



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 12:40 PM BST

PDB ID : 2VGF
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE: T384M mutant
Authors : Valentini, G.; Chiarelli, L.R.; Fortin, R.; Dolzan, M.; Galizzi, A.; Abraham, D.J.; Wang, C.; Bianchi, P.; Zanella, A.; Mattevi, A.
Deposited on : 2007-11-12
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

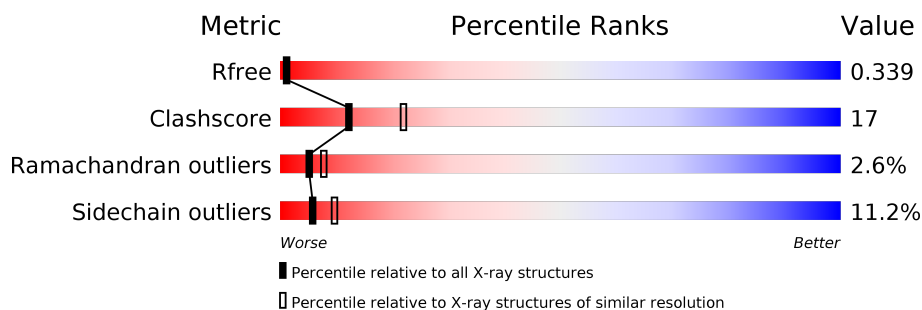
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	528	
1	B	528	
1	C	528	
1	D	528	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15550 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

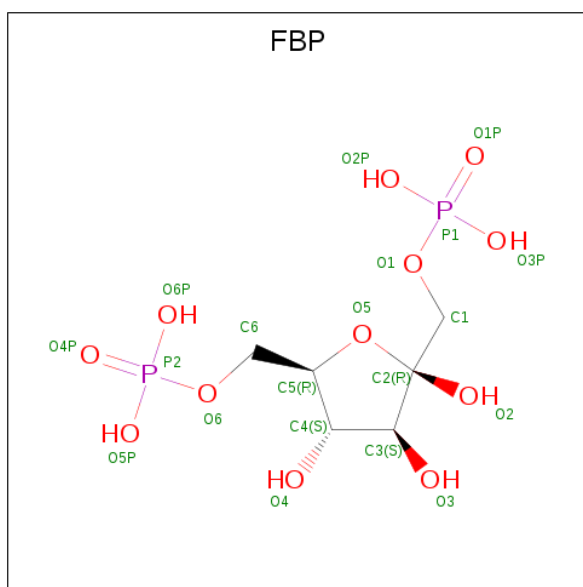
- Molecule 1 is a protein called PYRUVATE KINASE ISOZYMES R/L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3913	2458	709	727	19			
1	B	491	Total	C	N	O	S	0	0	0
			3720	2340	673	688	19			
1	C	517	Total	C	N	O	S	0	0	0
			3913	2458	709	727	19			
1	D	512	Total	C	N	O	S	7	0	0
			3880	2437	703	721	19			

There are 4 discrepancies between the modelled and reference sequences:

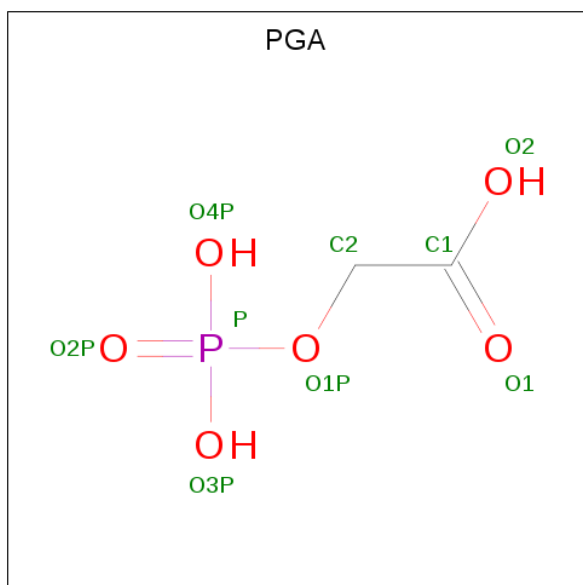
Chain	Residue	Modelled	Actual	Comment	Reference
A	384	MET	THR	engineered mutation	UNP P30613
B	384	MET	THR	engineered mutation	UNP P30613
C	384	MET	THR	engineered mutation	UNP P30613
D	384	MET	THR	engineered mutation	UNP P30613

- Molecule 2 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
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 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			9	2	6	1		
3	B	1	Total	C	O	P	0	0
			9	2	6	1		
3	C	1	Total	C	O	P	0	0
			9	2	6	1		
3	D	1	Total	C	O	P	0	0
			9	2	6	1		

- 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		

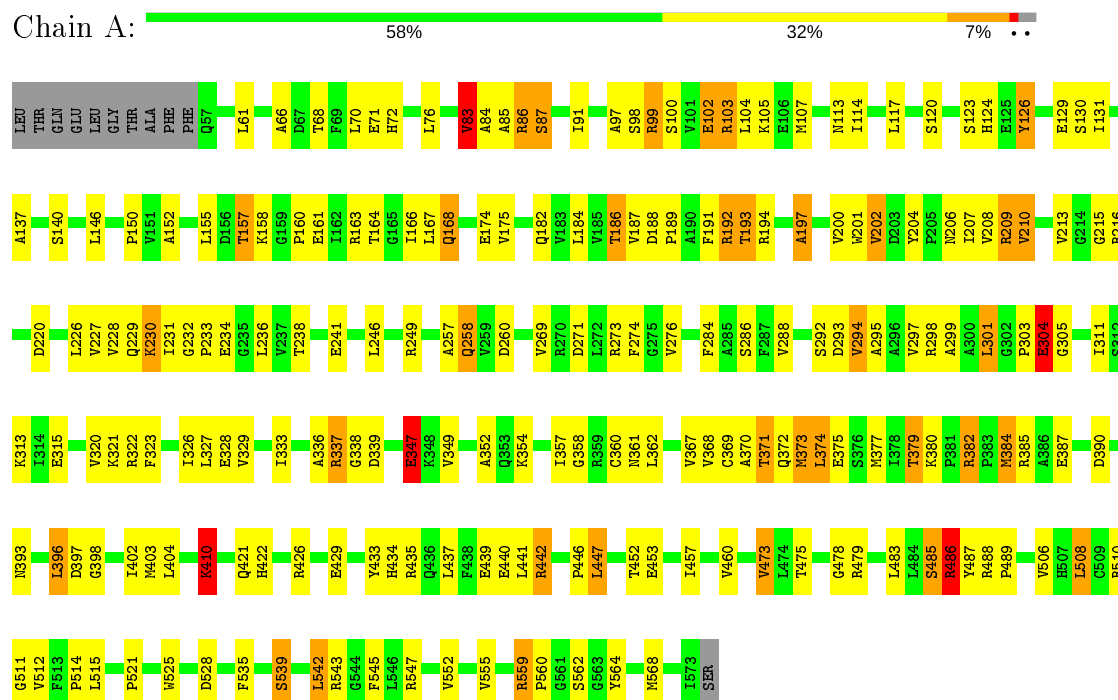
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

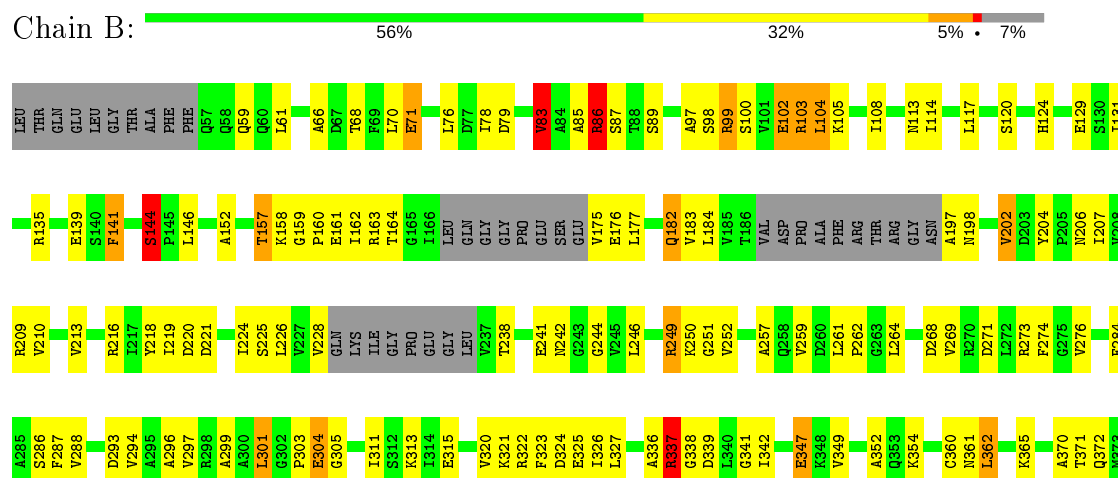
3 Residue-property plots

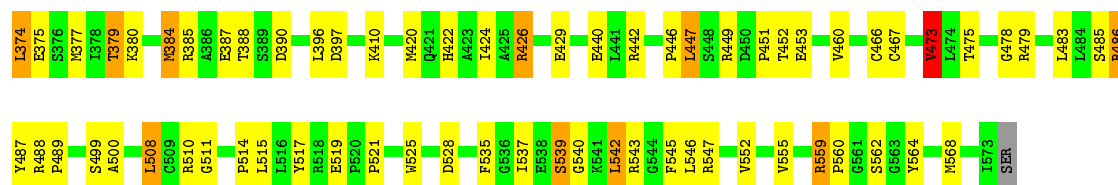
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



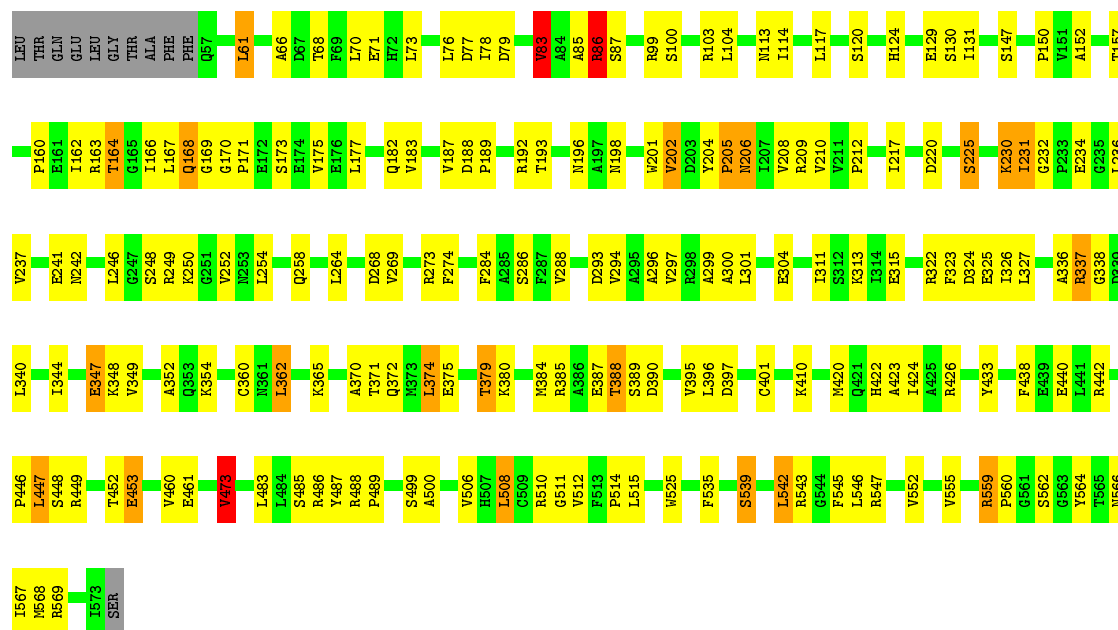
• Molecule 1: PYRUVATE KINASE ISOZYMES R/L





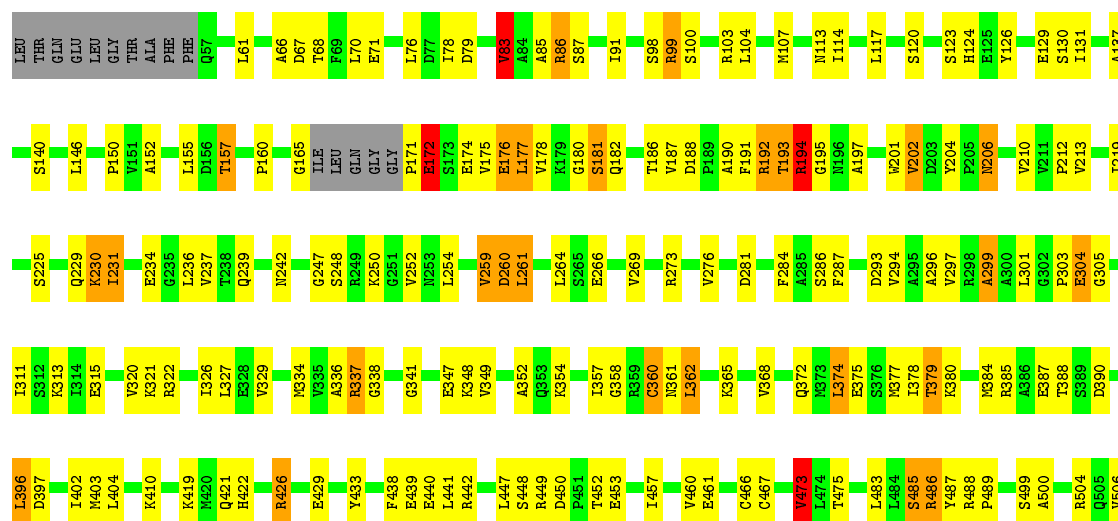
• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

Chain C: 63% 31%



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

Chain D: 58% 32% 6%



L507	L508	C509	R510	G511	V512	F513	F514	L515	P521	L525	D528	F535	S539	L542	R543	G544	F545	L546	R547	V552	V555	T556	G557	M558	R559	P560	G561	S562	G563	Y564	I567	M568	R569	L573	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.30 Å 172.98 Å 85.78 Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 19.98 – 2.75	Depositor EDS
% Data completeness (in resolution range)	93.7 (20.00-2.75) 93.7 (19.98-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.75 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.303 0.320 , 0.339	Depositor DCC
R_{free} test set	1103 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.7	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	0.85	EDS
Total number of atoms	15550	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: K, FBP, PGA, MN

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	1.00	11/3977 (0.3%)	0.94	13/5390 (0.2%)
1	B	1.04	8/3777 (0.2%)	0.90	11/5115 (0.2%)
1	C	1.02	7/3977 (0.2%)	0.89	9/5390 (0.2%)
1	D	1.94	25/3943 (0.6%)	1.24	17/5342 (0.3%)
All	All	1.31	51/15674 (0.3%)	1.00	50/21237 (0.2%)

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
1	D	0	3
All	All	0	4

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	172	GLU	CD-OE1	79.59	2.13	1.25
1	D	194	ARG	CZ-NH1	38.64	1.83	1.33
1	D	230	LYS	CE-NZ	32.91	2.31	1.49
1	D	176	GLU	CD-OE1	27.53	1.55	1.25
1	D	171	PRO	C-N	26.51	1.95	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ARG	NE-CZ-NH1	-43.84	98.38	120.30
1	D	171	PRO	O-C-N	-24.57	83.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	260	ASP	CB-CG-OD1	-23.99	96.71	118.30
1	A	382	ARG	NE-CZ-NH2	-18.45	111.08	120.30
1	D	192	ARG	NE-CZ-NH2	-15.14	112.73	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ARG	Sidechain
1	D	172	GLU	Sidechain
1	D	194	ARG	Sidechain
1	D	260	ASP	Sidechain

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	3913	0	3994	157	0
1	B	3720	0	3804	146	0
1	C	3913	0	3994	130	0
1	D	3880	0	3957	138	0
2	A	20	0	10	1	0
2	B	20	0	10	1	0
2	C	20	0	10	0	0
2	D	20	0	10	2	0
3	A	9	0	2	1	0
3	B	9	0	2	0	0
3	C	9	0	2	0	0
3	D	9	0	2	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15550	0	15797	530	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 17.

The worst 5 of 530 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:230:LYS:CG	1:D:230:LYS:CD	1.79	1.55
1:D:172:GLU:CG	1:D:172:GLU:CD	1.80	1.48
1:D:194:ARG:NH1	1:D:194:ARG:CZ	1.83	1.42
1:B:144:SER:OG	1:B:144:SER:CB	1.70	1.39
1:A:410:LYS:NZ	1:A:410:LYS:CE	1.88	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/528 (98%)	454 (88%)	44 (8%)	17 (3%)	4	5
1	B	483/528 (92%)	436 (90%)	38 (8%)	9 (2%)	8	14
1	C	515/528 (98%)	465 (90%)	37 (7%)	13 (2%)	5	9
1	D	508/528 (96%)	452 (89%)	43 (8%)	13 (3%)	5	8
All	All	2021/2112 (96%)	1807 (89%)	162 (8%)	52 (3%)	5	8

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ARG
1	B	447	LEU

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Mol	Chain	Res	Type
1	C	171	PRO
1	C	433	TYR
1	D	172	GLU

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	414/423 (98%)	366 (88%)	48 (12%)	5	8
1	B	394/423 (93%)	354 (90%)	40 (10%)	7	12
1	C	414/423 (98%)	366 (88%)	48 (12%)	5	8
1	D	411/423 (97%)	364 (89%)	47 (11%)	5	9
All	All	1633/1692 (96%)	1450 (89%)	183 (11%)	6	10

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	546	LEU
1	C	188	ASP
1	D	396	LEU
1	B	559	ARG
1	C	100	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	361	ASN
1	C	124	HIS
1	D	434	HIS
1	B	421	GLN
1	C	133	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FBP	C	580	-	18,20,20	1.08	1 (5%)	23,32,32	0.97	2 (8%)
2	FBP	A	580	-	18,20,20	0.89	1 (5%)	23,32,32	0.88	0
3	PGA	A	581	5,4	5,8,8	0.82	0	6,11,11	0.84	0
2	FBP	B	580	-	18,20,20	1.06	0	23,32,32	0.97	2 (8%)
3	PGA	C	581	5,4	5,8,8	0.96	0	6,11,11	0.88	0
3	PGA	B	581	5,4	5,8,8	0.84	0	6,11,11	1.00	1 (16%)
3	PGA	D	581	5,4	5,8,8	0.73	0	6,11,11	0.79	0
2	FBP	D	580	-	18,20,20	1.06	1 (5%)	23,32,32	1.04	1 (4%)

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	C	580	-	-	5/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	A	580	-	-	5/13/32/32	0/1/1/1
3	PGA	A	581	5,4	-	3/4/6/6	-
2	FBP	B	580	-	-	5/13/32/32	0/1/1/1
3	PGA	C	581	5,4	-	3/4/6/6	-
3	PGA	B	581	5,4	-	3/4/6/6	-
3	PGA	D	581	5,4	-	3/4/6/6	-
2	FBP	D	580	-	-	5/13/32/32	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	580	FBP	O2-C2	2.25	1.44	1.40
2	A	580	FBP	O2-C2	2.04	1.44	1.40
2	D	580	FBP	O2-C2	2.02	1.44	1.40

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	580	FBP	P2-O6-C6	2.51	125.22	118.30
2	B	580	FBP	O2P-P1-O1	2.28	112.81	106.73
2	C	580	FBP	O2P-P1-O1	2.28	112.80	106.73
3	B	581	PGA	O3P-P-O1P	2.20	112.60	106.73
2	B	580	FBP	P2-O6-C6	2.02	123.86	118.30

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	580	FBP	C6-O6-P2-O4P
2	C	580	FBP	C6-O6-P2-O5P
2	A	580	FBP	O5-C5-C6-O6
2	A	580	FBP	C6-O6-P2-O5P
2	A	580	FBP	C6-O6-P2-O6P

There are no ring outliers.

5 monomers are involved in 6 short contacts:

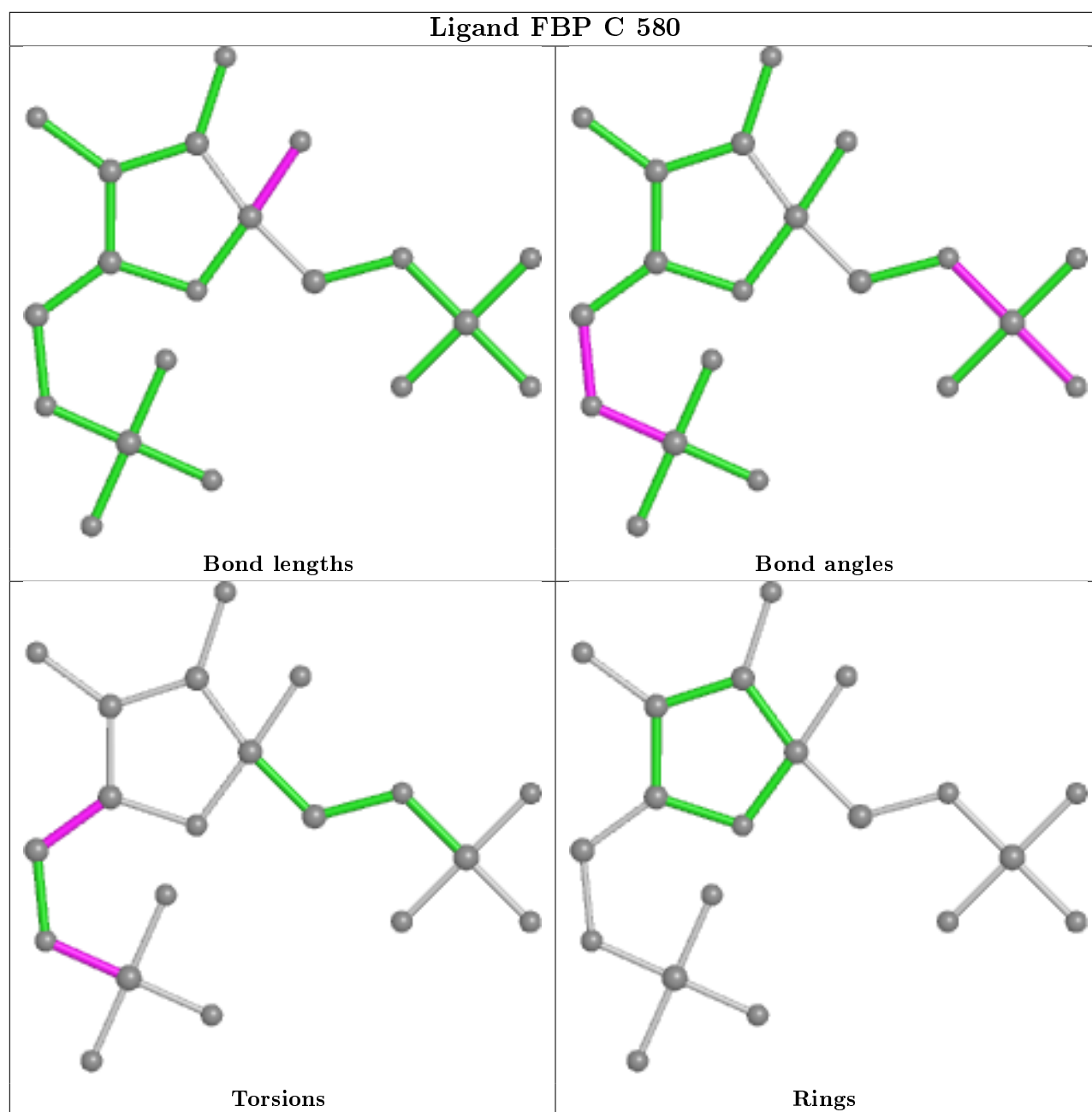
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	580	FBP	1	0

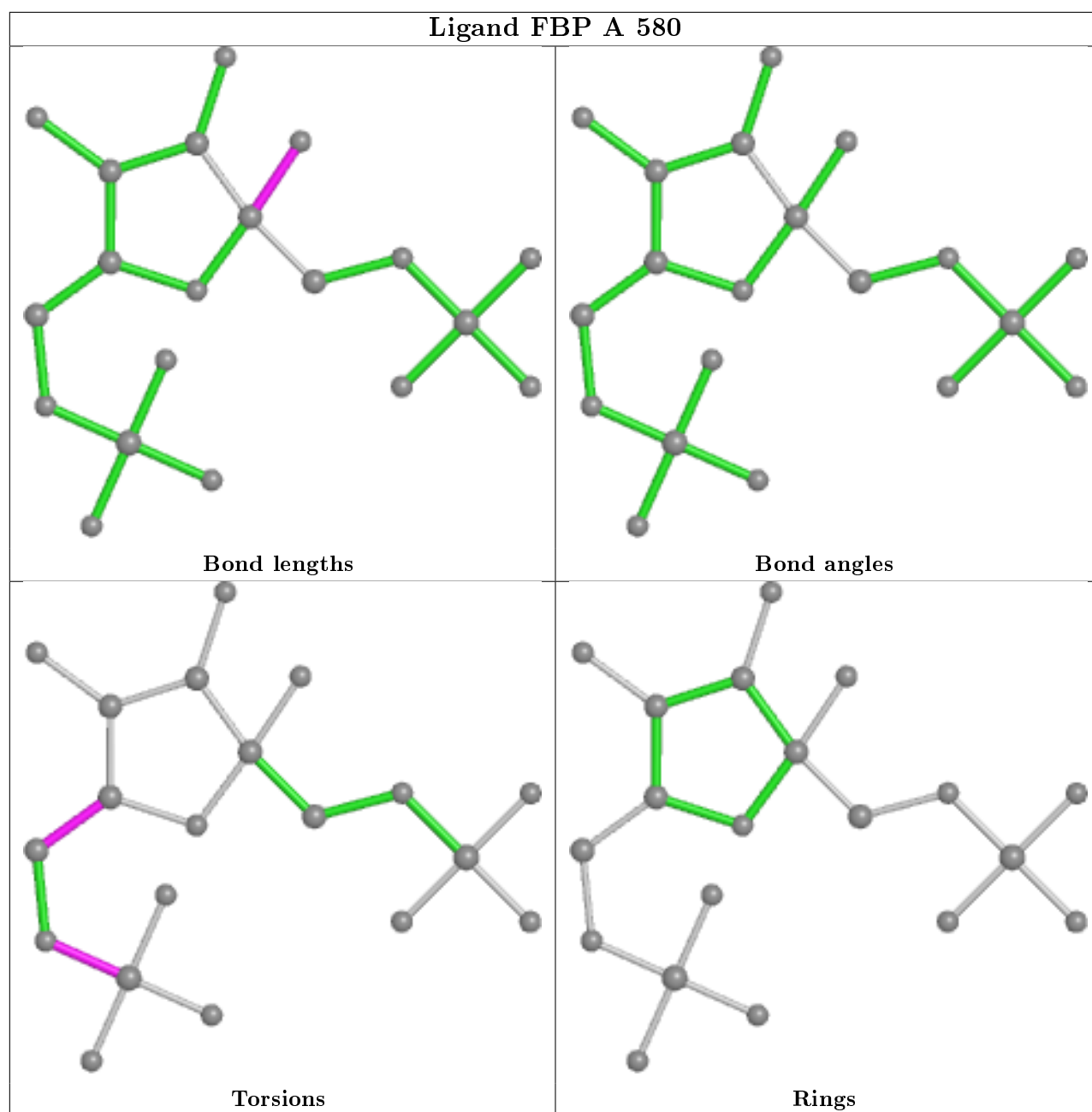
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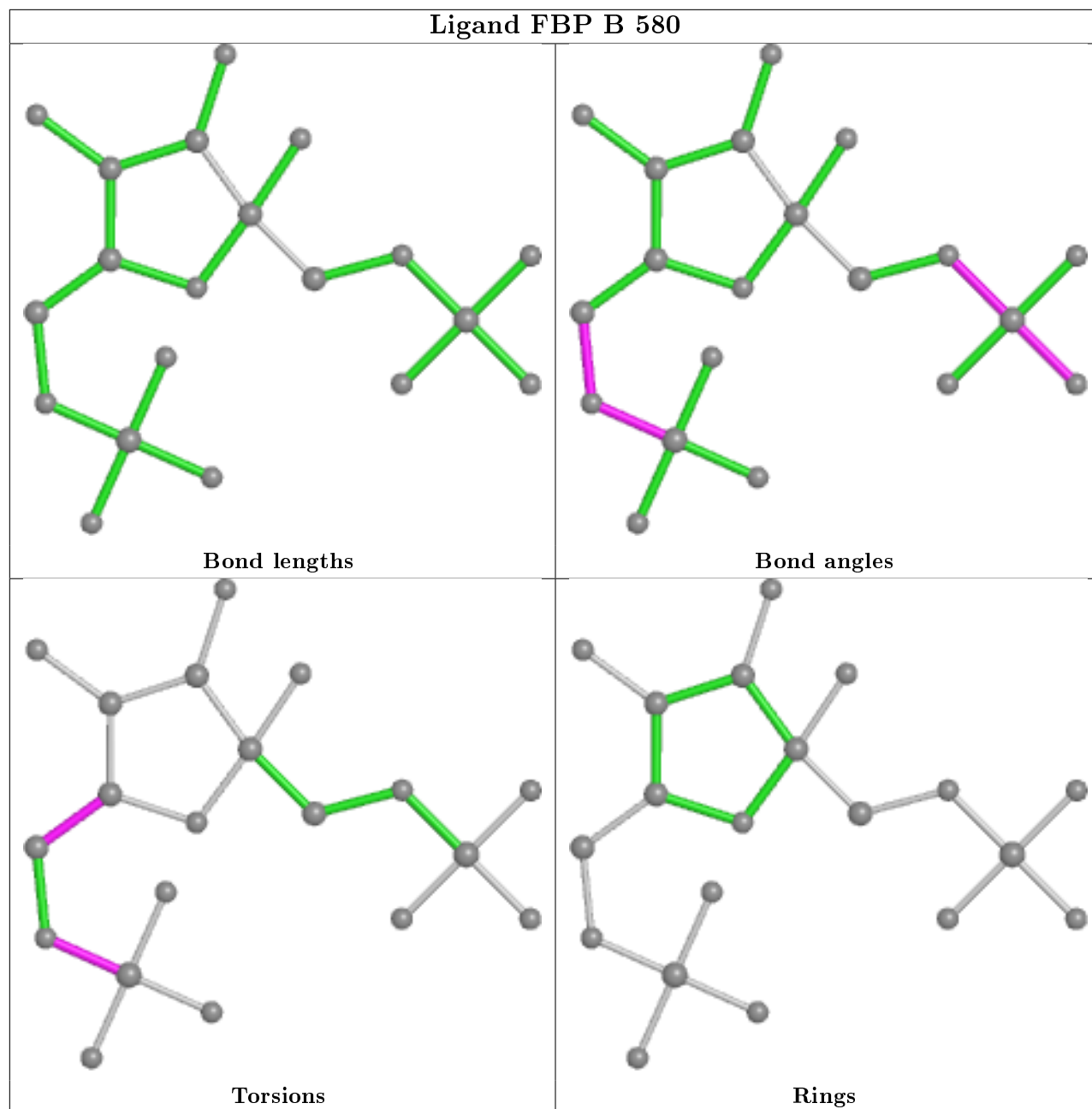
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	581	PGA	1	0
2	B	580	FBP	1	0
3	D	581	PGA	1	0
2	D	580	FBP	2	0

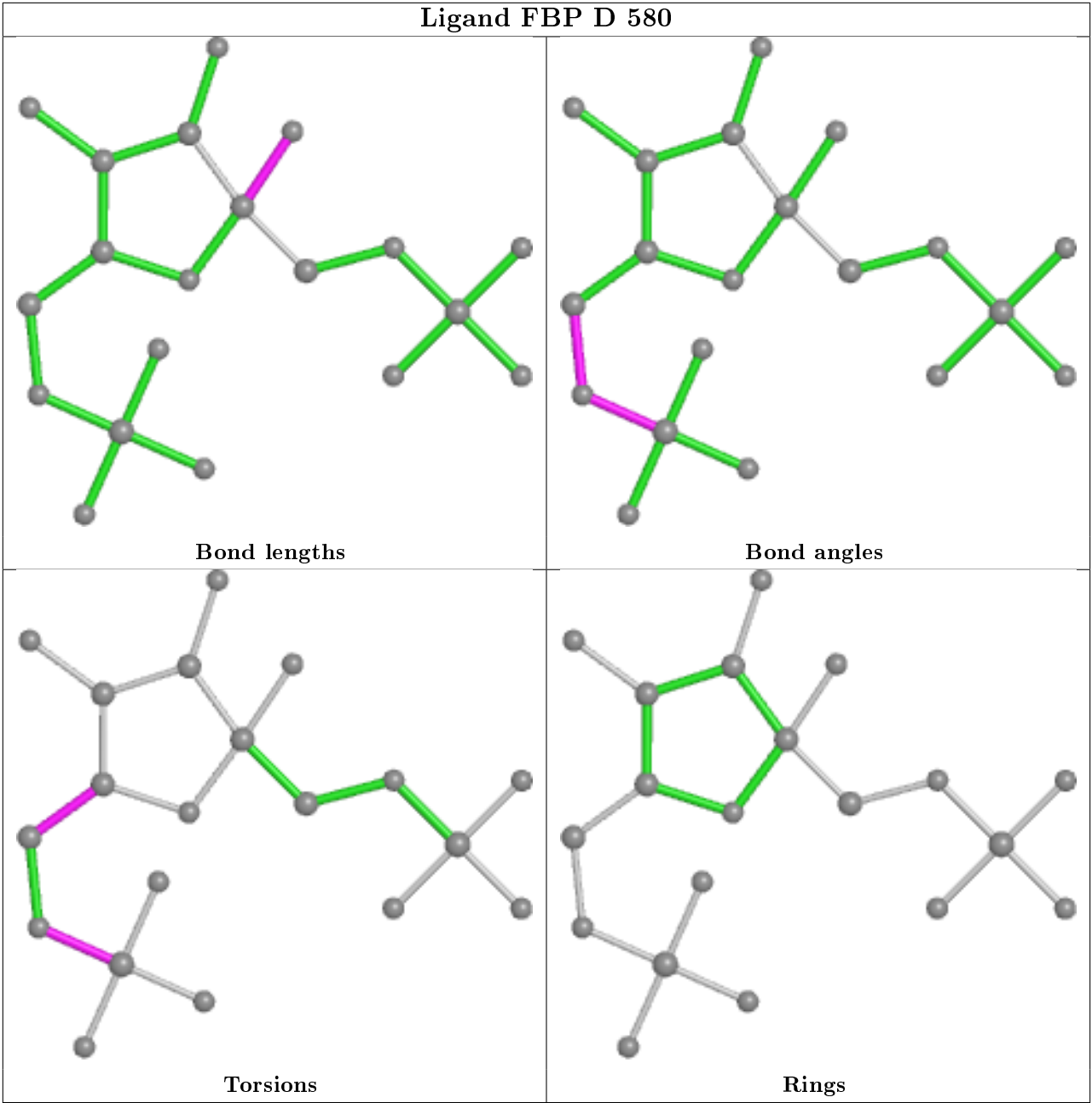
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand FBP B 580





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	171:PRO	C	172:GLU	N	1.95

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

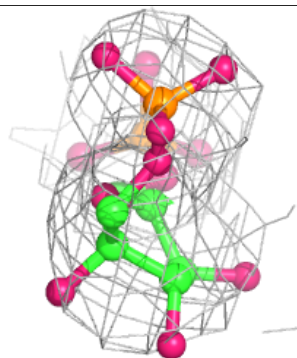
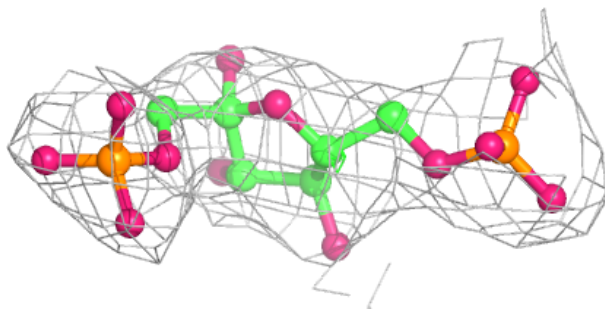
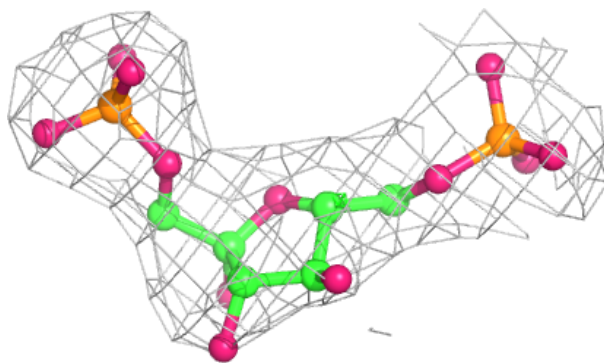
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

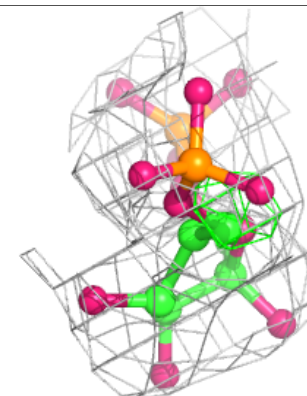
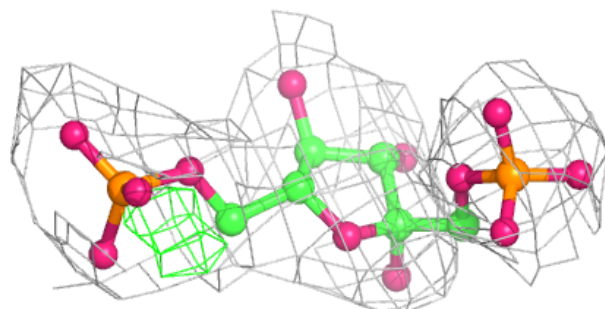
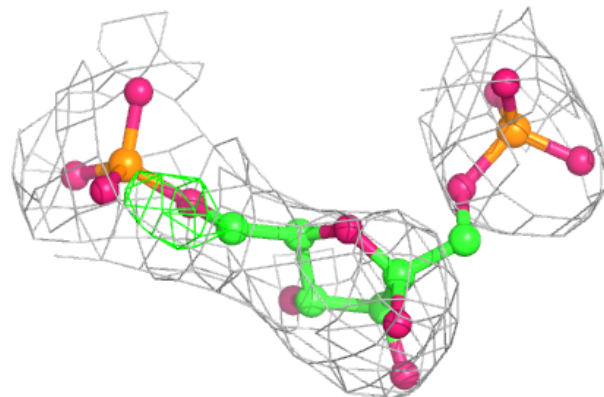
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP C 580:

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

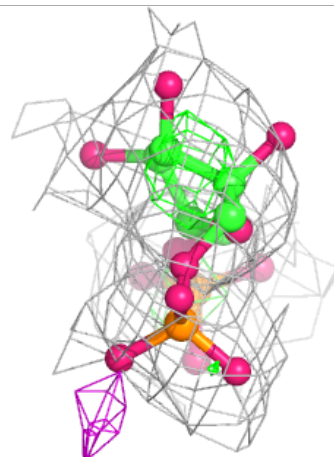
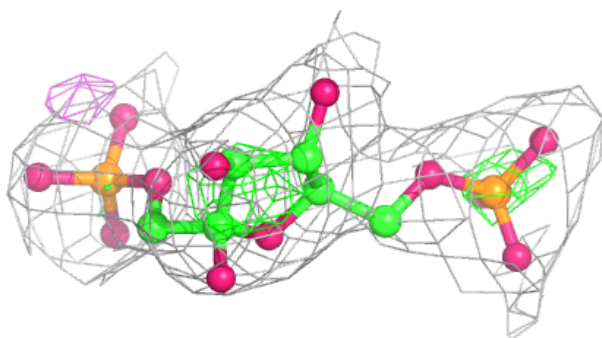
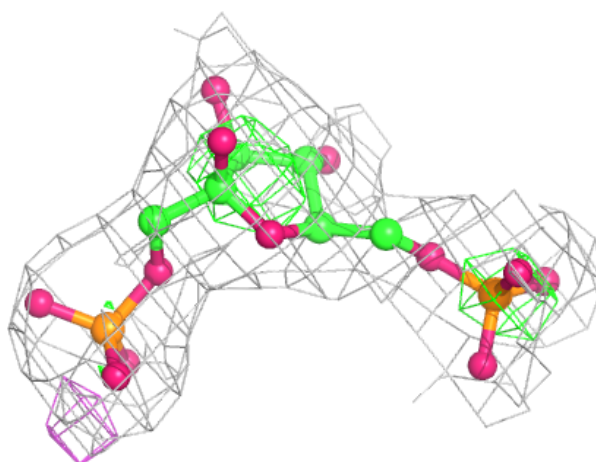
**Electron density around FBP A 580:**

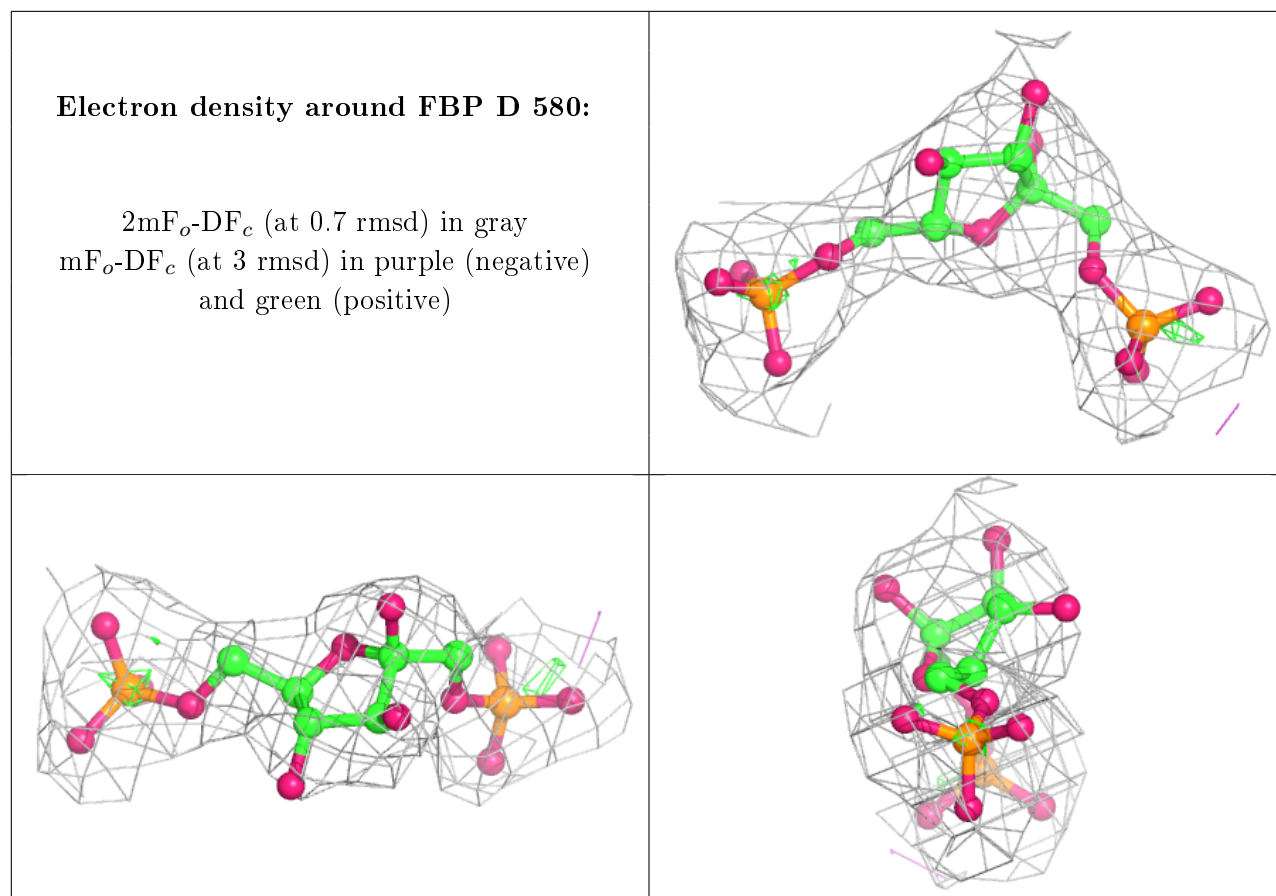
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FBP B 580:

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





6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.