALA	CA-C	5.43	1.60	1.52
1	A	492	PHE	C-O	-5.37	1.17	1.24
1	A	186	LYS	CA-C	5.30	1.59	1.52
1	A	354	ASP	C-O	-5.23	1.17	1.24
1	C	382	ALA	CA-C	-5.23	1.46	1.52
1	B	453	VAL	C-O	-5.17	1.18	1.24
1	B	88	ILE	C-O	-5.12	1.18	1.24
1	C	108	VAL	C-O	-5.09	1.18	1.24
1	A	197	VAL	C-O	-5.08	1.18	1.24
1	B	245	ILE	N-CA	-5.05	1.40	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ILE	N-CA-C	-6.68	106.49	111.90
1	D	211	LEU	CA-C-N	6.49	125.99	119.24
1	D	211	LEU	C-N-CA	6.49	125.99	119.24
1	D	226	ILE	CB-CA-C	-6.25	103.88	111.88
1	A	192	PHE	N-CA-C	6.12	118.16	108.79
1	C	164	ILE	N-CA-C	5.93	117.38	110.62
1	A	346	SER	N-CA-C	5.46	117.23	111.28
1	C	192	PHE	N-CA-C	5.28	116.87	108.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3963	0	4041	34	0
1	B	3949	0	4029	36	0
1	C	3963	0	4041	32	0
1	D	3963	0	4041	32	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	1	0
2	D	20	0	10	1	0
3	A	7	0	4	0	0
3	B	7	0	4	1	0
3	C	7	0	4	0	0
3	D	7	0	4	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
4	D	6	0	0	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	13	0	0	0	0
7	B	13	0	0	0	0
7	C	9	0	0	0	0
7	D	10	0	0	0	0
All	All	16023	0	16208	124	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 (124) 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:525:MET:HE3	1:C:525:MET:HE3	1.71	0.72
1:A:136:LYS:HG3	1:A:198:GLU:O	1.89	0.72
1:C:106:ARG:NH2	1:C:471:PRO:O	2.24	0.71
1:A:133:GLU:O	1:A:133:GLU:HG2	1.92	0.68
1:B:412:THR:HG22	1:B:512:LEU:HD21	1.74	0.68
1:C:218:LEU:O	1:C:219:PRO:C	2.37	0.66
1:D:123:LEU:HA	1:D:205:SER:HB3	1.82	0.61
1:D:515:TRP:CE3	1:D:516:ARG:HG2	2.35	0.61
1:D:323:PRO:HB3	1:D:465:LEU:O	2.00	0.60
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.84	0.59
1:B:143:THR:HA	1:B:191:ASP:O	2.02	0.59
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.87	0.57
1:D:515:TRP:CD2	1:D:516:ARG:HG2	2.40	0.56
1:C:393:GLN:O	1:C:397:GLU:HG3	2.06	0.56
1:A:243:SER:HA	1:A:270:LYS:HD3	1.89	0.55
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.42	0.55
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.42	0.54
1:A:370:TYR:N	1:A:371:PRO:CD	2.71	0.54
1:C:238:ASP:OD1	1:C:461:ARG:NE	2.40	0.54
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.90	0.52
1:B:92:ARG:O	1:B:96:GLU:HG2	2.10	0.52
1:A:334:MET:HA	1:A:337:LYS:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLU:CD	1:B:25:THR:HB	2.35	0.51
1:A:50:THR:HG22	1:A:366:ALA:HB2	1.91	0.51
1:B:99:ALA:O	1:B:100:SER:C	2.54	0.51
1:D:393:GLN:O	1:D:397:GLU:HG3	2.11	0.51
1:B:323:PRO:HB3	1:B:465:LEU:O	2.12	0.50
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.92	0.50
1:C:165:CYS:O	1:C:188:LYS:CE	2.60	0.50
1:D:28:GLU:O	1:D:32:ARG:HG3	2.11	0.50
1:C:311:LYS:HE3	1:D:353:LEU:CD1	2.41	0.50
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.94	0.50
1:D:514:GLY:HA3	2:D:601:FBP:O3	2.11	0.50
1:B:82:GLU:OE2	1:B:82:GLU:HA	2.11	0.50
1:D:145:ASP:HB3	1:D:148:TYR:HD2	1.77	0.49
1:A:525:MET:HE3	1:C:525:MET:CE	2.42	0.49
1:C:321:GLY:HA2	1:C:443:ARG:HG2	1.94	0.49
1:A:331:LEU:HD23	1:A:344:GLU:HB3	1.95	0.49
1:B:516:ARG:HB2	1:B:517:PRO:CD	2.43	0.48
1:A:226:ILE:O	1:A:227:GLN:C	2.54	0.48
1:D:309:ALA:HB1	1:D:313:MET:HE2	1.96	0.48
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.96	0.48
1:B:175:TYR:HE2	1:B:212:PRO:HG3	1.79	0.48
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.96	0.47
1:C:486:VAL:O	1:C:487:ASP:C	2.57	0.47
1:A:36:ASP:O	1:A:38:PRO:HD3	2.15	0.47
1:C:288:ASP:O	1:C:323:PRO:HD2	2.14	0.47
1:A:25:THR:HB	1:B:397:GLU:HG2	1.96	0.47
1:D:205:SER:O	1:D:206:LYS:HB2	2.15	0.47
1:D:272:GLU:HB3	1:D:293:ALA:HB3	1.96	0.47
1:A:443:ARG:O	1:A:443:ARG:HG2	2.15	0.47
1:A:22:MET:HA	1:A:22:MET:HE2	1.98	0.46
1:C:528:VAL:HG12	1:C:529:PRO:O	2.16	0.46
1:C:321:GLY:HA3	1:C:443:ARG:HD3	1.98	0.46
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.98	0.46
1:D:325:ILE:HG12	1:D:358:CYS:HB2	1.98	0.46
1:B:400:ARG:CZ	1:D:392:LEU:HD21	2.46	0.45
1:A:418:GLU:HG2	1:C:418:GLU:OE1	2.17	0.45
1:D:144:LEU:HD13	1:D:162:LYS:O	2.17	0.45
1:A:25:THR:HB	1:B:397:GLU:CG	2.46	0.45
1:A:416:ALA:HB2	1:A:512:LEU:HD11	1.98	0.45
1:C:127:SER:HB3	1:C:130:ALA:HB2	1.98	0.45
1:B:516:ARG:HB2	1:B:517:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:ALA:HB2	1:D:512:LEU:HD11	1.99	0.45
1:B:456:ASN:OD1	1:B:456:ASN:C	2.60	0.44
1:B:36:ASP:O	1:B:38:PRO:HD3	2.17	0.44
1:C:409:THR:HG23	1:C:522:THR:HB	1.99	0.44
1:D:40:ILE:HD12	1:D:42:ALA:HB3	1.99	0.44
1:A:337:LYS:HD2	1:B:180:LEU:HD22	1.98	0.44
1:B:188:LYS:HG2	1:B:189:GLY:H	1.82	0.44
1:D:190:ALA:O	1:D:191:ASP:CB	2.65	0.44
1:C:321:GLY:CA	1:C:443:ARG:HG2	2.48	0.44
1:C:438:ALA:HB1	1:C:469:ILE:HD13	1.99	0.44
1:B:141:LYS:HB3	1:B:156:ILE:HD13	1.99	0.43
1:B:228:ASP:O	1:B:231:PHE:HB3	2.18	0.43
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.01	0.43
1:C:514:GLY:HA3	2:C:601:FBP:O3	2.17	0.43
1:D:296:ASP:OD2	4:D:603:PYR:O	2.35	0.43
1:B:407:ASP:HA	1:B:408:PRO:HD2	1.90	0.43
1:B:325:ILE:HG12	1:B:358:CYS:HB2	2.00	0.43
1:A:136:LYS:CG	1:A:198:GLU:O	2.63	0.43
1:B:174:ILE:HG12	1:B:211:LEU:CD2	2.49	0.43
1:B:186:LYS:O	1:B:187:GLN:HG2	2.19	0.43
1:C:456:ASN:OD1	1:C:456:ASN:C	2.61	0.43
1:D:248:ALA:O	1:D:251:VAL:N	2.51	0.43
1:B:436:ARG:HG2	1:B:436:ARG:HH11	1.83	0.43
1:D:406:SER:O	1:D:408:PRO:HD3	2.19	0.43
1:D:71:VAL:HG22	1:D:109:ALA:HB3	2.00	0.43
1:B:503:PHE:CD1	1:B:530:VAL:HG21	2.53	0.42
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.53	0.42
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.49	0.42
1:A:301:ILE:HB	1:A:302:PRO:HD2	2.02	0.42
1:A:338:PRO:HB3	1:A:370:TYR:CE1	2.55	0.42
1:A:142:ILE:HA	1:A:157:LEU:O	2.20	0.42
1:C:112:LEU:C	1:C:112:LEU:HD23	2.45	0.42
1:D:84:HIS:O	1:D:87:THR:N	2.50	0.42
1:A:222:SER:O	1:A:226:ILE:HG13	2.19	0.42
1:A:456:ASN:C	1:A:456:ASN:OD1	2.63	0.42
1:D:164:ILE:HD12	1:D:193:LEU:HD11	2.02	0.42
1:B:14:GLN:O	1:B:14:GLN:HG3	2.20	0.42
1:C:168:VAL:O	1:C:188:LYS:HE3	2.20	0.42
1:C:297:LEU:O	1:C:301:ILE:HG12	2.19	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.84	0.41
1:B:48:ILE:HG12	1:B:71:VAL:HB	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:CYS:HB3	1:B:322:LYS:O	2.20	0.41
1:C:507:ASP:O	1:C:530:VAL:HG23	2.20	0.41
1:D:401:LEU:O	1:D:402:ALA:C	2.61	0.41
1:A:400:ARG:NH2	1:C:22:MET:O	2.53	0.41
1:B:175:TYR:CE2	1:B:212:PRO:HG3	2.55	0.41
1:C:332:GLU:HA	1:C:332:GLU:OE1	2.20	0.41
1:D:334:MET:HE3	1:D:338:PRO:O	2.21	0.41
1:B:142:ILE:O	1:B:192:PHE:HA	2.20	0.41
1:B:140:LEU:HD21	1:B:157:LEU:HD22	2.03	0.41
1:D:88:ILE:O	1:D:89:LYS:C	2.62	0.41
1:B:190:ALA:O	1:B:191:ASP:CB	2.68	0.41
1:A:40:ILE:HD12	1:A:42:ALA:HB3	2.02	0.41
1:B:178:ASP:OD1	1:B:178:ASP:N	2.53	0.41
1:C:144:LEU:HD13	1:C:162:LYS:O	2.20	0.41
1:C:223:GLU:OE2	1:C:223:GLU:N	2.49	0.41
1:D:125:LYS:H	1:D:125:LYS:HG3	1.71	0.41
1:B:159:LEU:HD12	1:B:164:ILE:CD1	2.51	0.40
1:C:143:THR:HG21	1:C:156:ILE:HD11	2.04	0.40
1:B:43:ARG:O	3:B:602:SER:HB2	2.21	0.40
1:A:60:THR:O	1:A:64:MET:HG2	2.21	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	516/551 (94%)	493 (96%)	22 (4%)	1 (0%)	43	58
1	B	511/551 (93%)	490 (96%)	19 (4%)	2 (0%)	30	42
1	C	516/551 (94%)	494 (96%)	19 (4%)	3 (1%)	21	31
1	D	516/551 (94%)	487 (94%)	25 (5%)	4 (1%)	16	24
All	All	2059/2204 (93%)	1964 (95%)	85 (4%)	10 (0%)	24	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	D	191	ASP
1	C	125	LYS
1	D	138	ALA
1	B	191	ASP
1	C	126	GLY
1	C	328	THR
1	D	206	LYS
1	D	328	THR
1	B	328	THR

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	426/453 (94%)	401 (94%)	25 (6%)	18	29
1	B	425/453 (94%)	398 (94%)	27 (6%)	16	26
1	C	426/453 (94%)	398 (93%)	28 (7%)	15	25
1	D	426/453 (94%)	397 (93%)	29 (7%)	14	23
All	All	1703/1812 (94%)	1594 (94%)	109 (6%)	16	26

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	A	123	LEU
1	A	125	LYS
1	A	127	SER
1	A	133	GLU
1	A	134	LEU
1	A	135	LYS
1	A	139	THR
1	A	154	GLU
1	A	156	ILE

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Mol	Chain	Res	Type
1	A	180	LEU
1	A	186	LYS
1	A	191	ASP
1	A	224	LYS
1	A	234	GLU
1	A	253	GLU
1	A	272	GLU
1	A	319	ARG
1	A	400	ARG
1	A	414	VAL
1	A	422	LYS
1	A	433	LYS
1	A	436	ARG
1	A	498	LYS
1	A	505	LYS
1	B	56	ARG
1	B	74	LEU
1	B	134	LEU
1	B	139	THR
1	B	156	ILE
1	B	162	LYS
1	B	169	GLU
1	B	172	SER
1	B	182	SER
1	B	194	VAL
1	B	224	LYS
1	B	260	GLU
1	B	261	LYS
1	B	272	GLU
1	B	275	GLU
1	B	285	GLU
1	B	396	GLU
1	B	400	ARG
1	B	401	LEU
1	B	404	ILE
1	B	424	CYS
1	B	431	LEU
1	B	443	ARG
1	B	504	LYS
1	B	505	LYS
1	B	508	VAL
1	B	512	LEU

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Mol	Chain	Res	Type
1	C	14	GLN
1	C	24	ASP
1	C	56	ARG
1	C	59	GLU
1	C	74	LEU
1	C	134	LEU
1	C	135	LYS
1	C	154	GLU
1	C	162	LYS
1	C	168	VAL
1	C	173	LYS
1	C	186	LYS
1	C	187	GLN
1	C	188	LYS
1	C	191	ASP
1	C	202	SER
1	C	226	ILE
1	C	256	LYS
1	C	272	GLU
1	C	346	SER
1	C	401	LEU
1	C	418	GLU
1	C	436	ARG
1	C	469	ILE
1	C	484	GLU
1	C	491	ASN
1	C	505	LYS
1	C	512	LEU
1	D	22	MET
1	D	40	ILE
1	D	58	VAL
1	D	97	SER
1	D	125	LYS
1	D	140	LEU
1	D	146	ASN
1	D	162	LYS
1	D	163	ASN
1	D	164	ILE
1	D	186	LYS
1	D	187	GLN
1	D	188	LYS
1	D	205	SER

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Mol	Chain	Res	Type
1	D	230	LYS
1	D	261	LYS
1	D	263	LYS
1	D	275	GLU
1	D	324	VAL
1	D	337	LYS
1	D	392	LEU
1	D	396	GLU
1	D	400	ARG
1	D	404	ILE
1	D	406	SER
1	D	430	VAL
1	D	480	GLU
1	D	505	LYS
1	D	508	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	378	GLN
1	B	78	HIS
1	B	227	GLN
1	B	391	HIS
1	C	155	ASN
1	C	184	GLN
1	C	439	HIS
1	D	155	ASN
1	D	187	GLN
1	D	318	ASN
1	D	458	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SER	B	602	-	4,6,6	0.70	0	2,7,7	1.92	1 (50%)
4	PYR	D	603	5	5,5,5	1.94	1 (20%)	3,6,6	2.38	1 (33%)
4	PYR	A	603	5	5,5,5	1.73	1 (20%)	3,6,6	0.83	0
3	SER	A	602	-	4,6,6	0.85	0	2,7,7	2.42	1 (50%)
2	FBP	B	601	-	18,20,20	0.76	0	21,32,32	1.15	3 (14%)
3	SER	C	602	-	4,6,6	1.30	1 (25%)	2,7,7	2.50	1 (50%)
2	FBP	D	601	-	18,20,20	1.01	1 (5%)	21,32,32	1.24	3 (14%)
4	PYR	B	603	5	5,5,5	1.54	1 (20%)	3,6,6	1.42	0
2	FBP	A	601	-	18,20,20	0.67	0	21,32,32	1.33	2 (9%)
2	FBP	C	601	-	18,20,20	0.78	0	21,32,32	1.27	3 (14%)
3	SER	D	602	-	4,6,6	0.98	0	2,7,7	2.79	1 (50%)
4	PYR	C	603	5	5,5,5	1.44	0	3,6,6	2.06	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SER	B	602	-	-	0/6/6/6	-
4	PYR	D	603	5	-	4/4/4/4	-
4	PYR	A	603	5	-	0/4/4/4	-
3	SER	A	602	-	-	0/6/6/6	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SER	C	602	-	-	0/6/6/6	-
2	FBP	D	601	-	-	3/13/32/32	0/1/1/1
4	PYR	B	603	5	-	0/4/4/4	-
2	FBP	A	601	-	-	9/13/32/32	0/1/1/1
2	FBP	C	601	-	-	5/13/32/32	0/1/1/1
3	SER	D	602	-	-	0/6/6/6	-
4	PYR	C	603	5	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	PYR	CA-C	-3.86	1.41	1.54
4	A	603	PYR	CA-C	-2.94	1.44	1.54
4	B	603	PYR	CA-C	-2.64	1.45	1.54
3	C	602	SER	OXT-C	-2.32	1.23	1.30
2	D	601	FBP	O5-C2	2.25	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	SER	OXT-C-O	-3.93	115.16	124.08
4	D	603	PYR	O3-CA-CB	3.64	127.93	119.77
3	C	602	SER	OXT-C-O	-3.53	116.06	124.08
3	A	602	SER	OXT-C-O	-3.41	116.34	124.08
2	A	601	FBP	O6P-P2-O5P	3.33	120.31	107.80
2	D	601	FBP	O3P-P1-O1	-2.79	99.39	106.67
4	C	603	PYR	OXT-C-CA	2.73	121.15	113.59
2	A	601	FBP	O5P-P2-O6	-2.67	99.70	106.67
3	B	602	SER	OXT-C-O	-2.65	118.06	124.08
2	B	601	FBP	O3P-P1-O1	-2.61	99.87	106.67
2	B	601	FBP	O3P-P1-O2P	2.47	117.06	107.80
2	D	601	FBP	O6P-P2-O5P	2.41	116.86	107.80
2	D	601	FBP	O3P-P1-O2P	2.33	116.53	107.80
2	C	601	FBP	O3P-P1-O1	-2.31	100.65	106.67
2	C	601	FBP	O3P-P1-O2P	2.19	116.01	107.80
2	C	601	FBP	O6P-P2-O5P	2.16	115.89	107.80
2	B	601	FBP	O6P-P2-O5P	2.05	115.50	107.80

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O1P
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	C	601	FBP	C1-O1-P1-O1P
4	D	603	PYR	O-C-CA-CB
4	D	603	PYR	OXT-C-CA-CB
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	C	601	FBP	C1-O1-P1-O3P
4	D	603	PYR	OXT-C-CA-O3
2	A	601	FBP	C6-O6-P2-O4P
2	D	601	FBP	C6-O6-P2-O4P
2	C	601	FBP	C1-O1-P1-O2P
4	D	603	PYR	O-C-CA-O3

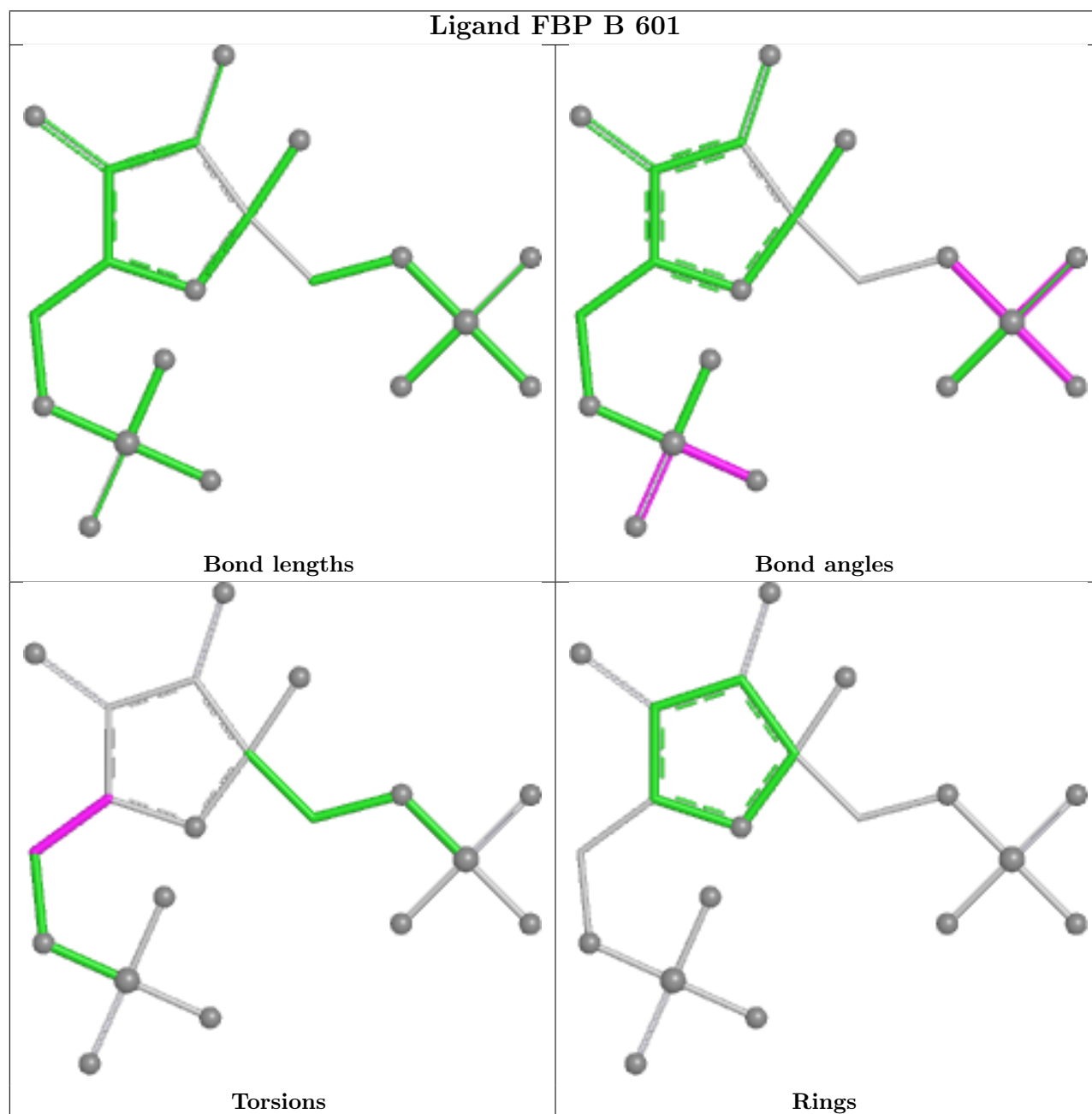
There are no ring outliers.

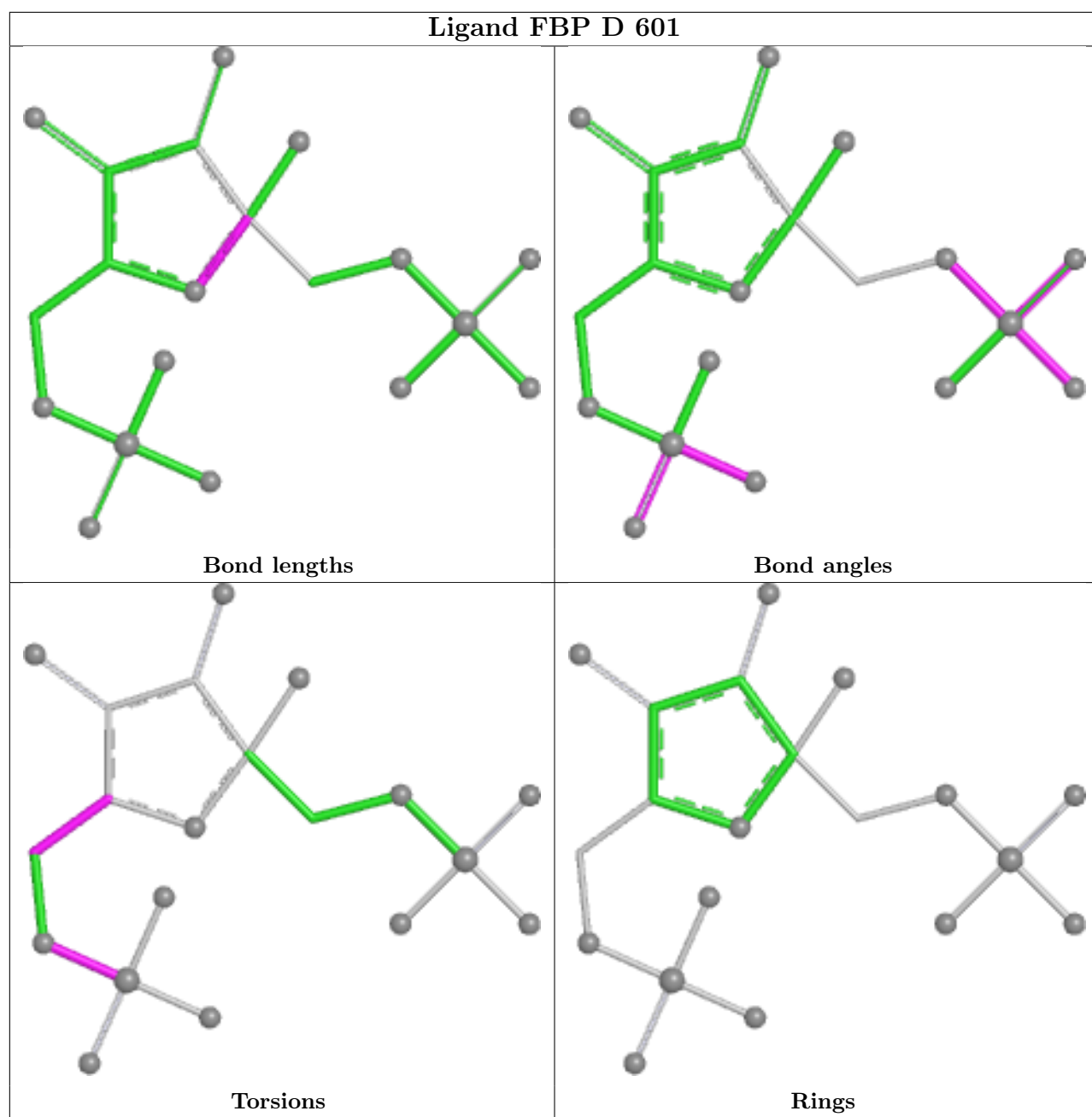
4 monomers are involved in 4 short contacts:

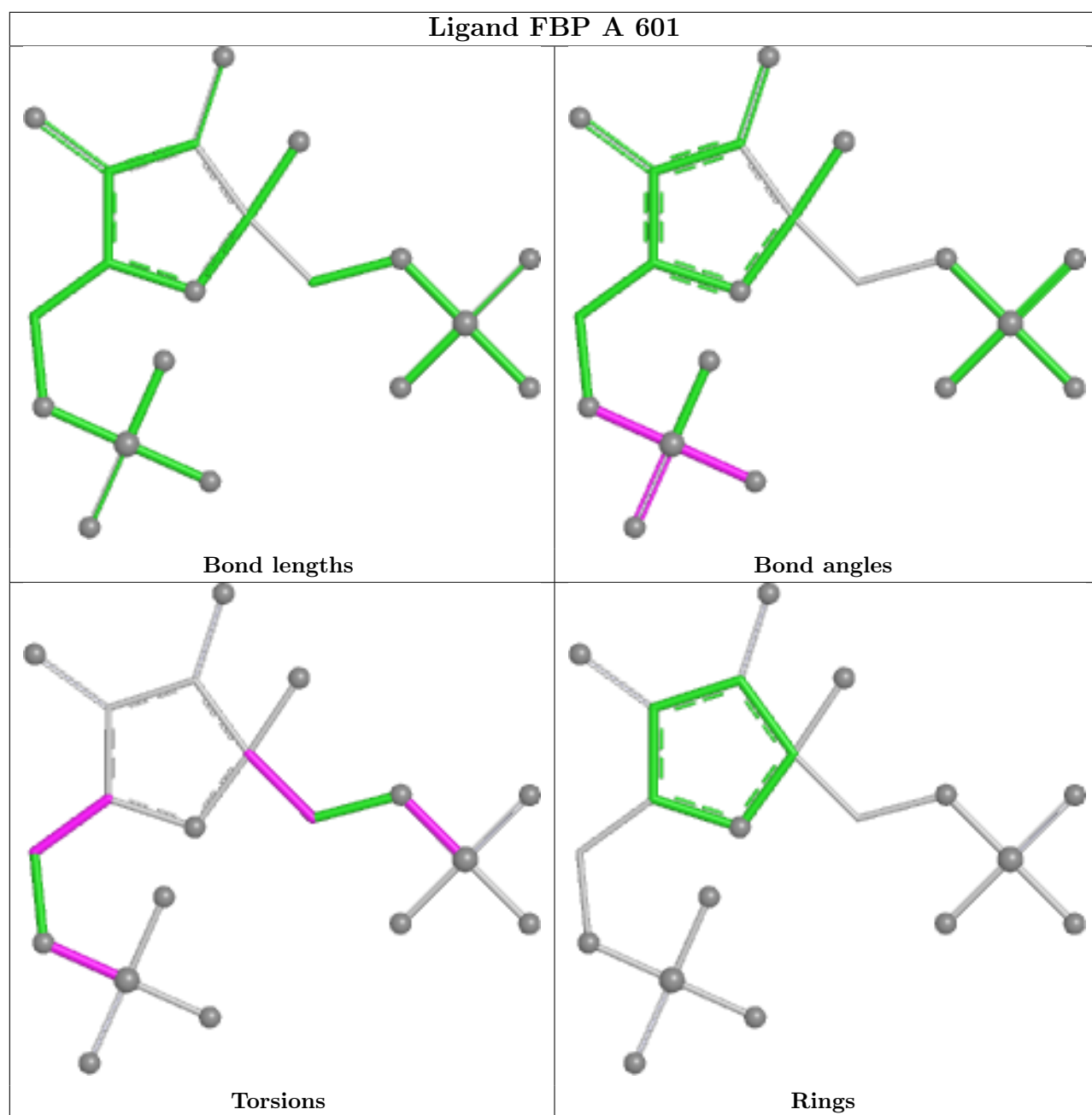
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	SER	1	0
4	D	603	PYR	1	0
2	D	601	FBP	1	0
2	C	601	FBP	1	0

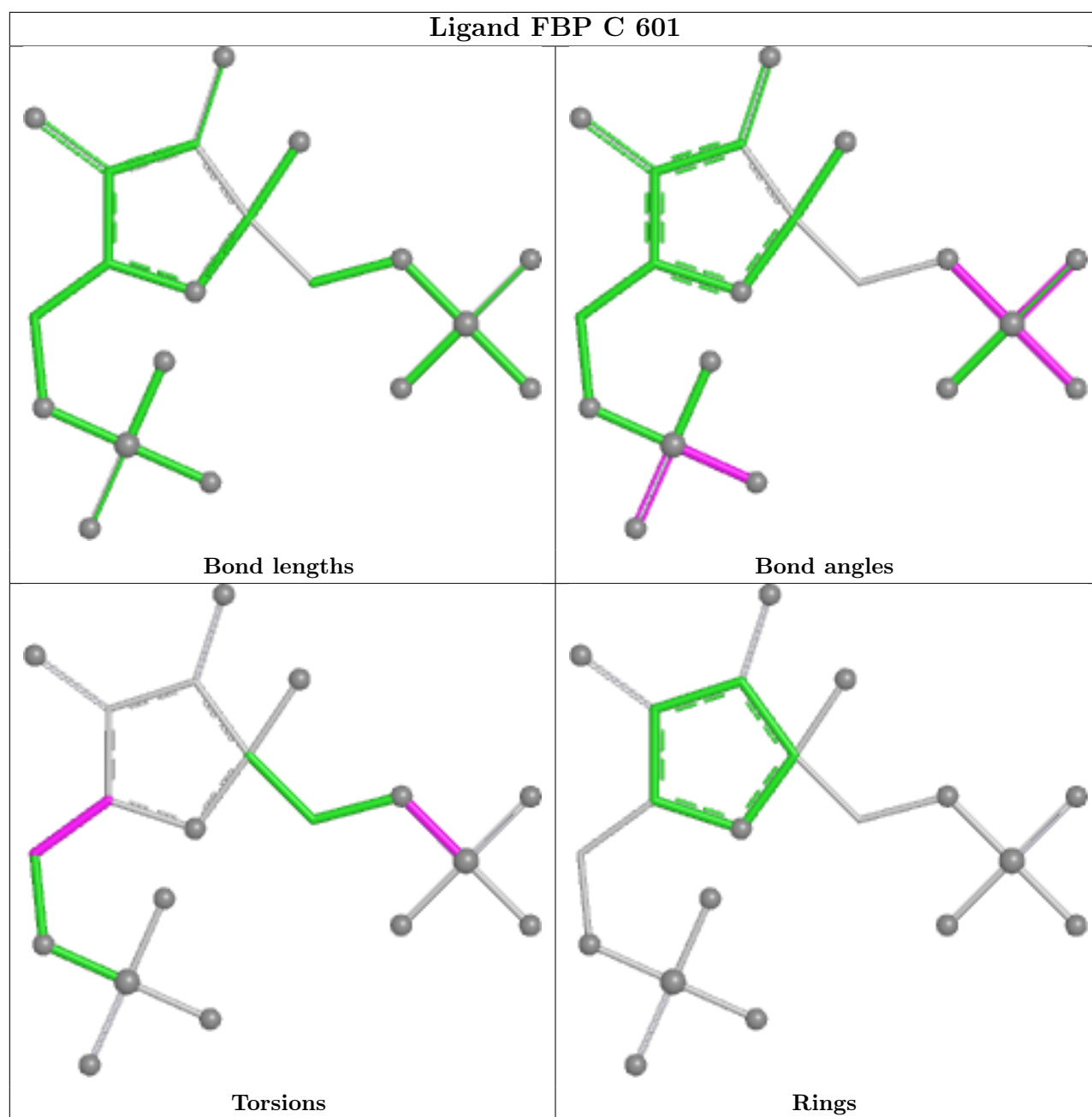
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	518/551 (94%)	-0.54	3 (0%) 85 83	19, 35, 61, 102	0
1	B	515/551 (93%)	-0.44	3 (0%) 85 83	23, 35, 81, 119	0
1	C	518/551 (94%)	-0.37	4 (0%) 82 80	23, 40, 77, 108	0
1	D	518/551 (94%)	-0.35	2 (0%) 88 87	23, 41, 79, 100	0
All	All	2069/2204 (93%)	-0.42	12 (0%) 85 83	19, 38, 77, 119	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	GLU	4.7
1	A	404	ILE	3.4
1	B	180	LEU	2.9
1	C	401	LEU	2.9
1	D	404	ILE	2.7
1	C	403	PRO	2.5
1	C	190	ALA	2.4
1	D	190	ALA	2.4
1	C	180	LEU	2.3
1	B	170	VAL	2.2
1	A	166	LYS	2.1
1	B	144	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

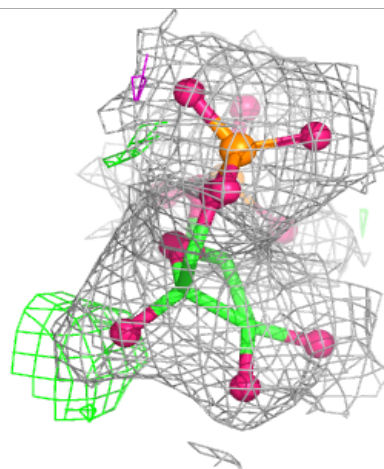
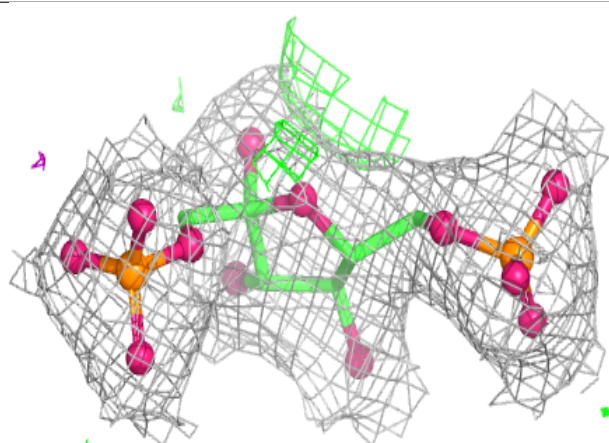
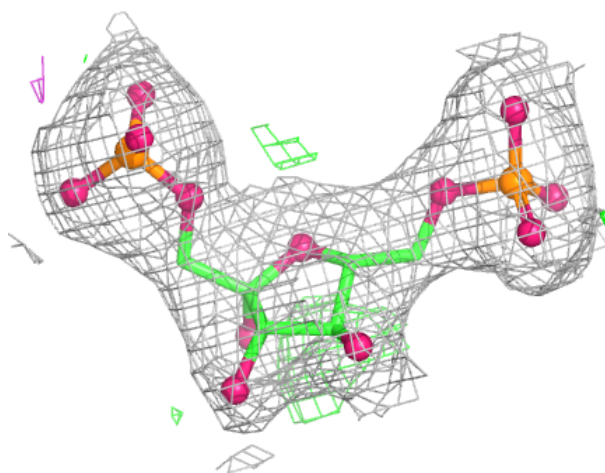
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SER	C	602	7/7	0.89	0.12	44,44,50,51	0
4	PYR	C	603	6/6	0.91	0.10	30,34,36,38	0
3	SER	D	602	7/7	0.92	0.09	42,46,50,55	0
3	SER	A	602	7/7	0.92	0.08	31,37,38,39	0
4	PYR	D	603	6/6	0.92	0.09	40,41,45,46	0
3	SER	B	602	7/7	0.93	0.09	39,44,47,47	0
6	K	C	605	1/1	0.94	0.06	44,44,44,44	0
5	MG	B	604	1/1	0.95	0.10	33,33,33,33	0
5	MG	D	604	1/1	0.95	0.10	46,46,46,46	0
4	PYR	B	603	6/6	0.95	0.07	24,25,32,35	0
4	PYR	A	603	6/6	0.96	0.07	36,38,38,41	0
6	K	D	605	1/1	0.96	0.06	52,52,52,52	0
6	K	B	605	1/1	0.97	0.07	42,42,42,42	0
5	MG	C	604	1/1	0.97	0.07	35,35,35,35	0
5	MG	A	604	1/1	0.97	0.07	28,28,28,28	0
6	K	A	605	1/1	0.98	0.03	44,44,44,44	0
2	FBP	A	601	20/20	0.98	0.05	22,28,33,36	0
2	FBP	C	601	20/20	0.98	0.05	27,31,40,41	0
2	FBP	D	601	20/20	0.98	0.05	20,26,31,31	0
2	FBP	B	601	20/20	0.99	0.04	21,25,32,34	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.

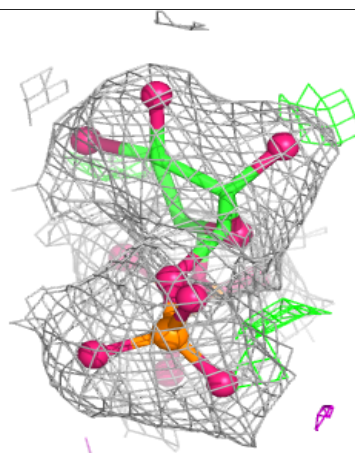
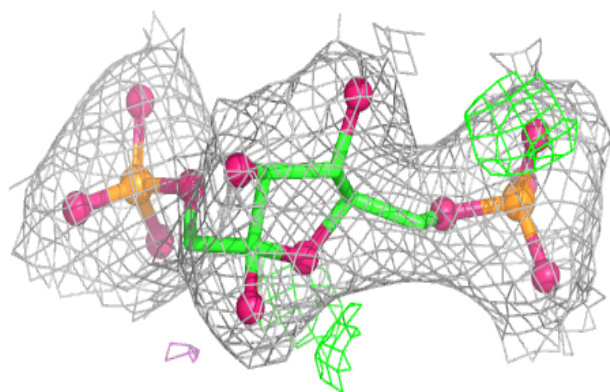
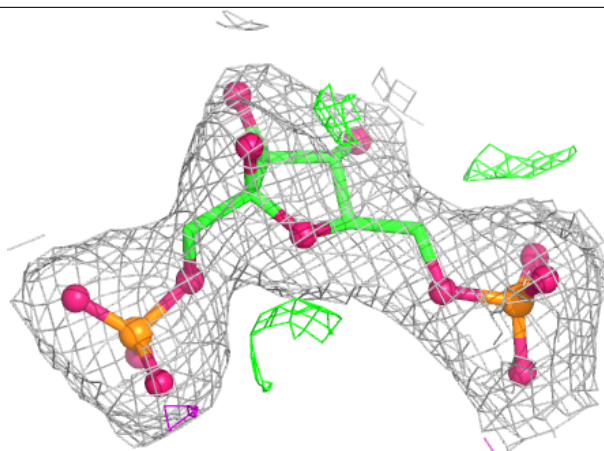
Electron density around FBP A 601:

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



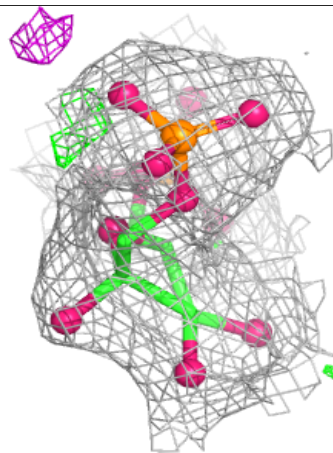
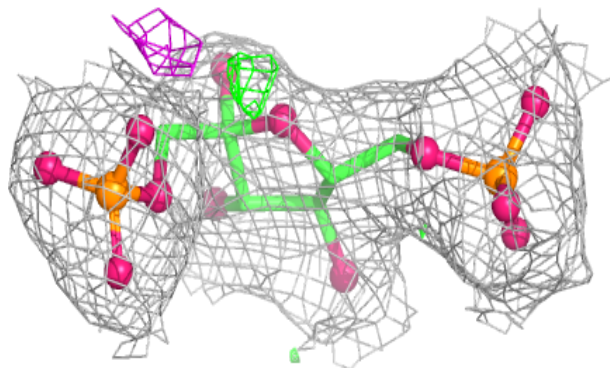
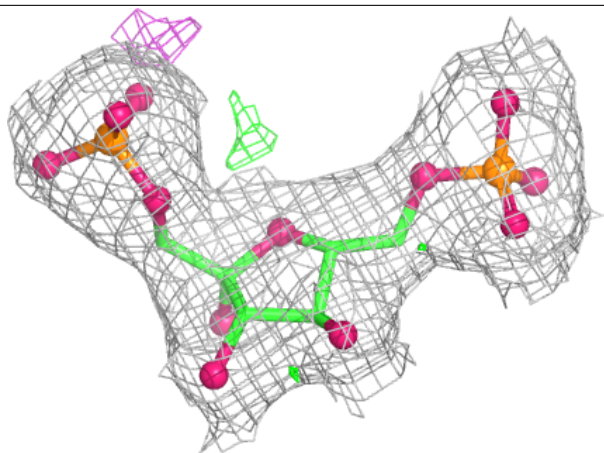
Electron density around FBP C 601:

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



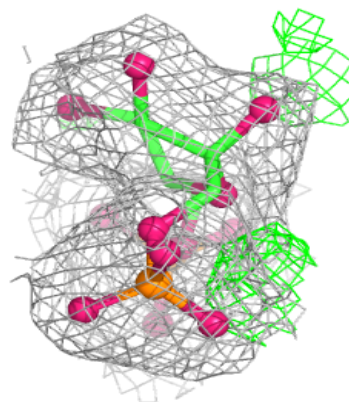
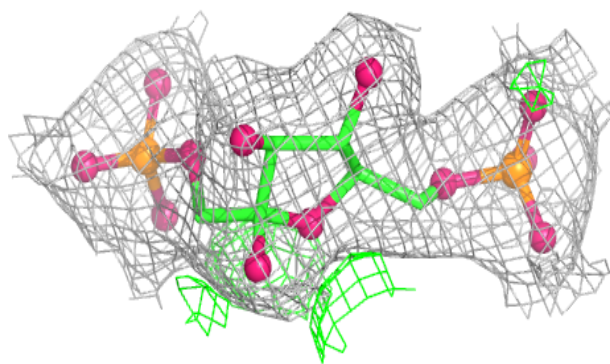
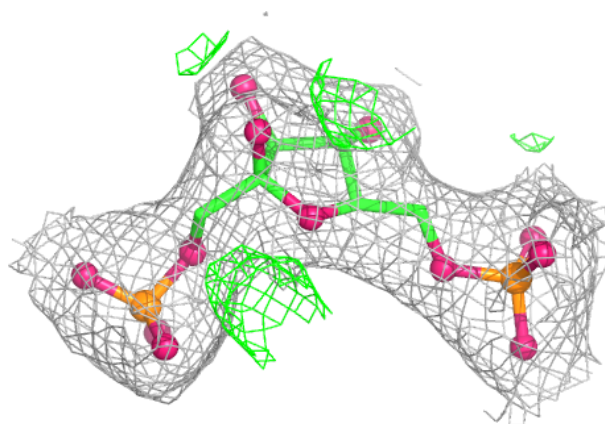
Electron density around FBP D 601:

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



Electron density around FBP B 601:

$2mF_o-DF_c$ (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.