



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:44 AM UTC

PDB ID : 3ME3 / pdb_00003me3
Title : Activator-Bound Structure of Human Pyruvate Kinase M2
Authors : Hong, B.; Dimov, S.; Tempel, W.; Auld, D.; Thomas, C.; Boxer, M.; Jianq, J.-K.; Skoumbourdis, A.; Min, S.; Southall, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Inglese, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2010-03-31
Resolution : 1.95 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](#) ①) 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

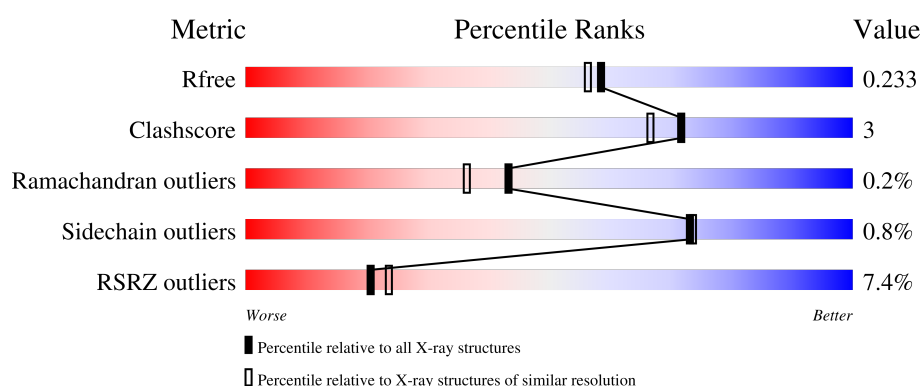
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	550	8% 87% 7% 6%
1	B	550	10% 83% 7% 9%
1	C	550	3% 86% 8% 6%
1	D	550	6% 84% 7% 8%

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
5	UNX	A	533	-	-	-	X
5	UNX	A	534	-	-	-	X
5	UNX	A	535	-	-	-	X
5	UNX	A	536	-	-	-	X
5	UNX	A	537	-	-	-	X
5	UNX	A	538	-	-	-	X
5	UNX	A	539	-	-	-	X
5	UNX	A	542	-	-	-	X
5	UNX	A	543	-	-	-	X
5	UNX	A	544	-	-	-	X
5	UNX	A	545	-	-	-	X
5	UNX	A	546	-	-	-	X
5	UNX	A	547	-	-	-	X
5	UNX	A	548	-	-	-	X
5	UNX	B	533	-	-	-	X
5	UNX	B	534	-	-	-	X
5	UNX	B	535	-	-	-	X
5	UNX	B	537	-	-	-	X
5	UNX	B	538	-	-	-	X
5	UNX	B	539	-	-	-	X
5	UNX	B	540	-	-	-	X
5	UNX	B	542	-	-	-	X
5	UNX	B	543	-	-	-	X
5	UNX	C	533	-	-	-	X
5	UNX	C	534	-	-	-	X
5	UNX	C	535	-	-	-	X
5	UNX	C	536	-	-	-	X
5	UNX	C	537	-	-	-	X
5	UNX	C	538	-	-	-	X
5	UNX	C	539	-	-	-	X
5	UNX	C	540	-	-	-	X
5	UNX	C	542	-	-	-	X
5	UNX	C	543	-	-	-	X
5	UNX	C	544	-	-	-	X
5	UNX	D	533	-	-	-	X
5	UNX	D	534	-	-	-	X
5	UNX	D	535	-	-	-	X
5	UNX	D	536	-	-	-	X
5	UNX	D	537	-	-	-	X
5	UNX	D	538	-	-	-	X
5	UNX	D	539	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16045 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 M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3854	2427	676	726	25			
1	B	498	Total	C	N	O	S	0	1	0
			3702	2323	664	691	24			
1	C	517	Total	C	N	O	S	0	0	0
			3866	2436	680	726	24			
1	D	504	Total	C	N	O	S	0	3	0
			3745	2360	663	698	24			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	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	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
B	-18	MET	-	expression tag	UNP P14618
B	-17	GLY	-	expression tag	UNP P14618

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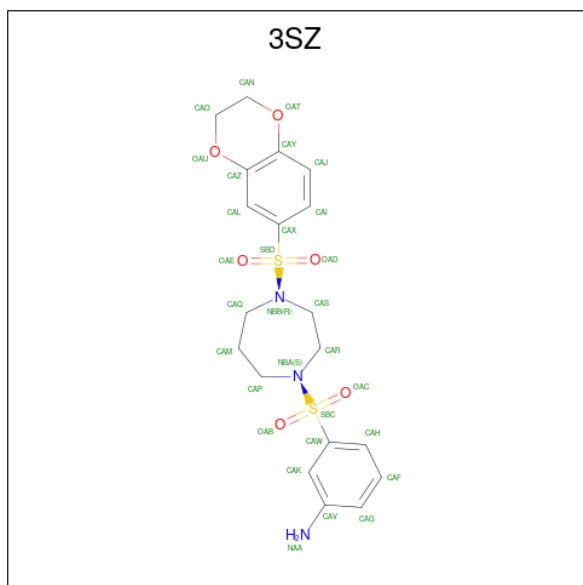
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
C	-18	MET	-	expression tag	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	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	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
D	-18	MET	-	expression tag	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618

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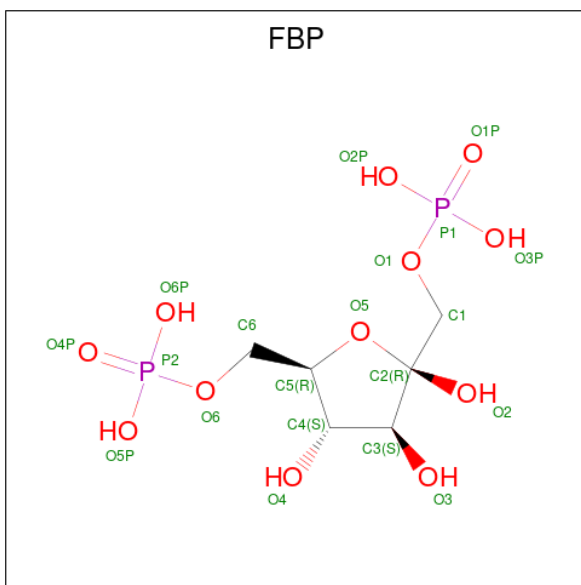
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618

- Molecule 2 is 3-{[4-(2,3-dihydro-1,4-benzodioxin-6-ylsulfonyl)-1,4-diazepan-1-yl]sulfonyl}aniline (CCD ID: 3SZ) (formula: C₁₉H₂₃N₃O₆S₂).



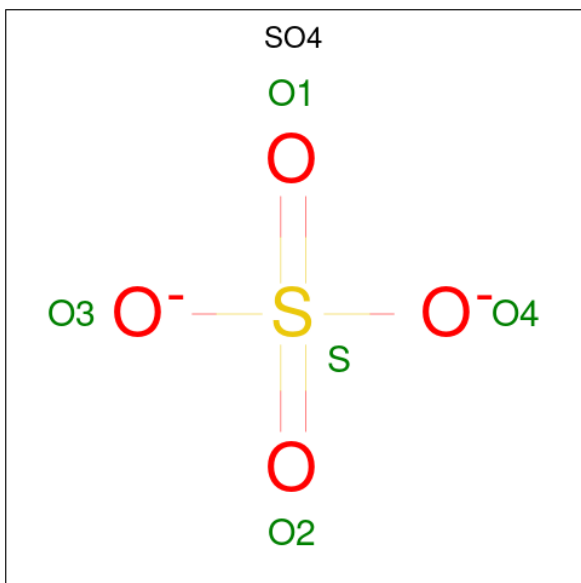
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	19	3	6	2		
2	D	1	Total	C	N	O	S	0	0
			30	19	3	6	2		

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C₆H₁₄O₁₂P₂).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total X 14 14	0	0
5	B	10	Total X 10 10	0	0
5	C	11	Total X 11 11	0	0
5	D	7	Total X 7 7	0	0

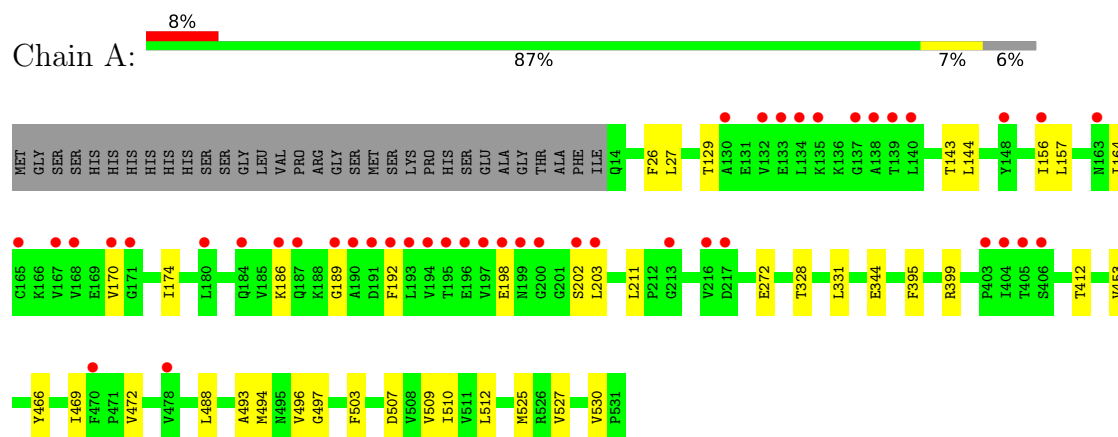
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	185	Total O 186 186	0	1
6	B	171	Total O 171 171	0	0
6	C	166	Total O 166 166	0	0
6	D	153	Total O 153 153	0	0

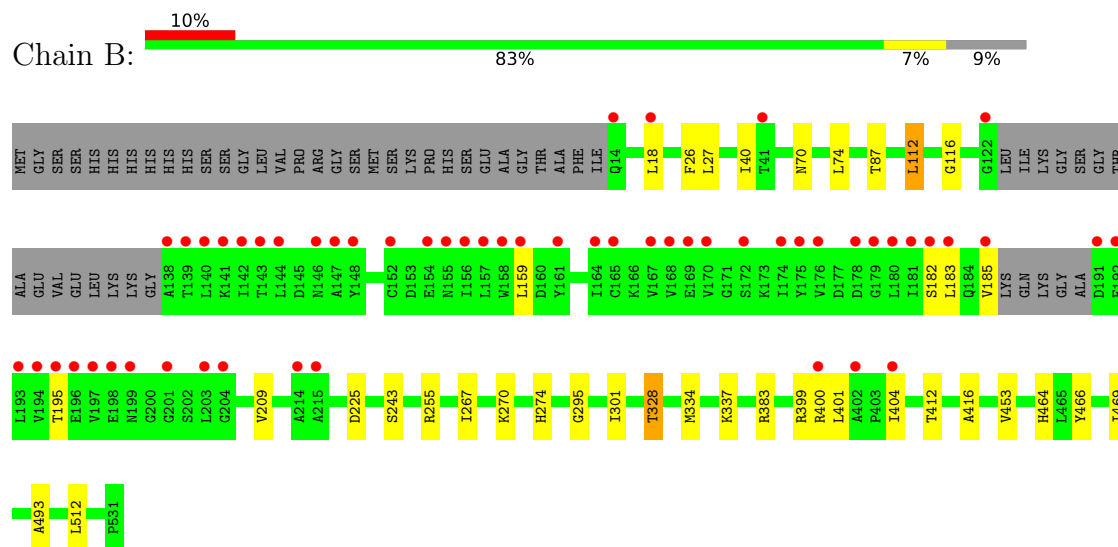
3 Residue-property plots [i](#)

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

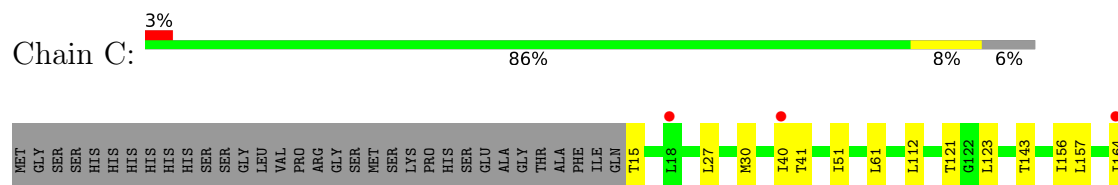
• Molecule 1: Pyruvate kinase isozymes M1/M2

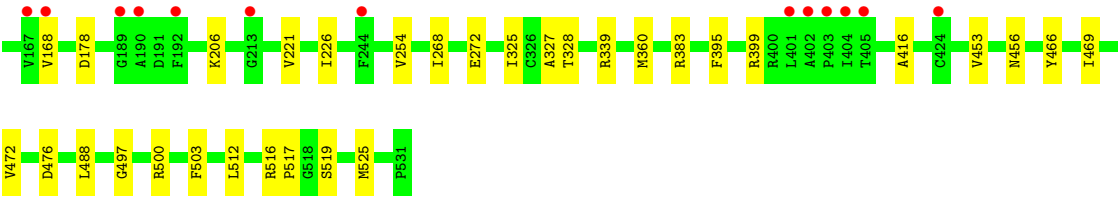


• Molecule 1: Pyruvate kinase isozymes M1/M2

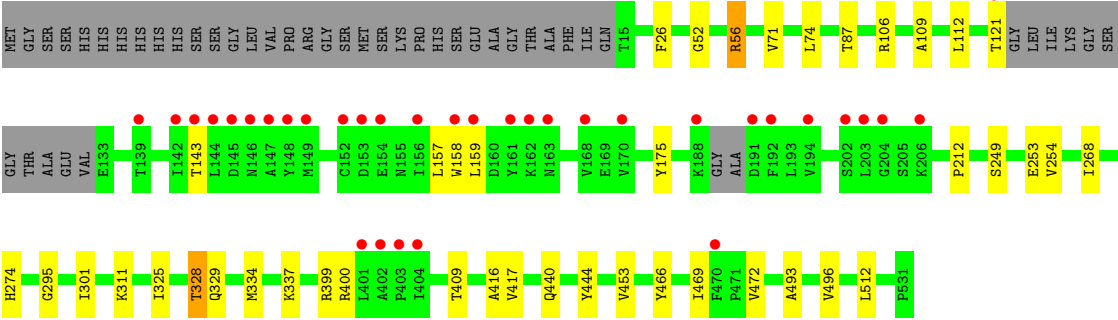
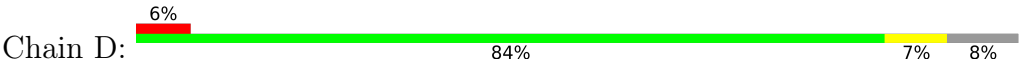


• Molecule 1: Pyruvate kinase isozymes M1/M2





● Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.88Å 152.56Å 93.04Å 90.00° 103.17° 90.00°	Depositor
Resolution (Å)	26.71 – 1.95 26.71 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.71-1.95) 99.6 (26.71-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.219 , 0.262 (Not available) , 0.233	Depositor DCC
R_{free} test set	1917 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16045	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, SO4, 3SZ, UNX

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	0.86	0/3918	0.88	0/5311
1	B	0.86	0/3765	0.91	0/5103
1	C	0.86	1/3930 (0.0%)	0.90	0/5325
1	D	0.85	1/3816 (0.0%)	0.89	0/5176
All	All	0.86	2/15429 (0.0%)	0.90	0/20915

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	254	VAL	CA-CB	6.12	1.62	1.54
1	C	254	VAL	CA-CB	5.64	1.61	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3854	0	3804	22	0
1	B	3702	0	3627	26	0
1	C	3866	0	3846	28	0
1	D	3745	0	3657	27	0
2	A	30	0	23	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	30	0	23	2	0
3	A	20	0	10	0	0
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	14	0	0	0	0
5	B	10	0	0	0	0
5	C	11	0	0	0	0
5	D	7	0	0	0	0
6	A	186	0	0	0	0
6	B	171	0	0	1	0
6	C	166	0	0	0	0
6	D	153	0	0	1	0
All	All	16045	0	15020	99	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 3.

All (99) 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:C:395:PHE:CZ	1:C:399:ARG:HD2	2.07	0.88
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.76	0.67
1:D:409:THR:CG2	1:D:440:GLN:OE1	2.42	0.67
1:B:112:LEU:HD23	1:B:112:LEU:C	2.20	0.67
1:A:144:LEU:HD11	1:A:164:ILE:HG22	1.79	0.64
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.79	0.63
1:A:395:PHE:CZ	1:A:399:ARG:HD2	2.34	0.63
1:D:409:THR:HG21	1:D:440:GLN:OE1	1.99	0.62
1:B:399:ARG:NH2	1:D:399:ARG:CD	2.65	0.60
1:B:182:SER:O	1:B:183:LEU:HD23	2.02	0.60
1:C:416:ALA:CB	1:C:512:LEU:HD21	2.33	0.58
1:C:488:LEU:HD23	1:C:488:LEU:O	2.06	0.56
1:A:525:MET:HE3	1:C:525:MET:HE3	1.87	0.56
1:A:27:LEU:HD23	1:B:401:LEU:HD12	1.87	0.55
1:C:488:LEU:HD23	1:C:488:LEU:C	2.32	0.55
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:THR:HG22	1:B:512:LEU:HD22	1.89	0.54
1:D:106[B]:ARG:CG	6:D:605:HOH:O	2.55	0.54
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.90	0.53
1:A:494:MET:HE1	1:A:509:VAL:HG21	1.90	0.53
2:A:540:3SZ:CAN	1:B:27:LEU:HD13	2.37	0.53
1:A:494:MET:HE1	1:A:509:VAL:CG2	2.39	0.53
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.92	0.52
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.45	0.52
1:D:249:SER:O	1:D:253:GLU:HG3	2.09	0.51
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.93	0.51
1:B:112:LEU:C	1:B:112:LEU:CD2	2.85	0.50
1:C:395:PHE:CE2	1:C:399:ARG:HD2	2.45	0.50
1:B:116:GLY:HA2	1:B:225:ASP:OD2	2.12	0.50
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.93	0.50
1:C:395:PHE:CE1	1:C:399:ARG:HD2	2.47	0.49
1:C:121:THR:HB	1:C:157:LEU:HD11	1.95	0.49
1:D:274:HIS:CE1	1:D:301:ILE:HG22	2.48	0.49
1:C:327:ALA:HB1	1:C:360:MET:HE2	1.95	0.48
1:C:123:LEU:HD21	1:C:206:LYS:HE3	1.95	0.48
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.97	0.47
1:C:453:VAL:HG22	1:C:472:VAL:CG2	2.45	0.47
2:A:540:3SZ:HAMA	1:B:26:PHE:CZ	2.49	0.46
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.45	0.46
1:D:175:TYR:CE1	1:D:212:PRO:HG3	2.51	0.46
1:D:74:LEU:HD21	1:D:87:THR:HG21	1.97	0.46
1:A:507:ASP:O	1:A:530:VAL:HG23	2.16	0.46
1:C:27:LEU:HD13	2:D:540:3SZ:CAN	2.46	0.46
1:D:268:ILE:HG21	1:D:325:ILE:HD12	1.97	0.46
1:C:476:ASP:OD2	1:C:488:LEU:HD21	2.16	0.46
1:C:30:MET:HE2	1:D:311:LYS:O	2.16	0.46
1:A:143:THR:HG21	1:A:156:ILE:HD11	1.97	0.45
1:A:488:LEU:C	1:A:488:LEU:HD23	2.41	0.45
1:D:112:LEU:C	1:D:112:LEU:HD23	2.41	0.45
1:A:510:ILE:HD12	1:A:527:VAL:HG22	1.98	0.45
1:D:121:THR:HB	1:D:157:LEU:HD11	1.99	0.45
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.97	0.45
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.98	0.45
1:C:516:ARG:HB2	1:C:517:PRO:CD	2.47	0.45
1:D:409:THR:HG22	1:D:440:GLN:OE1	2.13	0.45
1:D:52:GLY:O	1:D:56:ARG:HB3	2.17	0.45
1:A:412:THR:HG22	1:A:512:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:GLY:CA	1:D:328:THR:HG21	2.48	0.44
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.99	0.44
1:B:404:ILE:HD12	1:B:404:ILE:N	2.33	0.44
1:C:268:ILE:HG21	1:C:325:ILE:HD12	1.99	0.44
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.99	0.44
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.54	0.43
1:C:51:ILE:HD12	1:C:61:LEU:HD21	2.01	0.43
1:D:417:VAL:HG21	1:D:444:TYR:HB2	1.99	0.43
1:A:157:LEU:HD13	1:A:203:LEU:HD21	2.01	0.43
1:B:40:ILE:O	1:B:383:ARG:HD2	2.18	0.43
1:B:185:VAL:HA	1:B:195:THR:HG22	1.99	0.43
1:A:26:PHE:CE1	2:A:540:3SZ:HAPA	2.54	0.43
1:C:112:LEU:C	1:C:112:LEU:HD23	2.43	0.43
1:B:274:HIS:HB2	6:B:594:HOH:O	2.18	0.42
1:A:174:ILE:HG12	1:A:211:LEU:HD22	2.02	0.42
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.48	0.42
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.49	0.42
1:B:334:MET:HA	1:B:337:LYS:O	2.20	0.42
1:D:334:MET:HA	1:D:337:LYS:O	2.20	0.42
1:B:18:LEU:HD23	1:B:18:LEU:HA	1.84	0.42
1:C:143:THR:CG2	1:C:156:ILE:HD11	2.50	0.42
1:D:453:VAL:HG21	1:D:493:ALA:HB2	2.00	0.42
1:C:164:ILE:O	1:C:168:VAL:HG22	2.19	0.42
1:C:178:ASP:O	1:C:178:ASP:CG	2.62	0.42
1:A:170:VAL:HG13	1:A:186:LYS:O	2.20	0.41
1:A:189:GLY:HA3	1:A:192:PHE:CZ	2.56	0.41
1:D:26:PHE:CG	2:D:540:3SZ:HAR	2.55	0.41
1:D:143:THR:O	1:D:158:TRP:HA	2.20	0.41
1:D:121:THR:HG22	1:D:159:LEU:CD2	2.51	0.41
1:C:40:ILE:O	1:C:383:ARG:HD2	2.21	0.41
1:C:221:VAL:HG12	1:C:226:ILE:HG13	2.03	0.41
1:C:456:ASN:OD1	1:C:456:ASN:C	2.63	0.41
1:D:71:VAL:HG22	1:D:109:ALA:HB3	2.02	0.41
1:B:295:GLY:CA	1:B:328:THR:HG21	2.51	0.41
1:A:331:LEU:HD23	1:A:344:GLU:HB3	2.03	0.40
1:B:74:LEU:HD21	1:B:87:THR:CG2	2.50	0.40
1:C:41:THR:HG21	1:C:500:ARG:O	2.20	0.40
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.51	0.40
1:B:70:ASN:HB3	1:B:464:HIS:CG	2.56	0.40
1:B:159:LEU:CD2	1:B:209:VAL:HG21	2.51	0.40
2:A:540:3SZ:HAS	1:B:26:PHE:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:SER:HA	1:B:270:LYS:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	516/550 (94%)	504 (98%)	11 (2%)	1 (0%)	43	36
1	B	493/550 (90%)	482 (98%)	10 (2%)	1 (0%)	43	36
1	C	515/550 (94%)	505 (98%)	9 (2%)	1 (0%)	43	36
1	D	501/550 (91%)	490 (98%)	10 (2%)	1 (0%)	43	36
All	All	2025/2200 (92%)	1981 (98%)	40 (2%)	4 (0%)	43	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	D	328	THR

5.3.2 Protein sidechains [i](#)

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	392/452 (87%)	388 (99%)	4 (1%)	68	67
1	B	372/452 (82%)	369 (99%)	3 (1%)	73	74
1	C	397/452 (88%)	393 (99%)	4 (1%)	68	67
1	D	374/452 (83%)	372 (100%)	2 (0%)	81	82
All	All	1535/1808 (85%)	1522 (99%)	13 (1%)	73	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	198	GLU
1	A	202	SER
1	A	272	GLU
1	B	112	LEU
1	B	301	ILE
1	B	400	ARG
1	C	15	THR
1	C	272	GLU
1	C	339	ARG
1	C	519	SER
1	D	56	ARG
1	D	400	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	458	GLN
1	B	44	ASN
1	B	210	ASN
1	B	252	HIS
1	B	378	GLN
1	B	458	GLN
1	C	78	HIS
1	C	199	ASN
1	D	44	ASN
1	D	184	GLN
1	D	210	ASN
1	D	378	GLN
1	D	458	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 42 are unknown - leaving 10 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	C	541	-	18,20,20	0.98	1 (5%)	21,32,32	1.12	2 (9%)
4	SO4	D	532	-	4,4,4	0.31	0	6,6,6	0.26	0
4	SO4	B	532	-	4,4,4	0.40	0	6,6,6	0.26	0
4	SO4	A	532	-	4,4,4	0.33	0	6,6,6	0.36	0
3	FBP	B	541	-	18,20,20	0.79	0	21,32,32	1.05	1 (4%)
3	FBP	A	541	-	18,20,20	0.87	1 (5%)	21,32,32	1.07	2 (9%)
3	FBP	D	541	-	18,20,20	0.92	1 (5%)	21,32,32	1.09	1 (4%)
2	3SZ	D	540	-	33,33,33	2.54	9 (27%)	47,49,49	1.85	10 (21%)
4	SO4	C	532	-	4,4,4	0.18	0	6,6,6	0.25	0
2	3SZ	A	540	-	33,33,33	2.45	5 (15%)	47,49,49	2.09	9 (19%)

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	C	541	-	-	2/13/32/32	0/1/1/1
3	FBP	B	541	-	-	2/13/32/32	0/1/1/1
3	FBP	A	541	-	-	2/13/32/32	0/1/1/1
3	FBP	D	541	-	-	2/13/32/32	0/1/1/1
2	3SZ	D	540	-	-	3/24/42/42	0/4/4/4
2	3SZ	A	540	-	-	0/24/42/42	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	540	3SZ	OAD-SBD	7.23	1.51	1.43
2	D	540	3SZ	OAB-SBC	7.23	1.51	1.43
2	A	540	3SZ	OAB-SBC	7.08	1.51	1.43
2	A	540	3SZ	OAE-SBD	6.49	1.50	1.43
2	D	540	3SZ	OAD-SBD	6.25	1.50	1.43
2	A	540	3SZ	OAC-SBC	5.73	1.49	1.43
2	D	540	3SZ	OAC-SBC	5.34	1.49	1.43
2	D	540	3SZ	OAE-SBD	4.85	1.48	1.43
2	D	540	3SZ	CAX-SBD	-4.33	1.70	1.76
2	D	540	3SZ	SBC-NBA	4.15	1.69	1.63
2	D	540	3SZ	CAW-SBC	-3.28	1.72	1.76
3	C	541	FBP	O2-C2	3.18	1.46	1.40
3	D	541	FBP	O2-C2	3.02	1.45	1.40
3	A	541	FBP	O2-C2	2.24	1.44	1.40
2	D	540	3SZ	OAT-CAN	2.21	1.48	1.43
2	D	540	3SZ	CAP-NBA	-2.10	1.45	1.48
2	A	540	3SZ	OAT-CAN	2.01	1.48	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	540	3SZ	OAC-SBC-OAB	-6.90	108.83	119.59
2	A	540	3SZ	CAW-SBC-NBA	6.27	114.85	107.28
2	A	540	3SZ	OAE-SBD-OAD	-5.72	110.67	119.59
2	D	540	3SZ	OAE-SBD-OAD	-4.41	112.70	119.59
2	A	540	3SZ	OAD-SBD-NBB	4.20	110.64	106.69
2	D	540	3SZ	OAC-SBC-OAB	-3.95	113.42	119.59
2	A	540	3SZ	CAX-SBD-NBB	3.85	111.93	107.28
2	D	540	3SZ	OAE-SBD-CAX	3.80	112.82	108.10
2	D	540	3SZ	CAH-CAW-SBC	-3.78	115.98	119.73
2	D	540	3SZ	CAW-SBC-NBA	3.60	111.63	107.28
2	D	540	3SZ	CAS-NBB-CAQ	3.51	126.65	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	540	3SZ	CAK-CAW-SBC	3.41	123.01	119.30
3	B	541	FBP	O6-P2-O4P	3.30	115.36	106.44
2	D	540	3SZ	OAC-SBC-CAW	2.93	111.74	108.10
2	A	540	3SZ	CAS-NBB-CAQ	2.75	124.20	115.28
2	D	540	3SZ	CAV-CAK-CAW	-2.73	117.94	120.05
3	C	541	FBP	O6-P2-O4P	2.68	113.68	106.44
3	A	541	FBP	O3P-P1-O1P	2.57	120.85	110.83
2	D	540	3SZ	OAD-SBD-NBB	2.50	109.04	106.69
2	A	540	3SZ	CAK-CAW-SBC	2.47	121.99	119.30
2	A	540	3SZ	OAB-SBC-NBA	2.46	109.00	106.69
2	A	540	3SZ	OAC-SBC-CAW	2.20	110.84	108.10
3	A	541	FBP	O6-P2-O4P	2.18	112.33	106.44
3	D	541	FBP	O1-P1-O1P	-2.04	100.92	106.44
3	C	541	FBP	O5-C5-C6	2.03	114.28	109.50

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	541	FBP	C4-C5-C6-O6
3	B	541	FBP	C4-C5-C6-O6
3	C	541	FBP	C4-C5-C6-O6
3	D	541	FBP	C4-C5-C6-O6
3	A	541	FBP	O5-C5-C6-O6
3	B	541	FBP	O5-C5-C6-O6
3	C	541	FBP	O5-C5-C6-O6
2	D	540	3SZ	CAP-NBA-SBC-OAC
2	D	540	3SZ	CAQ-NBB-SBD-OAD
2	D	540	3SZ	CAS-NBB-SBD-OAE
3	D	541	FBP	O5-C5-C6-O6

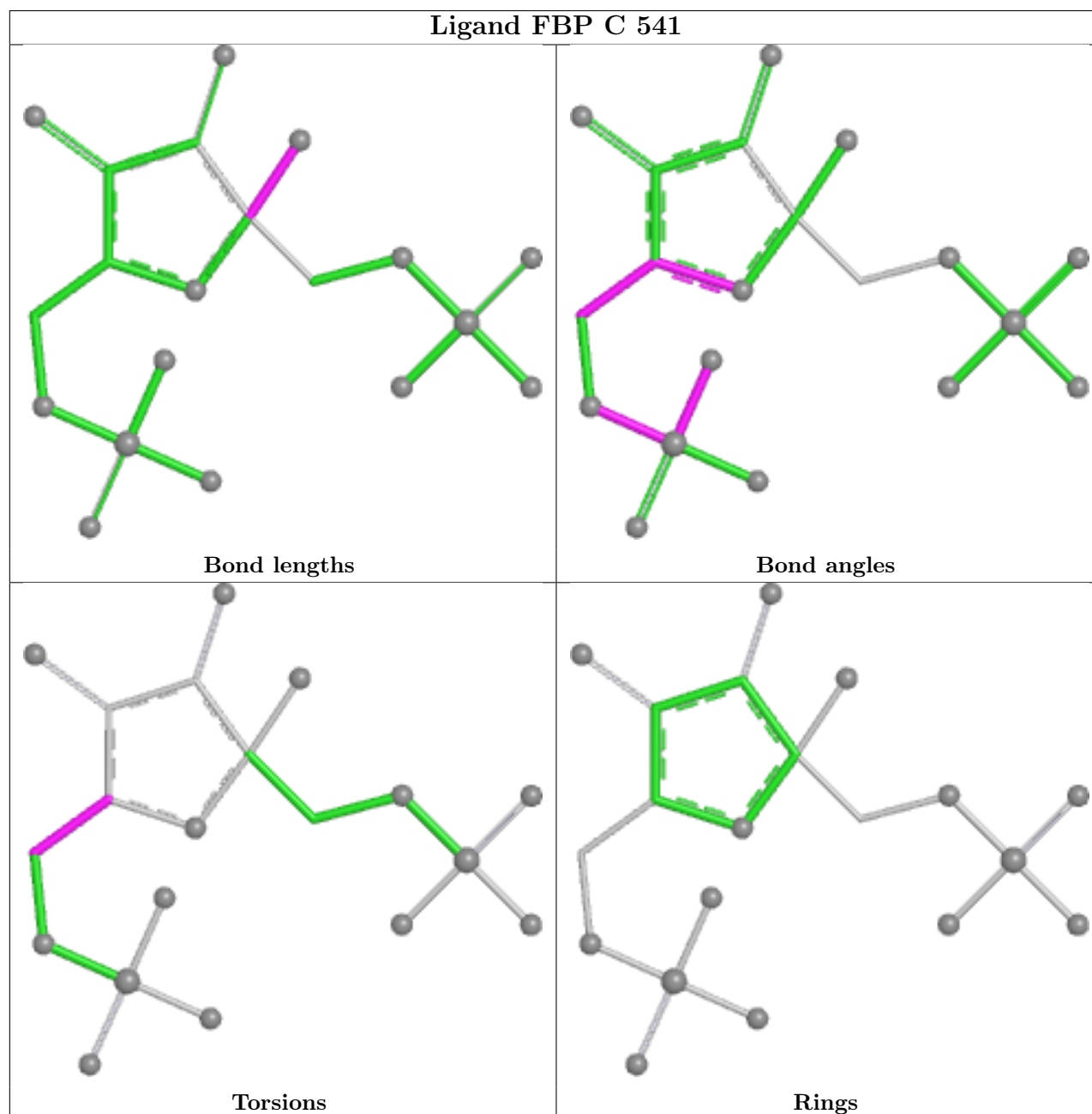
There are no ring outliers.

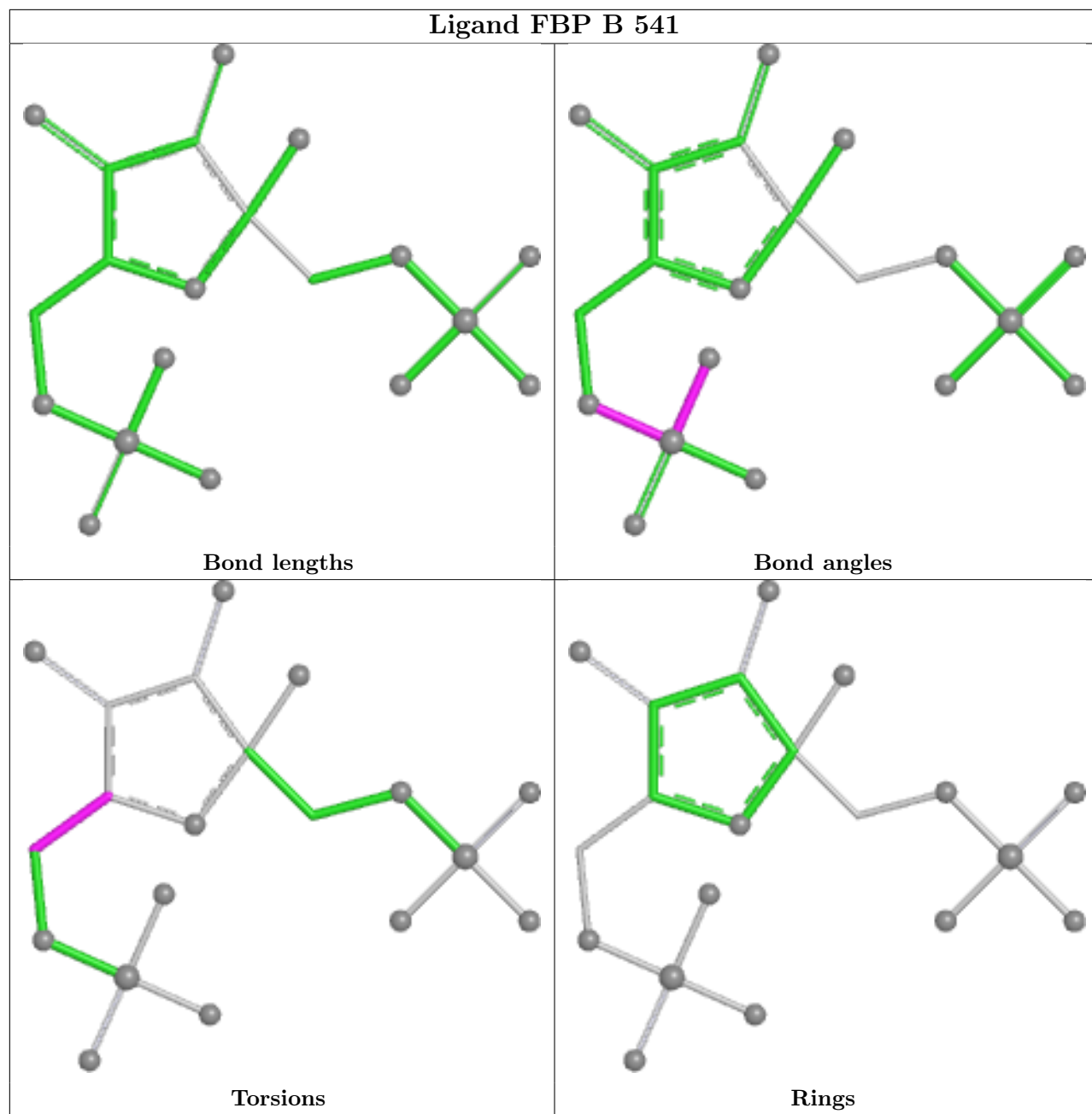
2 monomers are involved in 6 short contacts:

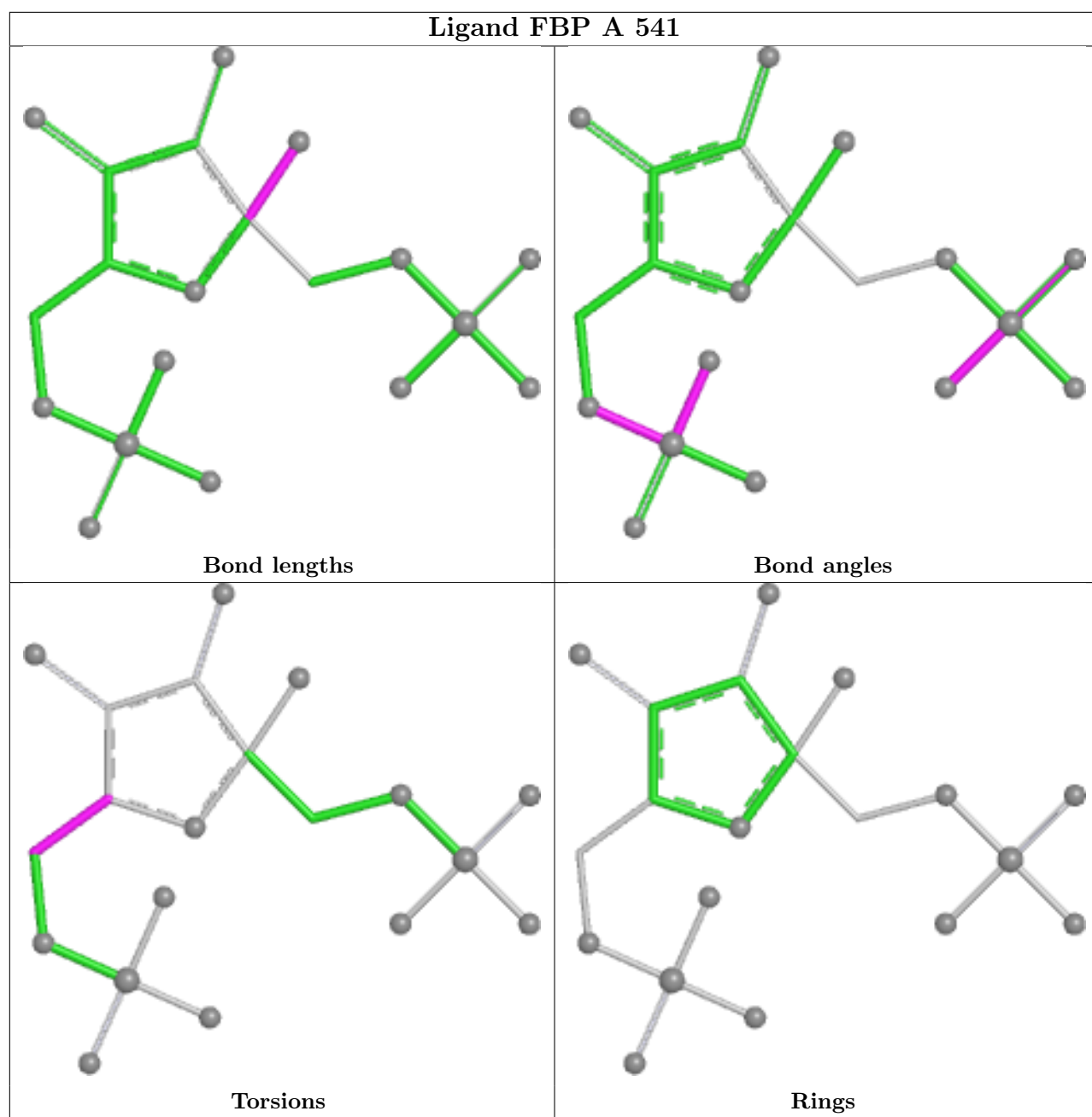
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	540	3SZ	2	0
2	A	540	3SZ	4	0

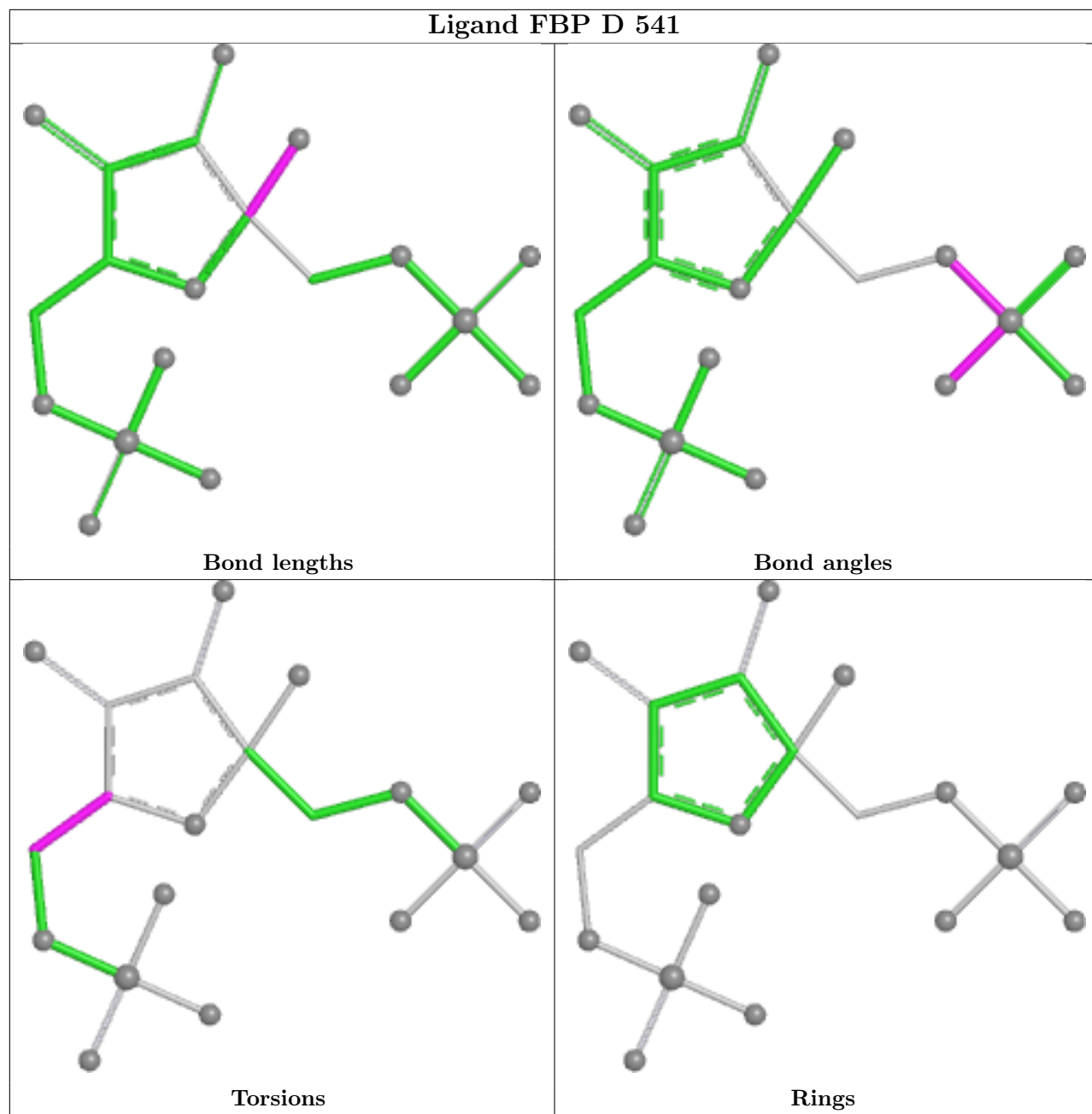
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

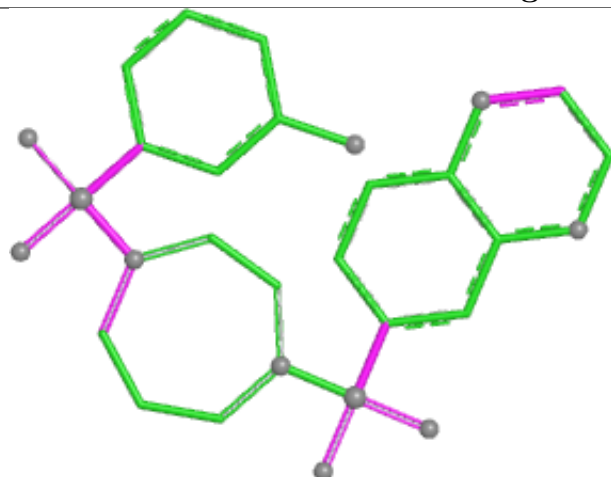




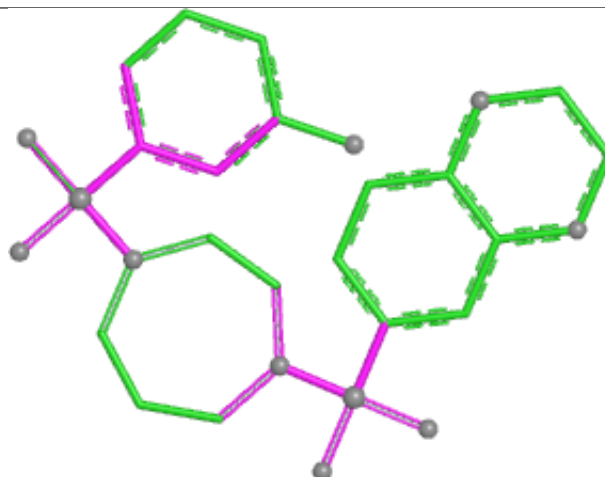




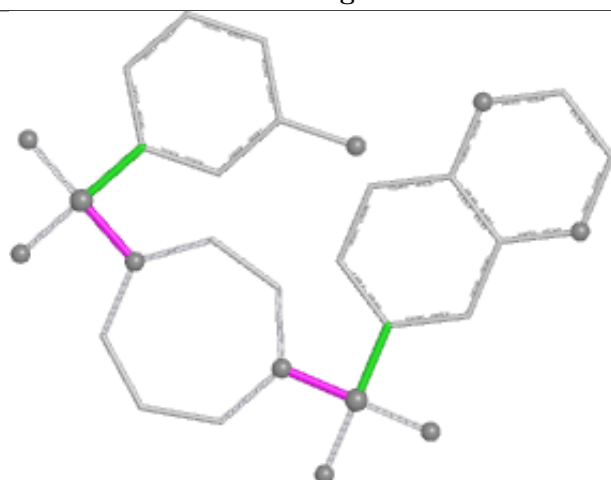
Ligand 3SZ D 540



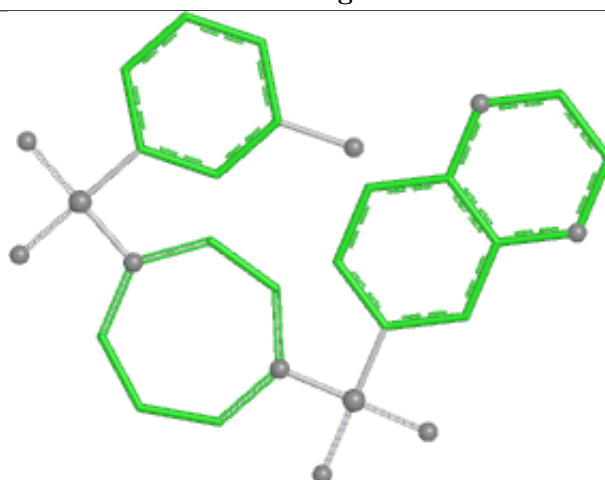
Bond lengths



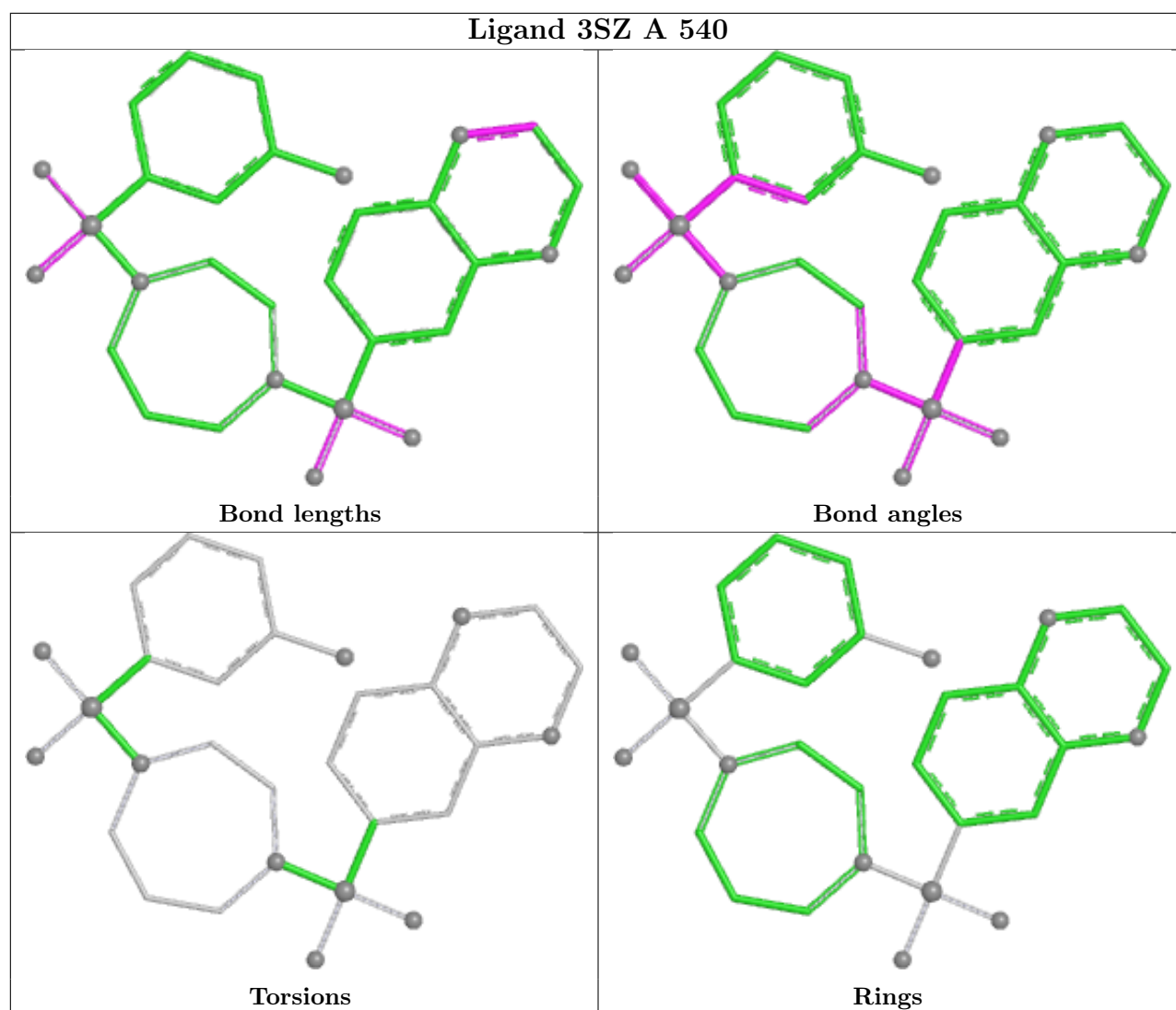
Bond angles



Torsions



Rings



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	518/550 (94%)	0.28	44 (8%) 16 19	16, 26, 54, 64	0
1	B	498/550 (90%)	0.40	56 (11%) 10 12	13, 26, 67, 79	1 (0%)
1	C	517/550 (94%)	0.23	16 (3%) 51 58	17, 27, 43, 53	0
1	D	504/550 (91%)	0.33	34 (6%) 24 27	12, 27, 53, 65	3 (0%)
All	All	2037/2200 (92%)	0.31	150 (7%) 20 23	12, 27, 54, 79	4 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	404	ILE	5.0
1	A	134	LEU	4.9
1	B	142	ILE	4.8
1	A	404	ILE	4.7
1	D	404	ILE	4.5
1	B	198	GLU	4.5
1	B	148	TYR	4.4
1	B	197	VAL	4.4
1	B	139	THR	4.3
1	A	189	GLY	4.1
1	B	143	THR	4.1
1	B	194	VAL	4.0
1	B	203	LEU	4.0
1	B	185	VAL	3.9
1	B	144	LEU	3.9
1	D	139	THR	3.9
1	B	159	LEU	3.8
1	B	138	ALA	3.8
1	A	138	ALA	3.8
1	B	170	VAL	3.7
1	B	192	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	137	GLY	3.6
1	B	167	VAL	3.6
1	D	144	LEU	3.6
1	A	168	VAL	3.6
1	B	193	LEU	3.6
1	C	401	LEU	3.6
1	A	187	GLN	3.5
1	D	156	ILE	3.5
1	A	171	GLY	3.5
1	B	157	LEU	3.4
1	D	402	ALA	3.4
1	B	183	LEU	3.4
1	B	41	THR	3.4
1	B	168	VAL	3.4
1	A	135	LYS	3.3
1	A	403	PRO	3.3
1	B	152	CYS	3.3
1	B	156	ILE	3.3
1	D	401	LEU	3.3
1	A	192	PHE	3.3
1	C	403	PRO	3.3
1	C	213	GLY	3.3
1	B	140	LEU	3.3
1	B	169	GLU	3.2
1	A	191	ASP	3.2
1	D	203	LEU	3.2
1	B	191	ASP	3.2
1	A	470	PHE	3.2
1	B	14	GLN	3.2
1	D	152	CYS	3.2
1	A	132	VAL	3.2
1	D	159	LEU	3.1
1	B	178	ASP	3.1
1	D	149	MET	3.1
1	B	147	ALA	3.1
1	A	405	THR	3.1
1	B	215	ALA	3.1
1	A	167	VAL	3.0
1	A	194	VAL	3.0
1	D	191	ASP	3.0
1	B	164	ILE	3.0
1	A	197	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	217	ASP	2.9
1	C	192	PHE	2.9
1	B	175	TYR	2.9
1	B	155	ASN	2.9
1	C	424	CYS	2.9
1	D	154	GLU	2.9
1	B	161	TYR	2.8
1	C	402	ALA	2.8
1	D	148	TYR	2.8
1	B	195	THR	2.8
1	A	203	LEU	2.8
1	B	181	ILE	2.8
1	B	165	CYS	2.7
1	B	176	VAL	2.7
1	B	174	ILE	2.7
1	A	202	SER	2.7
1	D	162	LYS	2.7
1	D	145	ASP	2.7
1	D	470	PHE	2.7
1	D	142	ILE	2.7
1	A	184	GLN	2.6
1	A	195	THR	2.6
1	B	196	GLU	2.6
1	D	192	PHE	2.6
1	D	158	TRP	2.6
1	A	478	VAL	2.6
1	B	402	ALA	2.6
1	A	193	LEU	2.5
1	A	148	TYR	2.5
1	D	204	GLY	2.5
1	D	163	ASN	2.5
1	B	18	LEU	2.5
1	D	403	PRO	2.5
1	A	130	ALA	2.4
1	D	121	THR	2.4
1	B	158	TRP	2.4
1	D	194	VAL	2.4
1	C	18	LEU	2.4
1	A	139	THR	2.4
1	A	196	GLU	2.4
1	D	168	VAL	2.4
1	B	182	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	147	ALA	2.3
1	D	146	ASN	2.3
1	B	400	ARG	2.3
1	C	190	ALA	2.3
1	B	122	GLY	2.3
1	B	204	GLY	2.3
1	C	168	VAL	2.3
1	B	154	GLU	2.3
1	A	140	LEU	2.3
1	B	146	ASN	2.3
1	A	199	ASN	2.3
1	D	202	SER	2.2
1	A	156	ILE	2.2
1	C	40	ILE	2.2
1	A	133	GLU	2.2
1	A	198	GLU	2.2
1	B	172	SER	2.2
1	A	170	VAL	2.2
1	D	153	ASP	2.2
1	A	165	CYS	2.2
1	A	180	LEU	2.2
1	B	179	GLY	2.2
1	C	189	GLY	2.2
1	B	214	ALA	2.2
1	A	406	SER	2.1
1	B	180	LEU	2.1
1	D	188	LYS	2.1
1	A	190	ALA	2.1
1	D	143	THR	2.1
1	A	200	GLY	2.1
1	C	167	VAL	2.1
1	A	186	LYS	2.1
1	B	141	LYS	2.1
1	D	206	LYS	2.1
1	A	216	VAL	2.1
1	D	170	VAL	2.1
1	D	161	TYR	2.0
1	C	405	THR	2.0
1	A	213	GLY	2.0
1	B	201	GLY	2.0
1	B	199	ASN	2.0
1	B	404	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	164	ILE	2.0
1	C	244	PHE	2.0
1	A	163	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	UNX	B	538	1/1	-0.75	1.45	2,2,2,2	1
5	UNX	B	534	1/1	-0.71	1.22	2,2,2,2	1
5	UNX	B	542	1/1	-0.64	1.30	2,2,2,2	1
5	UNX	C	544	1/1	-0.64	1.47	2,2,2,2	1
5	UNX	A	542	1/1	-0.48	1.25	2,2,2,2	1
5	UNX	A	547	1/1	-0.35	1.24	2,2,2,2	1
5	UNX	B	533	1/1	-0.28	1.19	2,2,2,2	1
5	UNX	A	543	1/1	-0.24	1.27	2,2,2,2	1
5	UNX	C	535	1/1	-0.23	1.54	2,2,2,2	1
5	UNX	D	537	1/1	-0.22	1.34	2,2,2,2	1
5	UNX	C	533	1/1	-0.18	1.23	2,2,2,2	1
5	UNX	A	533	1/1	-0.11	1.51	2,2,2,2	1
5	UNX	A	548	1/1	-0.10	1.23	2,2,2,2	1
5	UNX	A	545	1/1	-0.08	1.58	2,2,2,2	1
5	UNX	C	543	1/1	-0.08	1.20	2,2,2,2	1
5	UNX	B	543	1/1	-0.07	1.55	2,2,2,2	1
5	UNX	C	534	1/1	-0.07	1.31	2,2,2,2	1
5	UNX	C	539	1/1	-0.06	1.34	2,2,2,2	1
5	UNX	A	534	1/1	0.02	1.20	2,2,2,2	1

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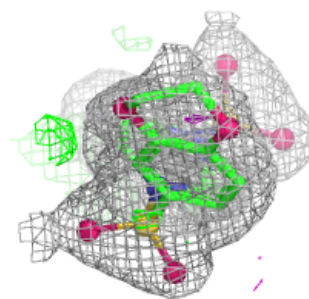
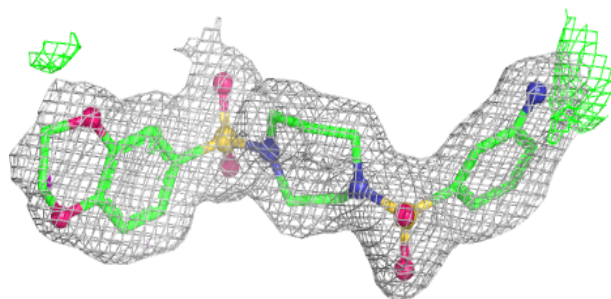
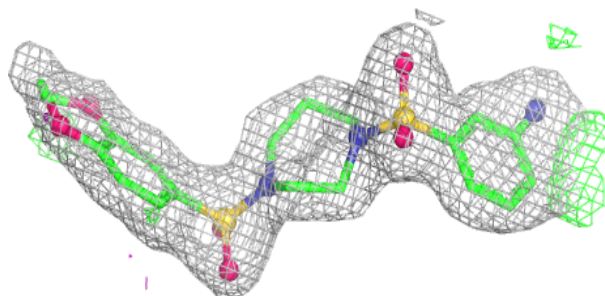
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	UNX	B	540	1/1	0.04	1.30	2,2,2,2	1
5	UNX	B	539	1/1	0.09	1.35	2,2,2,2	1
5	UNX	D	535	1/1	0.12	1.23	2,2,2,2	1
5	UNX	C	542	1/1	0.12	1.34	2,2,2,2	1
5	UNX	C	538	1/1	0.25	1.27	2,2,2,2	1
5	UNX	A	537	1/1	0.35	1.22	2,2,2,2	1
5	UNX	A	536	1/1	0.49	1.33	2,2,2,2	1
5	UNX	D	538	1/1	0.49	1.33	2,2,2,2	1
5	UNX	A	546	1/1	0.52	1.44	2,2,2,2	1
5	UNX	C	540	1/1	0.54	1.47	2,2,2,2	1
5	UNX	B	535	1/1	0.55	1.44	2,2,2,2	1
5	UNX	D	534	1/1	0.56	1.33	2,2,2,2	1
5	UNX	C	537	1/1	0.60	1.26	2,2,2,2	1
5	UNX	D	533	1/1	0.61	1.28	2,2,2,2	1
5	UNX	A	544	1/1	0.62	1.58	2,2,2,2	1
5	UNX	A	539	1/1	0.64	1.44	2,2,2,2	1
5	UNX	B	537	1/1	0.65	1.39	2,2,2,2	1
5	UNX	C	536	1/1	0.68	1.37	2,2,2,2	1
5	UNX	D	536	1/1	0.69	1.47	2,2,2,2	1
5	UNX	A	535	1/1	0.74	1.52	2,2,2,2	1
5	UNX	A	538	1/1	0.77	1.35	2,2,2,2	1
5	UNX	D	539	1/1	0.77	1.57	2,2,2,2	1
4	SO4	A	532	5/5	0.82	0.12	53,53,56,56	0
4	SO4	C	532	5/5	0.83	0.10	60,61,62,62	0
5	UNX	B	536	1/1	0.86	1.35	2,2,2,2	1
4	SO4	B	532	5/5	0.90	0.10	44,45,47,48	0
4	SO4	D	532	5/5	0.90	0.13	51,51,53,53	0
2	3SZ	A	540	30/30	0.94	0.09	25,32,35,37	0
2	3SZ	D	540	30/30	0.94	0.09	27,32,35,36	0
3	FBP	B	541	20/20	0.97	0.06	19,21,27,29	0
3	FBP	C	541	20/20	0.97	0.06	24,28,34,34	0
3	FBP	A	541	20/20	0.98	0.05	22,26,29,29	0
3	FBP	D	541	20/20	0.98	0.04	17,19,22,23	0

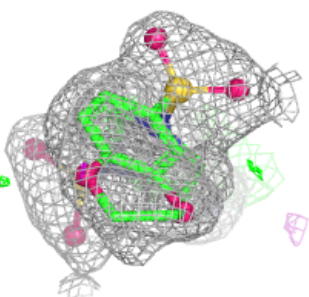
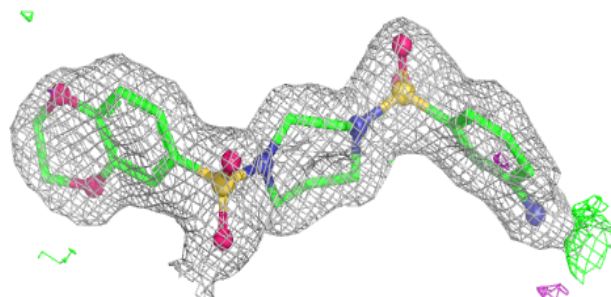
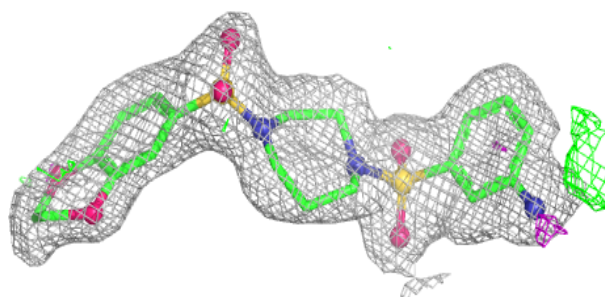
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3SZ A 540:

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

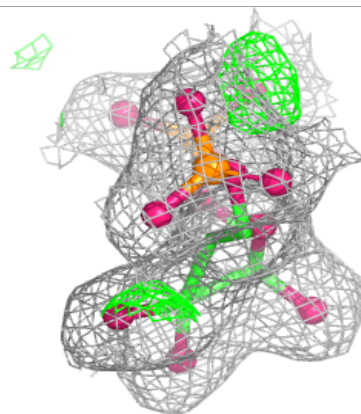
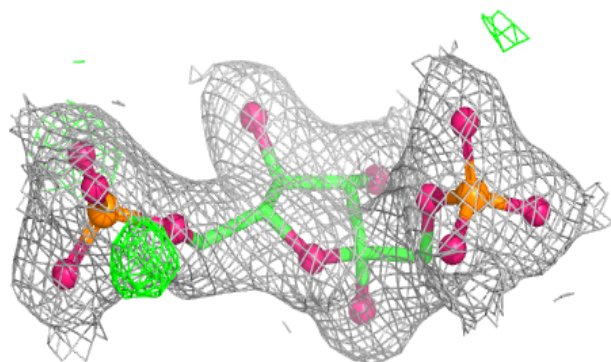
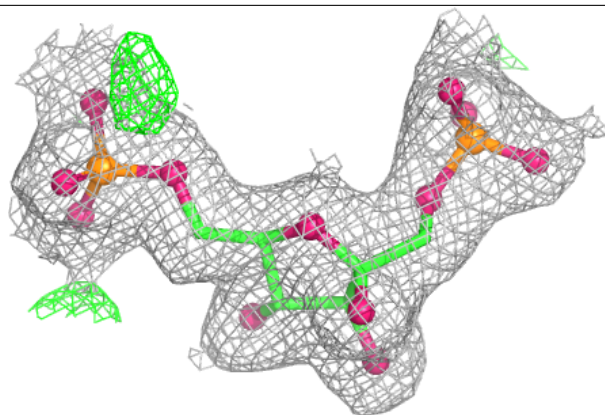
**Electron density around 3SZ D 540:**

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

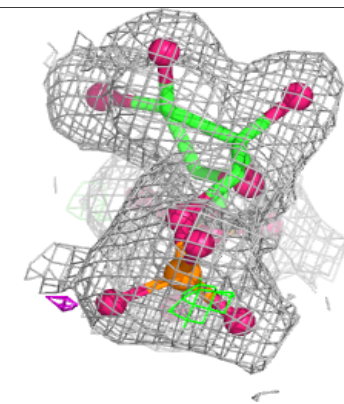
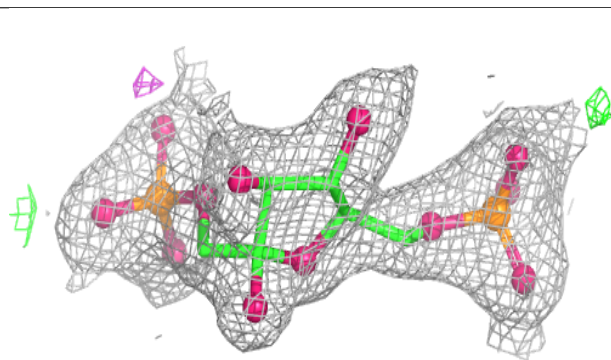
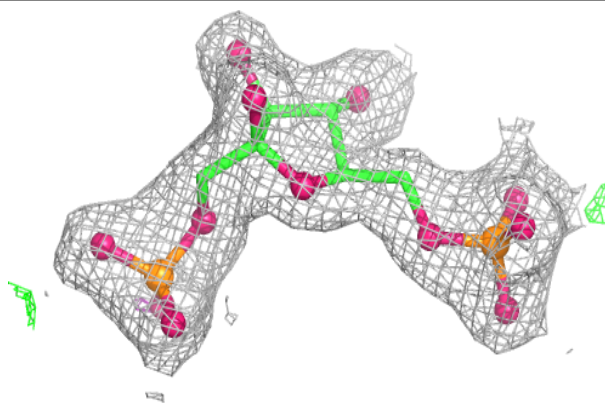


Electron density around FBP B 541:

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

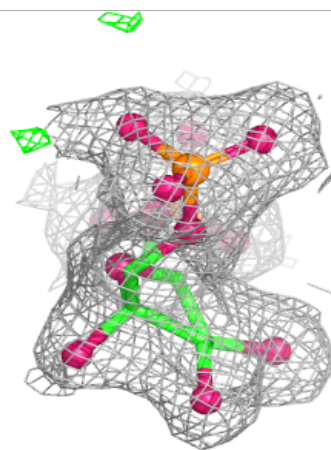
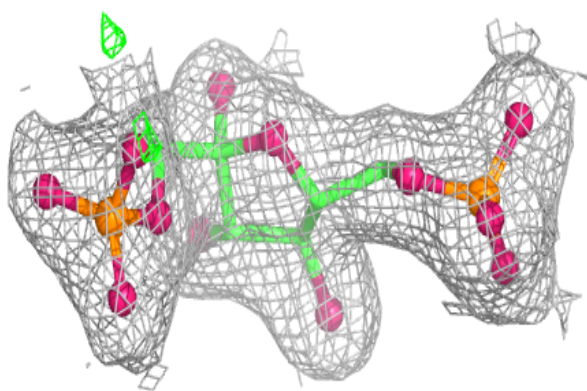
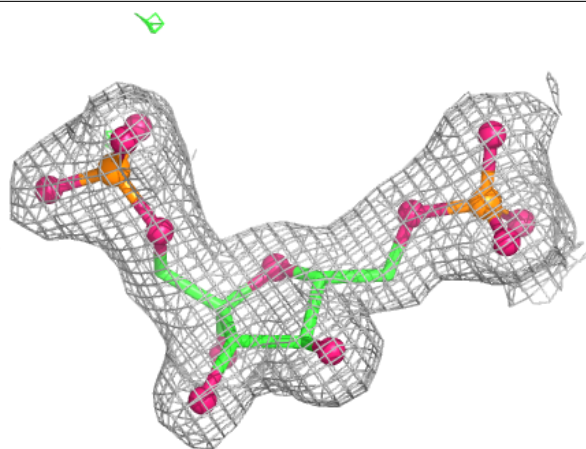
**Electron density around FBP C 541:**

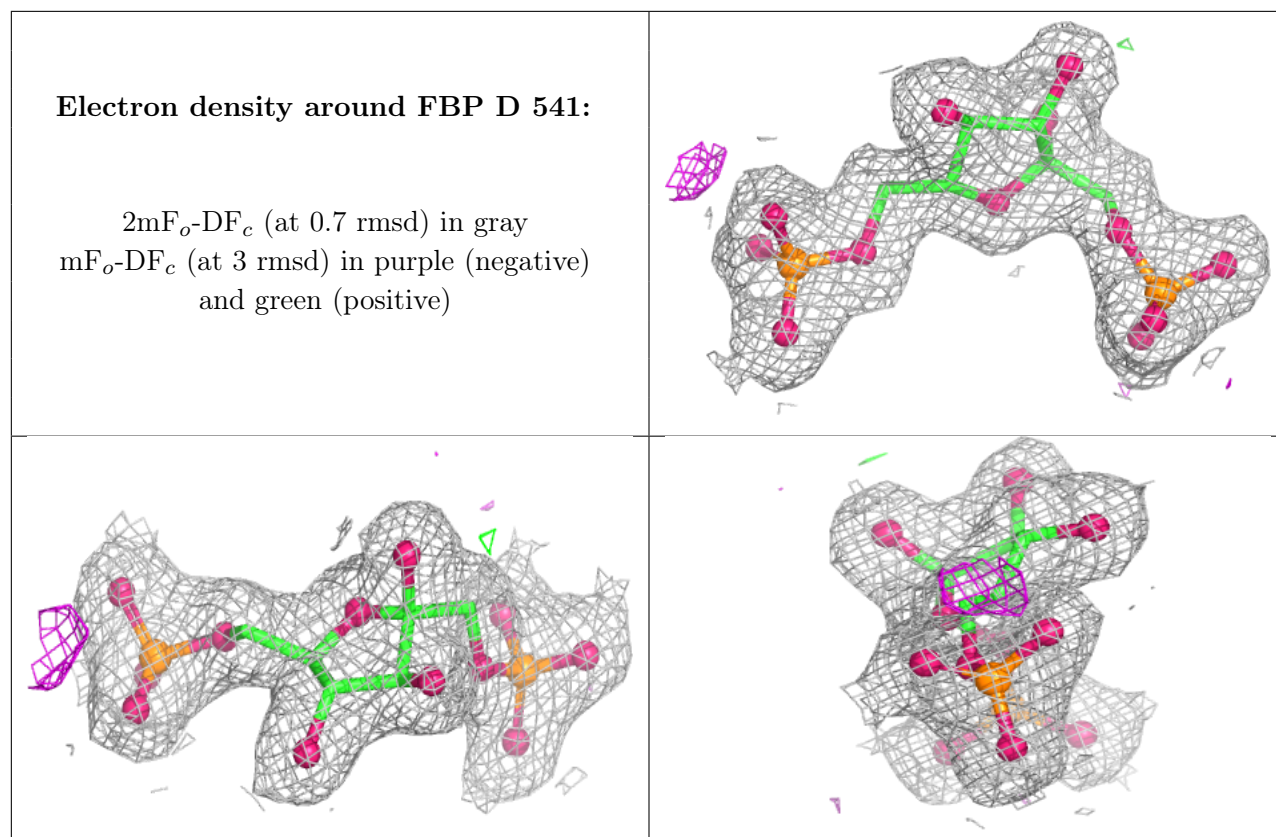
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FBP A 541:

$2mF_o-DF_c$ (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.