



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:27 AM BST

PDB ID : 4WJ8
Title : Human Pyruvate Kinase M2 Mutant C424A
Authors : Mitchell, T.; Yuan, M.; McNae, I.; Morgan, H.; Walkinshaw, M.D.
Deposited on : 2014-09-29
Resolution : 2.87 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

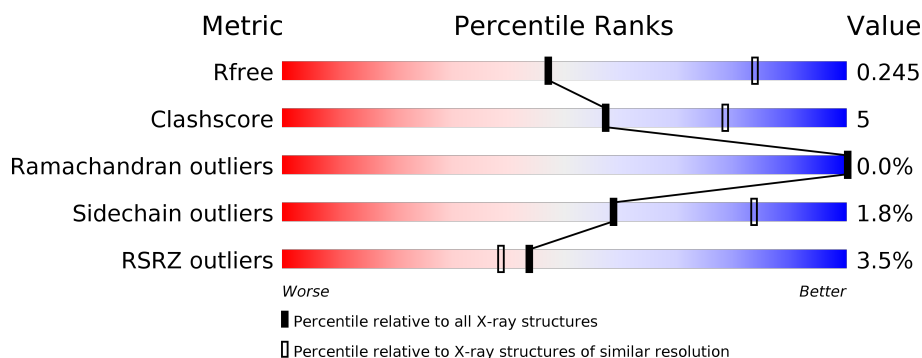
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	551	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>6%</div> </div> </div>
1	B	551	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>6%</div> </div> </div>
1	C	551	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	D	551	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16112 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
			3964	2492	704	744	24			
1	B	517	Total	C	N	O	S	0	0	0
			3955	2487	702	742	24			
1	C	516	Total	C	N	O	S	0	0	0
			3948	2483	701	740	24			
1	D	517	Total	C	N	O	S	0	0	0
			3955	2487	702	742	24			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	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	424	ALA	CYS	engineered mutation	UNP P14618

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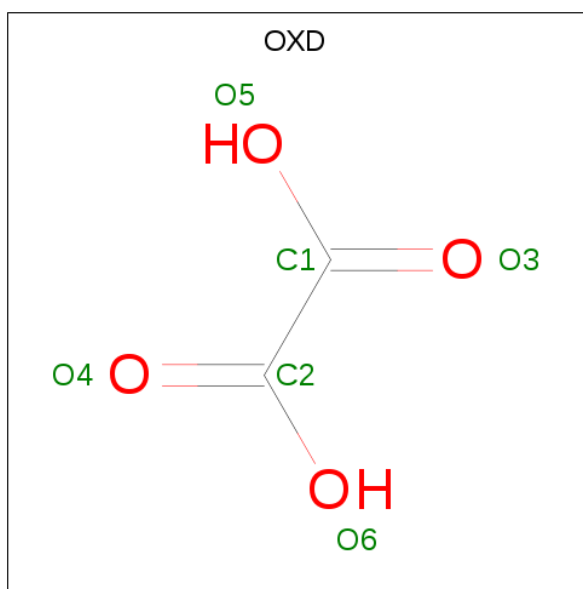
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression 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	424	ALA	CYS	engineered mutation	UNP P14618
C	-19	MET	-	initiating methionine	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	424	ALA	CYS	engineered mutation	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	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	424	ALA	CYS	engineered mutation	UNP P14618

- Molecule 2 is OXALIC ACID (three-letter code: OXD) (formula: C₂H₂O₄).



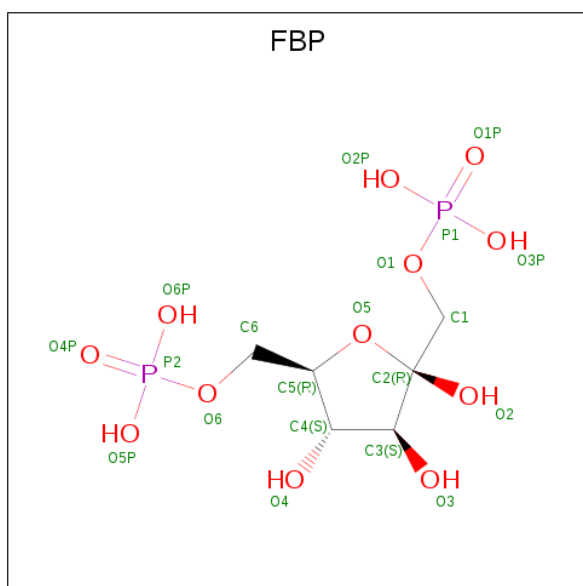
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		

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

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



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

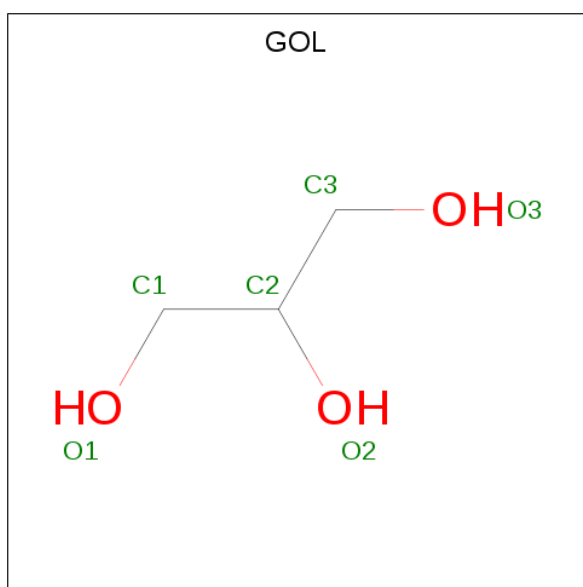
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



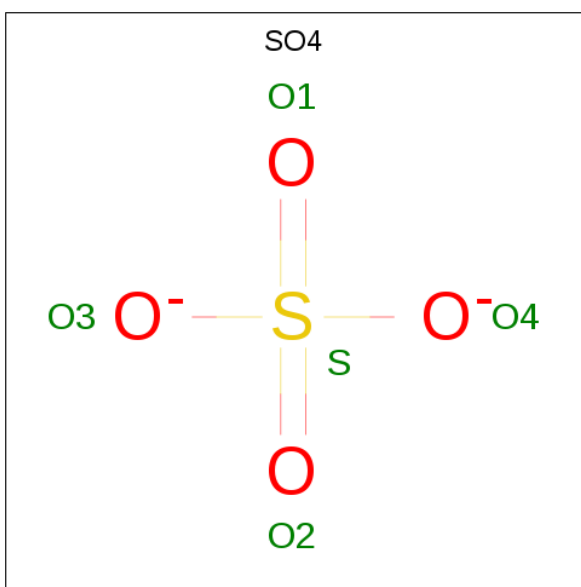
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		

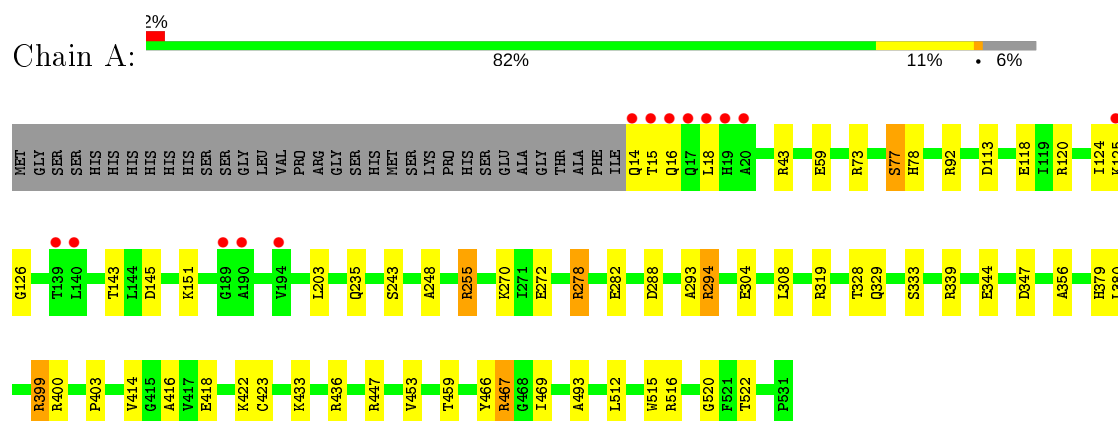
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	38	Total	O	0	0
			38	38		
9	B	52	Total	O	0	0
			52	52		
9	C	30	Total	O	0	0
			30	30		
9	D	43	Total	O	0	0
			43	43		

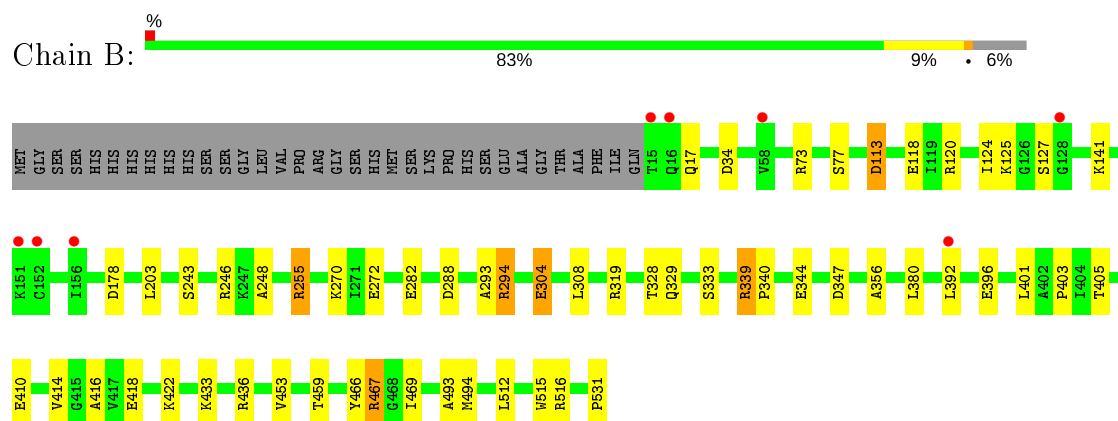
3 Residue-property plots [i](#)

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.

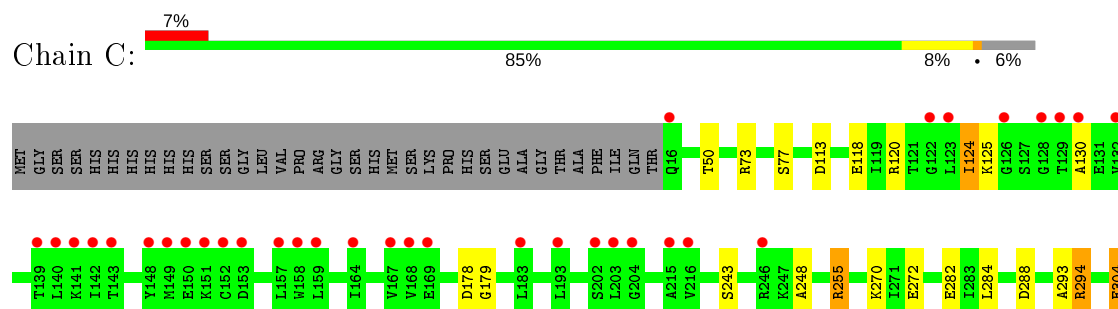
• Molecule 1: Pyruvate kinase PKM

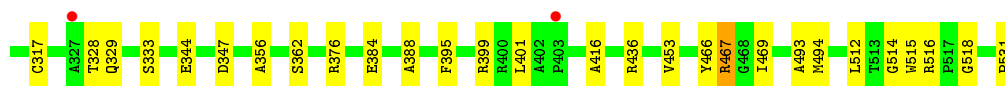


• Molecule 1: Pyruvate kinase PKM

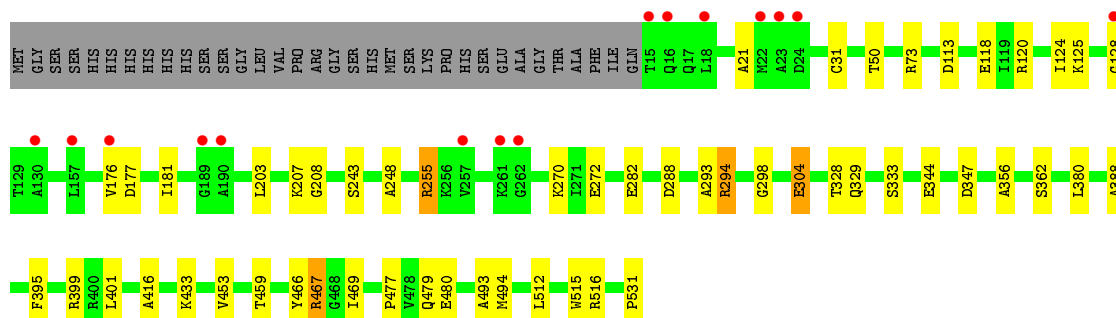
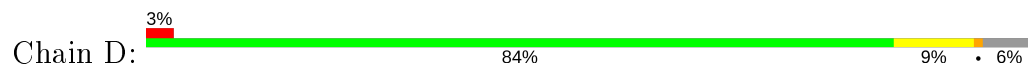


• Molecule 1: Pyruvate kinase PKM





• Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.36 Å 115.26 Å 109.40 Å 90.00° 114.43° 90.00°	Depositor
Resolution (Å)	49.88 – 2.87 49.88 – 2.87	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.88-2.87) 90.3 (49.88-2.87)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.200 , 0.243 0.203 , 0.245	Depositor DCC
R_{free} test set	2212 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16112	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: GOL, MG, FBP, K, SO4, OXD, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/4028	0.59	2/5440 (0.0%)
1	B	0.31	0/4019	0.56	0/5428
1	C	0.30	0/4012	0.56	0/5418
1	D	0.32	0/4019	0.58	0/5428
All	All	0.31	0/16078	0.57	2/21714 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	319	ARG	NE-CZ-NH2	-5.67	117.47	120.30

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	3964	0	4048	52	0
1	B	3955	0	4040	40	0
1	C	3948	0	4033	38	0
1	D	3955	0	4040	49	0
2	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
3	A	20	0	10	1	0
3	C	20	0	10	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	12	0	16	0	0
7	A	10	0	0	0	0
7	D	5	0	0	0	0
8	B	5	0	0	0	0
8	D	5	0	0	0	0
9	A	38	0	0	3	0
9	B	52	0	0	3	0
9	C	30	0	0	3	0
9	D	43	0	0	4	0
All	All	16112	0	16221	158	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 5.

All (158) 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:D:176:VAL:HG22	1:D:181:ILE:HB	1.21	1.08
1:C:124:ILE:HD11	1:C:130:ALA:HB3	1.09	1.08
1:B:73:ARG:NH1	1:B:113:ASP:OD2	1.87	1.04
1:B:339:ARG:NH2	1:D:298:GLY:O	2.00	0.94
1:C:124:ILE:HD11	1:C:130:ALA:CB	1.99	0.92
1:A:339:ARG:CZ	1:C:179:GLY:O	2.23	0.86
1:B:304:GLU:HG2	1:D:380:LEU:HB3	1.60	0.83
1:D:176:VAL:HG22	1:D:181:ILE:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:LEU:HD22	9:C:711:HOH:O	1.81	0.81
1:D:73:ARG:NH1	1:D:113:ASP:OD2	2.16	0.78
1:D:294:ARG:HD3	9:D:716:HOH:O	1.82	0.78
1:C:73:ARG:NH1	1:C:113:ASP:OD2	2.18	0.77
1:A:73:ARG:NH1	1:A:113:ASP:OD2	2.18	0.76
1:B:17:GLN:NE2	1:B:34:ASP:O	2.17	0.76
1:A:143:THR:HG22	1:A:145:ASP:H	1.52	0.74
1:A:243:SER:O	9:A:738:HOH:O	2.07	0.72
1:D:176:VAL:CG2	1:D:181:ILE:HB	2.10	0.71
1:D:176:VAL:CG2	1:D:181:ILE:HG13	2.24	0.68
1:C:124:ILE:CD1	1:C:130:ALA:HB3	2.05	0.68
1:B:339:ARG:HG2	1:B:340:PRO:HD2	1.77	0.67
1:D:176:VAL:O	1:D:208:GLY:O	2.14	0.66
1:A:143:THR:HG22	1:A:145:ASP:N	2.10	0.65
1:A:403:PRO:O	1:B:422:LYS:NZ	2.32	0.63
1:B:380:LEU:HB3	1:D:304:GLU:HG2	1.81	0.62
1:D:328:THR:N	9:D:716:HOH:O	1.94	0.62
1:A:380:LEU:HB3	1:C:304:GLU:HG2	1.82	0.61
1:A:14:GLN:HA	1:A:14:GLN:OE1	2.01	0.60
1:C:317:CYS:N	9:C:711:HOH:O	2.35	0.59
1:D:270:LYS:NZ	2:D:601:OXD:O4	2.35	0.59
1:D:176:VAL:HG21	1:D:181:ILE:HG13	1.84	0.59
1:D:479:GLN:HG3	1:D:480:GLU:HG3	1.86	0.58
1:B:333:SER:HB3	1:B:344:GLU:OE1	2.03	0.58
1:D:333:SER:HB3	1:D:344:GLU:OE1	2.03	0.57
1:A:333:SER:HB3	1:A:344:GLU:OE1	2.04	0.57
1:C:333:SER:HB3	1:C:344:GLU:OE1	2.04	0.57
1:D:176:VAL:HG23	1:D:177:ASP:N	2.18	0.57
1:C:124:ILE:HG13	1:C:125:LYS:H	1.71	0.55
1:A:143:THR:CG2	1:A:145:ASP:H	2.19	0.55
1:A:422:LYS:NZ	1:B:403:PRO:O	2.39	0.55
1:D:124:ILE:HG22	1:D:125:LYS:N	2.22	0.55
1:C:50:THR:OG1	1:C:362:SER:HA	2.06	0.55
1:A:125:LYS:N	1:A:126:GLY:HA2	2.21	0.55
1:A:328:THR:HG22	1:A:329:GLN:HG3	1.89	0.55
1:C:328:THR:HG22	1:C:329:GLN:HG3	1.89	0.54
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.89	0.54
1:B:243:SER:HA	1:B:270:LYS:HE3	1.90	0.54
1:C:514:GLY:HA3	3:C:601:FBP:O3	2.07	0.54
1:B:328:THR:HG22	1:B:329:GLN:HG3	1.90	0.54
1:A:243:SER:HA	1:A:270:LYS:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:SER:HA	1:C:270:LYS:HE3	1.90	0.54
1:D:243:SER:HA	1:D:270:LYS:HE3	1.90	0.54
1:D:50:THR:OG1	1:D:362:SER:HA	2.08	0.53
1:C:124:ILE:HG13	1:C:125:LYS:N	2.23	0.53
1:D:176:VAL:CG2	1:D:181:ILE:CG1	2.86	0.53
1:A:43:ARG:HE	1:A:379:HIS:CD2	2.27	0.52
1:A:59:GLU:OE2	9:A:711:HOH:O	2.19	0.52
1:A:43:ARG:HE	1:A:379:HIS:HD2	1.58	0.52
1:B:246:ARG:NH1	9:B:752:HOH:O	2.43	0.52
1:A:436:ARG:NH1	1:A:520:GLY:HA2	2.26	0.51
1:C:124:ILE:O	1:C:125:LYS:HG3	2.10	0.51
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.94	0.49
1:A:339:ARG:NH1	1:C:179:GLY:O	2.45	0.49
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.95	0.49
1:B:515:TRP:CD2	1:B:516:ARG:HG2	2.47	0.49
1:C:515:TRP:CD2	1:C:516:ARG:HG2	2.48	0.49
1:D:124:ILE:HD11	1:D:203:LEU:O	2.13	0.49
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.94	0.48
1:D:176:VAL:CG2	1:D:181:ILE:CB	2.83	0.48
1:D:294:ARG:CD	9:D:716:HOH:O	2.50	0.48
1:A:124:ILE:HD11	1:A:203:LEU:O	2.13	0.48
1:A:436:ARG:HH11	1:A:520:GLY:HA2	1.79	0.48
1:B:118:GLU:OE2	1:B:120:ARG:NH1	2.43	0.48
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.96	0.48
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.96	0.48
1:B:113:ASP:CG	9:B:713:HOH:O	2.52	0.47
1:A:399:ARG:HG3	1:A:400:ARG:N	2.28	0.47
1:A:515:TRP:CD2	1:A:516:ARG:HG2	2.48	0.47
1:D:515:TRP:CD2	1:D:516:ARG:HG2	2.49	0.47
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.95	0.47
1:A:304:GLU:CG	1:C:384:GLU:HG3	2.45	0.47
1:B:141:LYS:HE2	9:B:729:HOH:O	2.13	0.47
1:B:124:ILE:HD11	1:B:203:LEU:O	2.14	0.47
1:B:308:LEU:HD21	1:D:388:ALA:HB2	1.96	0.47
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.96	0.47
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.97	0.47
1:C:118:GLU:OE2	1:C:120:ARG:NH1	2.44	0.47
1:C:50:THR:CB	1:C:362:SER:HA	2.45	0.47
1:D:118:GLU:OE2	1:D:120:ARG:NH1	2.45	0.47
1:A:422:LYS:HE3	1:B:410:GLU:HG2	1.96	0.46
1:B:294:ARG:NH2	1:B:347:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:NH1	1:A:235:GLN:O	2.48	0.46
1:D:21:ALA:HB2	9:D:741:HOH:O	2.14	0.46
1:B:125:LYS:C	1:B:127:SER:H	2.18	0.46
1:A:423:CYS:HA	1:B:405:THR:O	2.16	0.46
1:A:418:GLU:CG	1:B:414:VAL:HG12	2.44	0.46
1:D:177:ASP:OD1	1:D:207:LYS:HD2	2.14	0.46
1:D:294:ARG:NH2	1:D:347:ASP:OD1	2.49	0.46
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.96	0.46
1:D:50:THR:CB	1:D:362:SER:HA	2.46	0.46
1:D:494:MET:HG2	1:D:531:PRO:HD2	1.98	0.45
1:A:272:GLU:HG3	1:A:293:ALA:HB3	1.98	0.45
1:D:50:THR:HG1	1:D:362:SER:HA	1.81	0.45
1:D:477:PRO:O	1:D:479:GLN:N	2.50	0.45
1:A:294:ARG:NH2	1:A:347:ASP:OD1	2.48	0.45
1:A:422:LYS:CE	1:B:410:GLU:HG2	2.47	0.45
1:C:294:ARG:NH2	1:C:347:ASP:OD1	2.48	0.45
1:C:494:MET:HG2	1:C:531:PRO:HD2	1.99	0.45
1:A:118:GLU:OE2	1:A:120:ARG:NH1	2.45	0.45
1:A:399:ARG:HD2	1:B:418:GLU:OE2	2.17	0.45
1:C:50:THR:HG1	1:C:362:SER:HA	1.81	0.45
1:A:278:ARG:NH1	9:A:724:HOH:O	2.49	0.45
1:C:518:GLY:O	3:C:601:FBP:O4	2.20	0.45
1:D:272:GLU:HG3	1:D:293:ALA:HB3	1.98	0.45
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.47	0.45
1:C:376:ARG:HB3	9:C:703:HOH:O	2.17	0.44
1:C:453:VAL:CG2	1:C:493:ALA:HB2	2.47	0.44
1:A:522:THR:OG1	3:A:602:FBP:H61	2.18	0.44
1:C:248:ALA:HB2	1:C:282:GLU:HG2	1.99	0.44
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.48	0.44
1:A:77:SER:O	1:A:78:HIS:CD2	2.70	0.44
1:C:272:GLU:HG3	1:C:293:ALA:HB3	1.99	0.44
1:B:248:ALA:HB2	1:B:282:GLU:HG2	1.99	0.44
1:A:308:LEU:HD21	1:C:388:ALA:HB2	1.98	0.43
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.48	0.43
1:B:272:GLU:HG3	1:B:293:ALA:HB3	1.99	0.43
1:A:339:ARG:NH2	1:C:179:GLY:O	2.50	0.43
1:A:248:ALA:HB2	1:A:282:GLU:HG2	2.00	0.43
1:B:319:ARG:HD3	1:D:31:CYS:SG	2.58	0.43
1:D:248:ALA:HB2	1:D:282:GLU:HG2	1.99	0.43
1:B:304:GLU:HG2	1:D:380:LEU:CB	2.41	0.43
1:B:356:ALA:O	1:B:467:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ARG:NH2	1:C:288:ASP:OD2	2.52	0.42
1:C:356:ALA:O	1:C:467:ARG:NH1	2.51	0.42
1:B:255:ARG:NH2	1:B:288:ASP:OD2	2.53	0.42
1:C:50:THR:HB	1:C:362:SER:HA	2.02	0.42
1:D:356:ALA:O	1:D:467:ARG:NH1	2.51	0.42
1:D:124:ILE:HG22	1:D:125:LYS:H	1.82	0.42
1:A:356:ALA:O	1:A:467:ARG:NH1	2.51	0.42
1:A:125:LYS:HA	1:A:151:LYS:HA	2.01	0.42
1:A:16:GLN:CD	1:A:447:ARG:HD2	2.40	0.42
1:A:18:LEU:HD23	1:A:18:LEU:O	2.20	0.42
1:D:255:ARG:NH2	1:D:288:ASP:OD2	2.53	0.42
1:A:124:ILE:HG22	1:A:125:LYS:H	1.85	0.42
1:A:414:VAL:HG12	1:B:418:GLU:CG	2.50	0.42
1:B:433:LYS:O	1:B:459:THR:HG21	2.20	0.42
1:B:515:TRP:CE3	1:B:516:ARG:HG2	2.55	0.41
1:A:515:TRP:CE3	1:A:516:ARG:HG2	2.55	0.41
1:C:515:TRP:CE3	1:C:516:ARG:HG2	2.56	0.41
1:D:515:TRP:CE3	1:D:516:ARG:HG2	2.56	0.41
1:A:433:LYS:O	1:A:459:THR:HG21	2.21	0.41
1:A:255:ARG:NH2	1:A:288:ASP:OD2	2.53	0.41
1:A:143:THR:HG21	1:A:145:ASP:HB3	2.03	0.41
1:C:395:PHE:O	1:C:399:ARG:HG3	2.21	0.41
1:D:433:LYS:O	1:D:459:THR:HG21	2.21	0.41
1:B:319:ARG:CD	1:D:31:CYS:SG	3.09	0.40
1:B:392:LEU:O	1:B:396:GLU:HB2	2.20	0.40
1:D:176:VAL:CG2	1:D:177:ASP:N	2.82	0.40
1:D:395:PHE:O	1:D:399:ARG:HG3	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%)	499 (97%)	17 (3%)	0	100	100
1	B	515/551 (94%)	495 (96%)	20 (4%)	0	100	100
1	C	514/551 (93%)	497 (97%)	17 (3%)	0	100	100
1	D	515/551 (94%)	497 (96%)	17 (3%)	1 (0%)	47	76
All	All	2060/2204 (94%)	1988 (96%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	128	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	425/452 (94%)	418 (98%)	7 (2%)	62	85
1	B	424/452 (94%)	414 (98%)	10 (2%)	49	78
1	C	423/452 (94%)	414 (98%)	9 (2%)	53	80
1	D	424/452 (94%)	419 (99%)	5 (1%)	71	89
All	All	1696/1808 (94%)	1665 (98%)	31 (2%)	59	83

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	77	SER
1	A	255	ARG
1	A	278	ARG
1	A	294	ARG
1	A	399	ARG
1	A	467	ARG
1	B	77	SER
1	B	113	ASP
1	B	178	ASP

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Mol	Chain	Res	Type
1	B	255	ARG
1	B	294	ARG
1	B	304	GLU
1	B	339	ARG
1	B	401	LEU
1	B	436	ARG
1	B	467	ARG
1	C	77	SER
1	C	124	ILE
1	C	178	ASP
1	C	255	ARG
1	C	294	ARG
1	C	304	GLU
1	C	401	LEU
1	C	436	ARG
1	C	467	ARG
1	D	255	ARG
1	D	294	ARG
1	D	304	GLU
1	D	401	LEU
1	D	467	ARG

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	78	HIS
1	A	163	ASN
1	A	274	HIS
1	A	379	HIS
1	B	163	ASN
1	C	163	ASN
1	D	16	GLN
1	D	163	ASN

5.3.3 RNA ⓘ

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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	FBP	A	602	-	18,20,20	0.69	0	23,32,32	1.06	2 (8%)
3	FBP	C	601	-	18,20,20	0.75	1 (5%)	23,32,32	1.16	1 (4%)
2	OXD	D	601	5	0,5,5	0.00	-	0,6,6	0.00	-
8	SO4	B	602	-	4,4,4	0.30	0	6,6,6	0.16	0
2	OXD	B	601	5	0,5,5	0.00	-	0,6,6	0.00	-
7	PO4	D	602	-	4,4,4	0.89	0	6,6,6	0.44	0
2	OXD	C	602	5	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	D	607	-	5,5,5	0.21	0	5,5,5	0.42	0
6	GOL	A	605	-	5,5,5	0.27	0	5,5,5	0.31	0
8	SO4	D	603	-	4,4,4	0.37	0	6,6,6	0.17	0
6	GOL	C	605	-	5,5,5	0.16	0	5,5,5	0.67	0
6	GOL	B	605	-	5,5,5	0.32	0	5,5,5	0.16	0
2	OXD	A	601	5	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	D	606	-	5,5,5	0.16	0	5,5,5	0.30	0
7	PO4	A	606	-	4,4,4	0.92	0	6,6,6	0.44	0
7	PO4	A	607	-	4,4,4	0.87	0	6,6,6	0.41	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
3	FBP	A	602	-	-	5/13/32/32	0/1/1/1
3	FBP	C	601	-	-	9/13/32/32	0/1/1/1
2	OXD	B	601	5	-	0/0/4/4	-
6	GOL	D	607	-	-	2/4/4/4	-
2	OXD	D	601	5	-	0/0/4/4	-
6	GOL	A	605	-	-	0/4/4/4	-
6	GOL	C	605	-	-	2/4/4/4	-
6	GOL	B	605	-	-	4/4/4/4	-
2	OXD	A	601	5	-	0/0/4/4	-
6	GOL	D	606	-	-	0/4/4/4	-
2	OXD	C	602	5	-	0/0/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	FBP	O2-C2	2.09	1.44	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	FBP	O5-C5-C6	2.15	114.18	109.45
3	C	601	FBP	O3P-P1-O2P	2.04	115.45	107.64
3	A	602	FBP	P2-O6-C6	2.01	123.84	118.30

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	FBP	C6-O6-P2-O4P
3	A	602	FBP	C6-O6-P2-O5P
3	A	602	FBP	C6-O6-P2-O6P
3	C	601	FBP	C1-O1-P1-O3P
3	C	601	FBP	O1-C1-C2-O2
3	C	601	FBP	O1-C1-C2-C3
3	C	601	FBP	O1-C1-C2-O5
3	C	601	FBP	C4-C5-C6-O6
6	C	605	GOL	O1-C1-C2-C3
6	B	605	GOL	O1-C1-C2-C3
6	B	605	GOL	C1-C2-C3-O3
6	D	607	GOL	C1-C2-C3-O3
6	B	605	GOL	O2-C2-C3-O3

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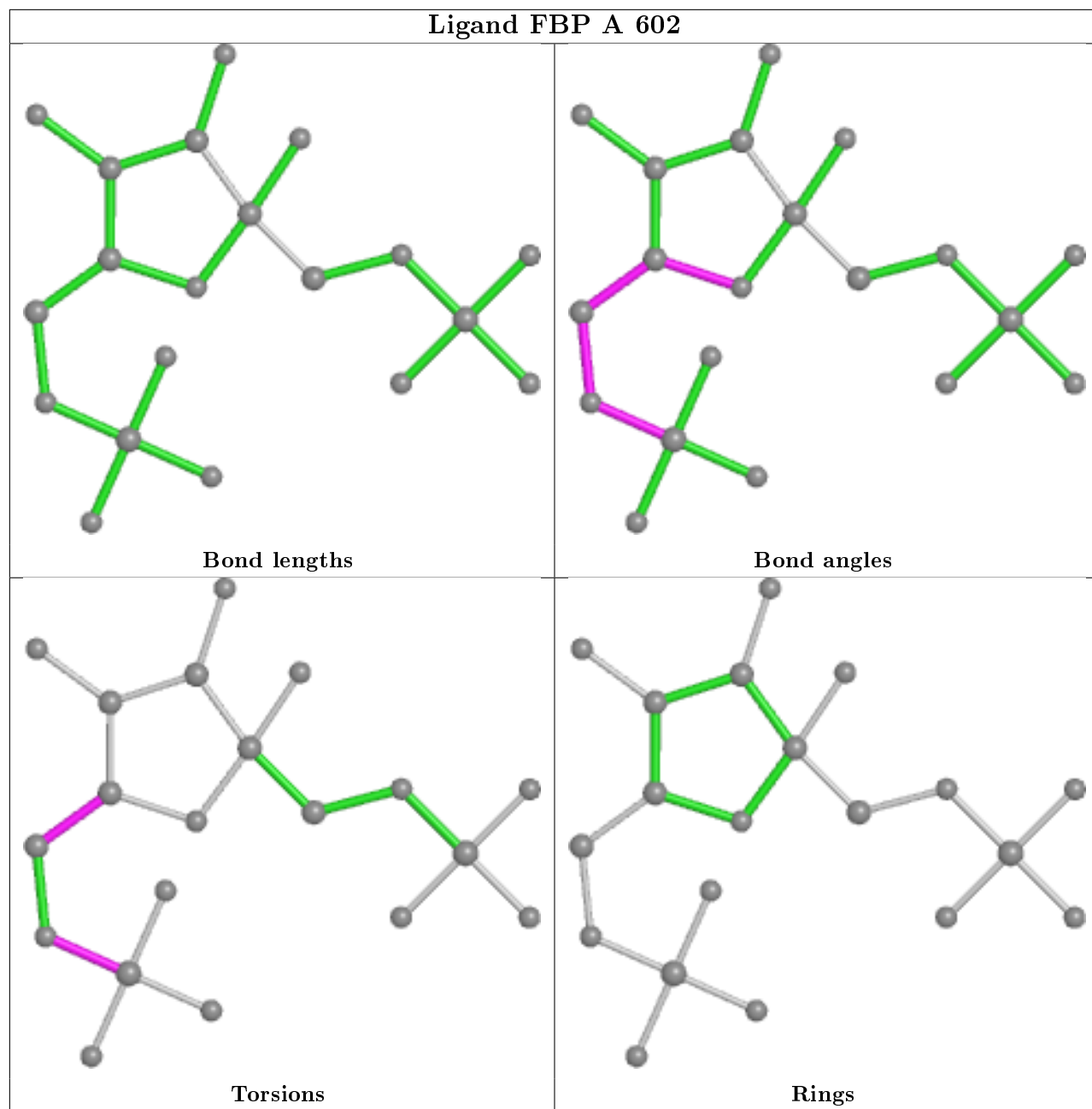
Mol	Chain	Res	Type	Atoms
3	C	601	FBP	O5-C5-C6-O6
6	C	605	GOL	O1-C1-C2-O2
6	B	605	GOL	O1-C1-C2-O2
3	C	601	FBP	C6-O6-P2-O4P
6	D	607	GOL	O2-C2-C3-O3
3	C	601	FBP	C1-O1-P1-O2P
3	C	601	FBP	C1-O1-P1-O1P
3	A	602	FBP	C4-C5-C6-O6
3	A	602	FBP	O5-C5-C6-O6

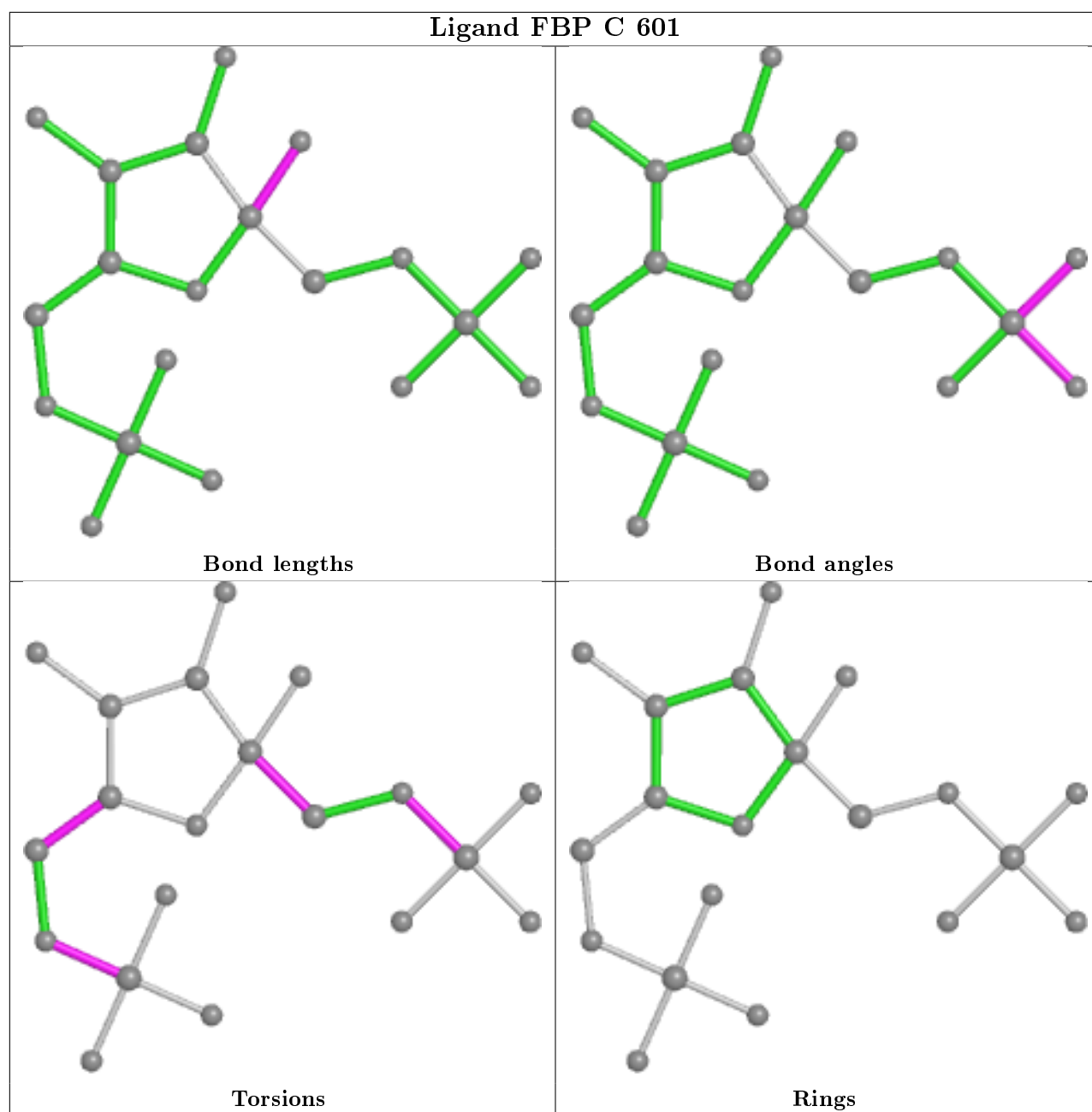
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	FBP	1	0
3	C	601	FBP	2	0
2	D	601	OXD	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%)	0.09	13 (2%) 57 55	44, 65, 109, 156	0
1	B	517/551 (93%)	-0.02	8 (1%) 73 73	42, 64, 97, 147	0
1	C	516/551 (93%)	0.38	36 (6%) 16 12	48, 79, 127, 151	0
1	D	517/551 (93%)	0.01	15 (2%) 51 48	40, 60, 102, 173	1 (0%)
All	All	2068/2204 (93%)	0.12	72 (3%) 44 39	40, 67, 115, 173	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	THR	6.1
1	A	14	GLN	6.1
1	C	16	GLN	5.3
1	A	17	GLN	4.9
1	D	189	GLY	4.9
1	C	157	LEU	4.9
1	D	15	THR	4.8
1	A	20	ALA	4.5
1	C	128	GLY	4.4
1	C	148	TYR	4.0
1	D	16	GLN	4.0
1	C	153	ASP	3.8
1	A	16	GLN	3.8
1	A	190	ALA	3.8
1	C	149	MET	3.7
1	C	168	VAL	3.6
1	C	140	LEU	3.6
1	C	216	VAL	3.6
1	D	130	ALA	3.6
1	C	167	VAL	3.6
1	A	18	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	3.4
1	C	158	TRP	3.4
1	B	128	GLY	3.3
1	C	122	GLY	3.3
1	C	215	ALA	3.2
1	C	204	GLY	3.2
1	C	141	LYS	3.2
1	A	139	THR	3.2
1	C	123	LEU	3.1
1	C	142	ILE	3.0
1	B	392	LEU	2.9
1	B	156	ILE	2.9
1	A	125	LYS	2.8
1	C	203	LEU	2.8
1	B	151	LYS	2.8
1	D	24	ASP	2.8
1	C	403	PRO	2.7
1	C	126	GLY	2.7
1	D	190	ALA	2.6
1	C	159	LEU	2.6
1	C	246	ARG	2.6
1	C	143	THR	2.6
1	C	152	CYS	2.6
1	C	151	LYS	2.6
1	D	262	GLY	2.6
1	D	18	LEU	2.6
1	B	15	THR	2.5
1	C	150	GLU	2.5
1	D	176	VAL	2.5
1	D	23	ALA	2.4
1	C	169	GLU	2.3
1	D	128	GLY	2.3
1	B	152	CYS	2.3
1	C	193	LEU	2.3
1	B	16	GLN	2.3
1	A	19	HIS	2.3
1	C	129	THR	2.3
1	A	140	LEU	2.2
1	B	58	VAL	2.2
1	C	139	THR	2.2
1	D	261	LYS	2.2
1	C	327	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	132	VAL	2.1
1	D	157	LEU	2.1
1	C	164	ILE	2.1
1	D	22	MET	2.1
1	C	202	SER	2.1
1	C	130	ALA	2.1
1	D	257	VAL	2.1
1	C	183	LEU	2.0
1	A	189	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	K	B	604	1/1	0.92	0.07	72,72,72,72	0
3	FBP	C	601	20/20	0.92	0.26	67,118,146,147	0
3	FBP	A	602	20/20	0.93	0.25	59,99,116,118	0
4	K	A	603	1/1	0.93	0.10	71,71,71,71	0
6	GOL	D	606	6/6	0.94	0.20	69,70,72,74	0
7	PO4	A	606	5/5	0.94	0.15	79,80,80,83	0
6	GOL	C	605	6/6	0.94	0.17	61,61,61,62	0
7	PO4	D	602	5/5	0.94	0.17	77,78,80,83	0
6	GOL	A	605	6/6	0.94	0.18	73,75,77,78	0
6	GOL	D	607	6/6	0.95	0.29	65,66,74,79	0
4	K	C	604	1/1	0.95	0.06	73,73,73,73	0
7	PO4	A	607	5/5	0.95	0.20	82,84,87,87	0
2	OXD	D	601	6/6	0.96	0.14	50,52,55,57	0
5	MG	B	603	1/1	0.97	0.14	49,49,49,49	0

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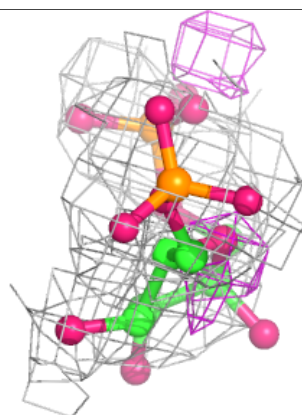
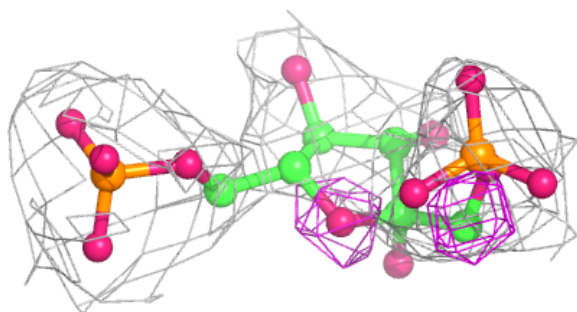
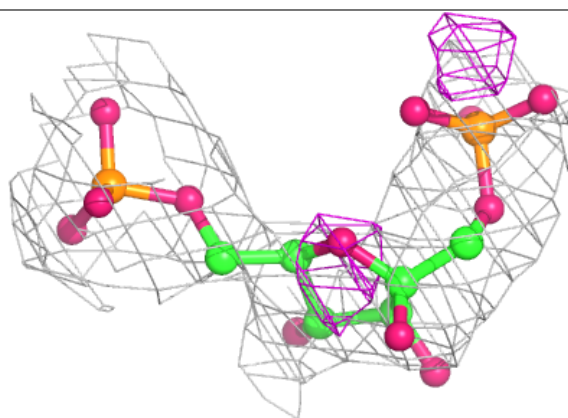
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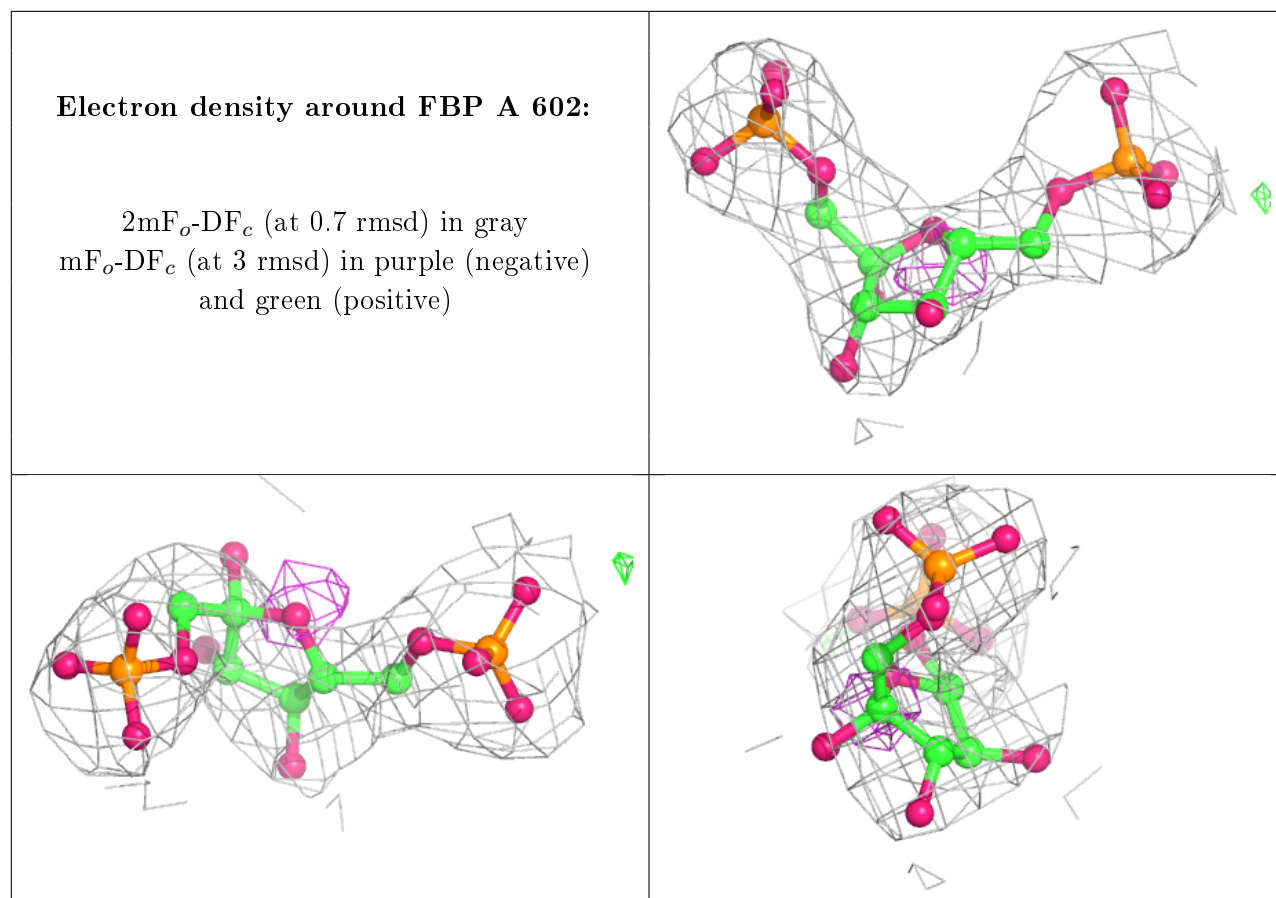
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OXD	B	601	6/6	0.97	0.12	50,52,54,54	0
6	GOL	B	605	6/6	0.97	0.14	59,61,61,62	0
2	OXD	C	602	6/6	0.97	0.10	63,67,68,69	0
5	MG	C	603	1/1	0.97	0.06	59,59,59,59	0
8	SO4	B	602	5/5	0.97	0.12	59,60,64,64	0
4	K	D	605	1/1	0.98	0.08	58,58,58,58	0
2	OXD	A	601	6/6	0.98	0.16	49,50,53,54	0
8	SO4	D	603	5/5	0.98	0.09	56,57,60,63	0
5	MG	D	604	1/1	0.98	0.18	46,46,46,46	0
5	MG	A	604	1/1	0.98	0.21	47,47,47,47	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 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 ⓘ

There are no such residues in this entry.