



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:20 PM UTC

PDB ID : 3GR4 / pdb_00003gr4
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 : 2009-03-24
Resolution : 1.60 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

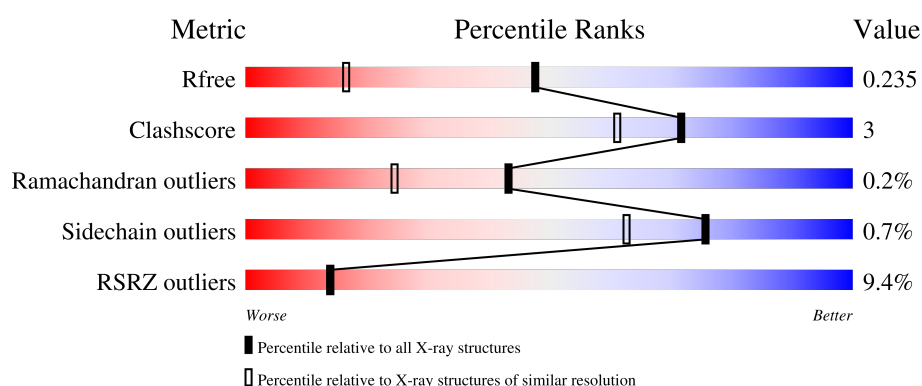
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	10% 87% 7% 6%
1	B	550	13% 85% 6% 8%
1	C	550	4% 89% 6% •
1	D	550	9% 86% 6% 7%

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	532	-	-	-	X
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	B	533	-	-	-	X
5	UNX	B	534	-	-	-	X
5	UNX	B	535	-	-	-	X
5	UNX	B	536	-	-	-	X
5	UNX	B	537	-	-	-	X
5	UNX	C	532	-	-	-	X
5	UNX	C	533	-	-	-	X
5	UNX	D	532	-	-	-	X
5	UNX	D	533	-	-	-	X
5	UNX	D	534	-	-	-	X
5	UNX	D	535	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16503 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	519	Total	C	N	O	S	0	2	0
			3885	2453	676	731	25			
1	B	505	Total	C	N	O	S	0	3	0
			3754	2361	663	706	24			
1	C	515	Total	C	N	O	S	0	4	0
			3847	2430	672	721	24			
1	D	509	Total	C	N	O	S	0	4	0
			3808	2398	679	706	25			

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

Continued on next page...

Continued from previous page...

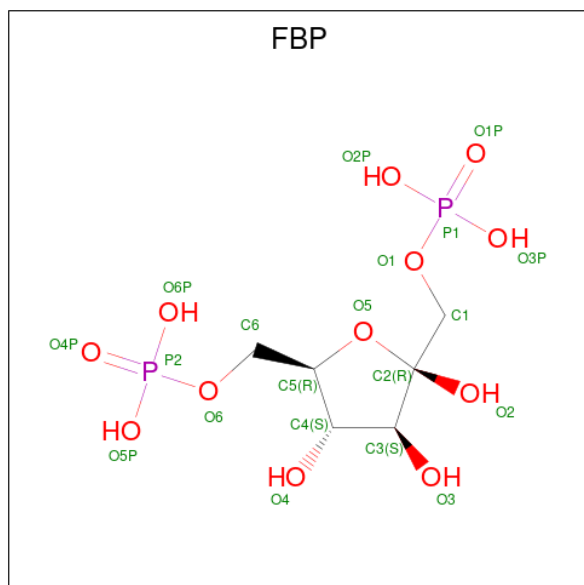
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

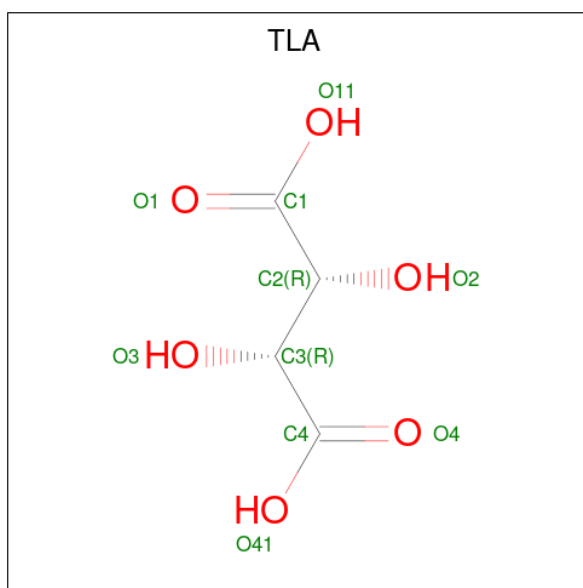
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP 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 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



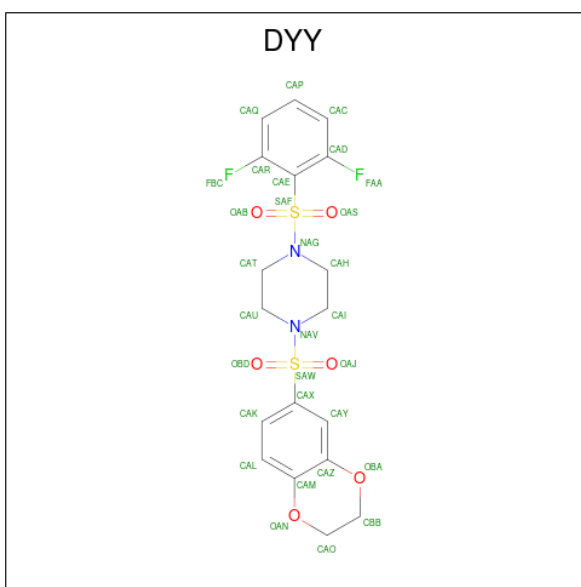
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			6	1	4	1		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is 1-[(2,6-difluorophenyl)sulfonyl]-4-(2,3-dihydro-1,4-benzodioxin-6-ylsulfonyl)perazine (CCD ID: DYY) (formula: $C_{18}H_{18}F_2N_2O_6S_2$).

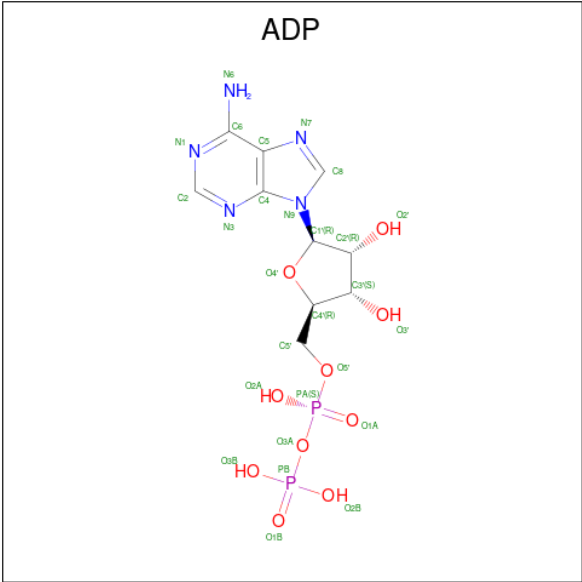


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 60	C 36	F 4	N 4	O 12	S 4	0	1
4	D	1	Total 60	C 36	F 4	N 4	O 12	S 4	0	1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	X	0	0
			6	6		
5	B	6	Total	X	0	0
			6	6		
5	C	2	Total	X	0	0
			2	2		
5	D	4	Total	X	0	0
			4	4		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			18	5	1	10	2		

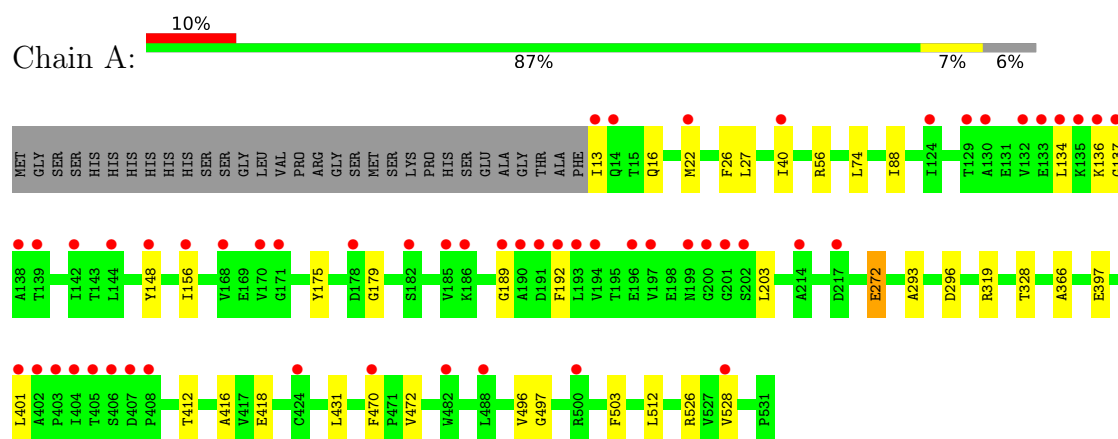
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	245	Total	O	0	0
			245	245		
7	B	237	Total	O	0	0
			237	237		
7	C	228	Total	O	0	0
			228	228		
7	D	207	Total	O	0	0
			207	207		

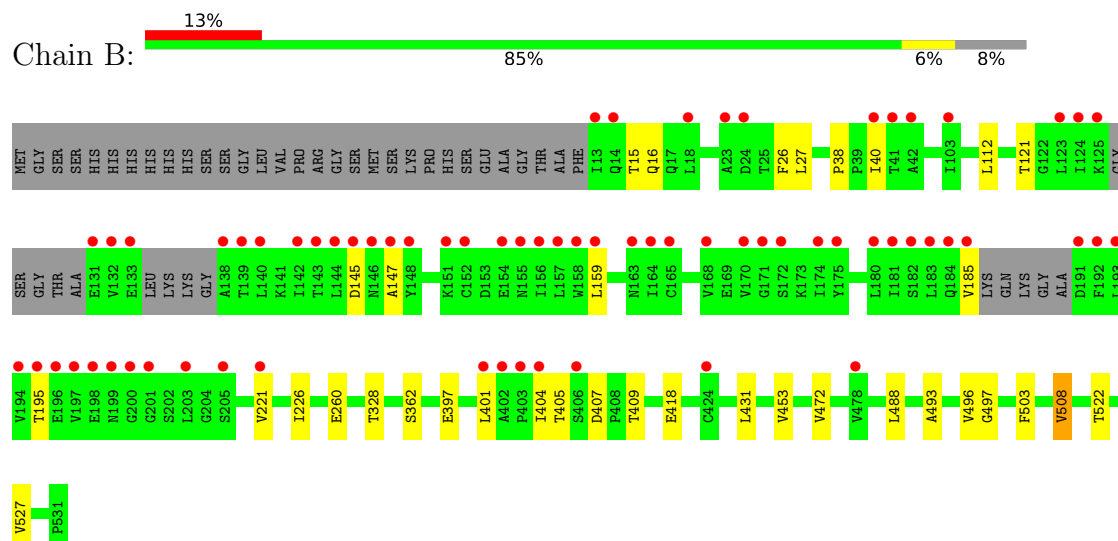
3 Residue-property plots

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 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.

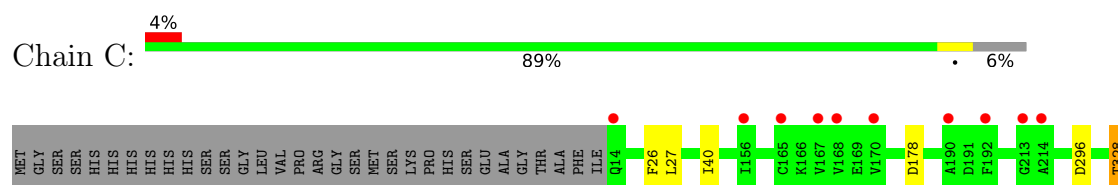
• Molecule 1: Pyruvate kinase isozymes M1/M2

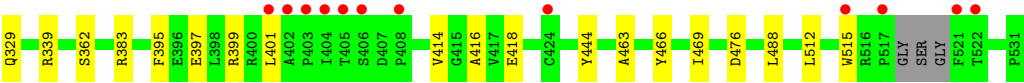


• Molecule 1: Pyruvate kinase isozymes M1/M2

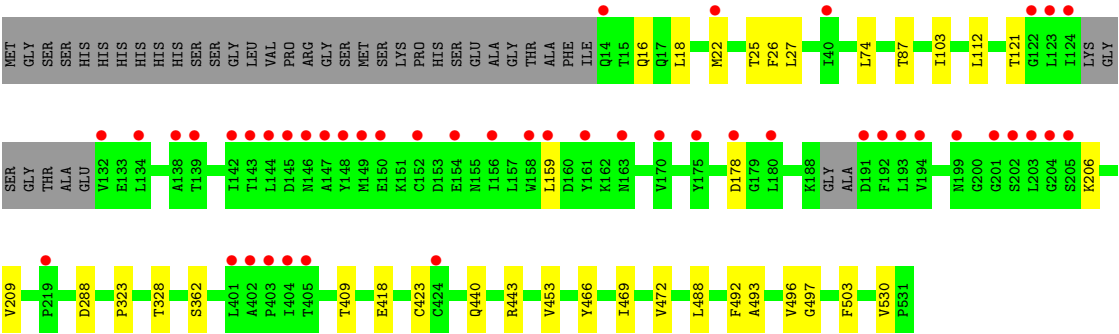
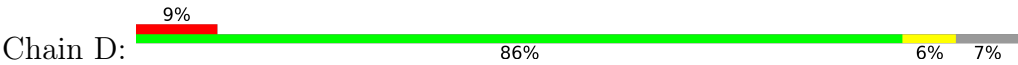


• Molecule 1: Pyruvate kinase isozymes M1/M2





● 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	81.28Å 153.21Å 93.14Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-1.60) 96.3 (30.00-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0088, prodrgr	Depositor
R, R_{free}	0.208 , 0.231 0.212 , 0.235	Depositor DCC
R_{free} test set	2916 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16503	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, DYY, UNX, TLA, ADP

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	0.90	1/3960 (0.0%)	0.83	1/5367 (0.0%)
1	B	0.87	1/3819 (0.0%)	0.81	0/5177
1	C	0.87	1/3920 (0.0%)	0.80	0/5315
1	D	0.85	1/3877 (0.0%)	0.82	0/5255
All	All	0.87	4/15576 (0.0%)	0.82	1/21114 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	362	SER	CA-C	7.45	1.56	1.52
1	B	362	SER	CA-C	5.53	1.55	1.52
1	C	362	SER	CA-C	5.46	1.55	1.52
1	A	366	ALA	CA-CB	-5.36	1.44	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	N-CA-CB	-5.11	102.47	110.44

There are no chirality outliers.

There are no planarity outliers.

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	3885	0	3853	30	0
1	B	3754	0	3664	29	0
1	C	3847	0	3821	26	0
1	D	3808	0	3728	31	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	6	0	0	0	0
2	D	20	0	10	0	0
3	A	10	0	4	0	0
3	B	20	0	8	0	0
3	C	20	0	8	0	0
3	D	20	0	8	0	0
4	A	60	0	36	9	0
4	D	60	0	36	8	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	2	0	0	0	0
5	D	4	0	0	0	0
6	A	18	0	8	0	0
7	A	245	0	0	0	0
7	B	237	0	0	0	0
7	C	228	0	0	1	0
7	D	207	0	0	0	0
All	All	16503	0	15204	102	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 (102) 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:B:418[B]:GLU:HG3	1:D:418:GLU:HG2	1.58	0.83
1:D:74:LEU:HD11	1:D:87:THR:HG21	1.69	0.73
1:A:526:ARG:HD3	1:C:515:TRP:CD2	2.24	0.72
1:C:27:LEU:HD13	4:D:550[A]:DYY:CAO	2.20	0.72
1:A:16:GLN:HG2	1:A:40:ILE:HG23	1.77	0.67
1:B:418[B]:GLU:OE2	1:D:418:GLU:OE2	2.14	0.66
1:D:121:THR:HG22	1:D:159:LEU:CD2	2.28	0.64
1:C:397:GLU:O	1:C:401:LEU:HD13	1.98	0.63
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.83	0.61
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.82	0.60
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.85	0.59
1:B:121:THR:HG22	1:B:159:LEU:CD2	2.32	0.59
1:B:418[B]:GLU:HG3	1:D:418:GLU:CG	2.29	0.59
1:B:488:LEU:HD23	1:B:488:LEU:C	2.28	0.59
1:B:185:VAL:HA	1:B:195:THR:HG22	1.83	0.58
1:D:488:LEU:C	1:D:488:LEU:HD23	2.28	0.58
1:D:26:PHE:CE1	4:D:550[B]:DYY:HAI	2.39	0.57
1:A:27:LEU:HD13	4:A:550[A]:DYY:CAO	2.34	0.57
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.87	0.57
1:A:13:ILE:HD11	1:A:22:MET:SD	2.45	0.56
1:B:121:THR:HG22	1:B:159:LEU:HD21	1.87	0.56
1:A:26:PHE:CE1	4:A:550[A]:DYY:HAI	2.41	0.55
1:C:488:LEU:C	1:C:488:LEU:HD23	2.33	0.54
1:D:121:THR:O	1:D:206:LYS:HA	2.08	0.54
1:A:418:GLU:OE2	1:C:418:GLU:OE2	2.26	0.53
1:C:401:LEU:HD11	1:D:25:THR:HG21	1.91	0.53
1:C:476:ASP:OD2	1:C:488:LEU:HD21	2.08	0.53
1:D:74:LEU:HD11	1:D:87:THR:CG2	2.38	0.53
1:A:319:ARG:HD3	1:A:401:LEU:HD13	1.90	0.53
1:B:112:LEU:HD23	1:B:112:LEU:C	2.34	0.52
1:B:508:VAL:CG2	1:B:527:VAL:CG1	2.87	0.52
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.91	0.52
1:D:27:LEU:HD13	4:D:550[B]:DYY:CAO	2.40	0.52
1:A:148:TYR:CD1	1:A:156:ILE:HD13	2.45	0.52
4:A:550[A]:DYY:HAL	1:B:397:GLU:OE1	2.10	0.51
1:C:26:PHE:CE1	4:D:550[A]:DYY:HAI	2.45	0.51
1:D:121:THR:HG22	1:D:159:LEU:HD21	1.92	0.51
1:B:508:VAL:HG21	1:B:527:VAL:CG1	2.40	0.51
1:B:404:ILE:HD13	1:D:22:MET:HE1	1.91	0.51
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.93	0.51
1:B:15:THR:HG22	1:B:38:PRO:HG2	1.93	0.51
1:B:221:VAL:HG12	1:B:226:ILE:HG13	1.93	0.51
1:A:189:GLY:HA3	1:A:192:PHE:CZ	2.46	0.50
1:A:272:GLU:HG2	1:A:293:ALA:HB3	1.93	0.50
4:A:550[B]:DYY:HAI	1:B:26:PHE:CE1	2.45	0.50
1:D:26:PHE:CD1	4:D:550[B]:DYY:HAI	2.47	0.50
1:A:74:LEU:HD11	1:A:88:ILE:HG13	1.93	0.50
1:D:16:GLN:HG3	1:D:18:LEU:HG	1.93	0.49
1:A:27:LEU:HD23	1:B:401:LEU:HD12	1.95	0.49
1:A:526:ARG:HD3	1:C:515:TRP:CG	2.48	0.49
1:A:412:THR:HG22	1:A:512:LEU:HD22	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:VAL:CG2	1:B:527:VAL:HG13	2.43	0.49
1:B:16:GLN:HG3	1:B:40:ILE:HG23	1.95	0.48
1:A:27:LEU:HD13	4:A:550[A]:DYY:HAOA	1.94	0.48
1:C:401:LEU:HD22	1:D:27:LEU:HD23	1.96	0.48
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.96	0.48
1:A:526:ARG:HD3	1:C:515:TRP:CE3	2.49	0.47
1:A:134:LEU:HD11	1:A:203:LEU:HD22	1.95	0.47
1:C:414[B]:VAL:HG22	1:C:444:TYR:CE2	2.50	0.47
4:A:550[B]:DYY:CAO	1:B:27:LEU:HD13	2.45	0.47
1:B:418[B]:GLU:HG3	1:D:418:GLU:CB	2.44	0.47
1:C:414[B]:VAL:HG22	1:C:444:TYR:CZ	2.50	0.47
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.96	0.47
1:C:26:PHE:CG	4:D:550[B]:DYY:HAT	2.50	0.47
1:D:103:ILE:HD13	1:D:492:PHE:CE1	2.50	0.46
1:B:405:THR:O	1:D:423:CYS:HA	2.15	0.46
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.51	0.45
4:A:550[B]:DYY:FBC	4:A:550[B]:DYY:OAS	2.24	0.45
1:B:407:ASP:OD1	1:B:409[B]:THR:OG1	2.33	0.45
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.51	0.45
1:B:145:ASP:OD2	1:B:147:ALA:HB3	2.16	0.45
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.52	0.45
1:B:409[A]:THR:HG23	1:B:522:THR:HB	1.99	0.44
1:C:178:ASP:O	1:C:178:ASP:CG	2.61	0.44
1:A:418:GLU:CG	1:C:414[B]:VAL:HG12	2.47	0.43
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.47	0.43
1:A:175:TYR:HB3	1:A:179:GLY:HA2	2.00	0.43
1:D:453:VAL:HG21	1:D:493:ALA:HB2	2.00	0.43
1:D:112:LEU:C	1:D:112:LEU:HD23	2.43	0.43
1:A:26:PHE:CG	4:A:550[B]:DYY:HAT	2.54	0.43
1:C:329:GLN:CD	7:C:835:HOH:O	2.60	0.43
1:B:418[B]:GLU:CG	1:D:418:GLU:HG2	2.39	0.42
1:C:27:LEU:HD13	4:D:550[A]:DYY:HAO	1.99	0.42
1:C:27:LEU:HD13	4:D:550[A]:DYY:HAOA	2.00	0.42
1:C:40:ILE:O	1:C:383:ARG:HD2	2.19	0.42
1:D:503:PHE:CD1	1:D:530:VAL:HG21	2.55	0.41
1:A:397:GLU:OE1	4:A:550[B]:DYY:HAL	2.20	0.41
1:A:189:GLY:HA3	1:A:192:PHE:CE2	2.56	0.41
1:D:409:THR:HG21	1:D:440:GLN:OE1	2.20	0.41
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.50	0.41
1:A:136:LYS:HG2	1:A:137:GLY:N	2.35	0.41
1:C:401:LEU:N	1:C:401:LEU:HD12	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:GLN:O	1:D:443:ARG:HG2	2.21	0.41
1:C:328:THR:HG22	1:C:329:GLN:HG3	2.03	0.40
1:D:288:ASP:O	1:D:323:PRO:HD2	2.21	0.40
1:C:463:ALA:HB1	1:C:469:ILE:HG21	2.04	0.40
1:D:159:LEU:HD22	1:D:209:VAL:HG21	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	519/550 (94%)	510 (98%)	8 (2%)	1 (0%)	43	24
1	B	500/550 (91%)	492 (98%)	7 (1%)	1 (0%)	43	24
1	C	515/550 (94%)	505 (98%)	9 (2%)	1 (0%)	43	24
1	D	507/550 (92%)	496 (98%)	10 (2%)	1 (0%)	43	24
All	All	2041/2200 (93%)	2003 (98%)	34 (2%)	4 (0%)	43	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	C	328	THR
1	D	328	THR
1	B	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	399/452 (88%)	395 (99%)	4 (1%)	68	50
1	B	376/452 (83%)	373 (99%)	3 (1%)	73	59
1	C	391/452 (86%)	389 (100%)	2 (0%)	81	70
1	D	381/452 (84%)	380 (100%)	1 (0%)	86	78
All	All	1547/1808 (86%)	1537 (99%)	10 (1%)	76	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	GLU
1	A	296	ASP
1	A	431	LEU
1	A	528	VAL
1	B	260	GLU
1	B	431	LEU
1	B	508	VAL
1	C	296	ASP
1	C	339	ARG
1	D	178	ASP

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	44	ASN
1	A	210	ASN
1	A	252	HIS
1	A	491	ASN
1	B	16	GLN
1	B	44	ASN
1	B	252	HIS
1	C	44	ASN
1	C	78	HIS
1	C	187	GLN
1	C	274	HIS
1	C	458	GLN
1	D	44	ASN
1	D	78	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	235	GLN
1	D	458	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 18 are unknown - 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	TLA	B	538	-	9,9,9	1.09	0	12,12,12	1.17	1 (8%)
3	TLA	D	542	-	9,9,9	1.13	1 (11%)	12,12,12	0.93	1 (8%)
6	ADP	A	538	-	16,18,29	1.16	1 (6%)	24,28,45	1.72	5 (20%)
3	TLA	C	542	-	9,9,9	1.19	0	12,12,12	1.11	0
3	TLA	D	543	-	9,9,9	1.10	0	12,12,12	1.18	2 (16%)
2	FBP	A	541	-	18,20,20	0.93	1 (5%)	21,32,32	0.72	1 (4%)
2	FBP	C	541	-	5,5,20	1.32	1 (20%)	7,7,32	1.07	0
4	DYY	D	550[B]	-	33,33,33	2.88	6 (18%)	48,50,50	2.51	13 (27%)
4	DYY	A	550[A]	-	33,33,33	2.46	6 (18%)	48,50,50	2.20	10 (20%)
4	DYY	A	550[B]	-	33,33,33	3.07	7 (21%)	48,50,50	2.48	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DYY	D	550[A]	-	33,33,33	2.69	6 (18%)	48,50,50	2.20	12 (25%)
3	TLA	A	542	-	9,9,9	1.16	0	12,12,12	1.00	1 (8%)
3	TLA	B	542	-	9,9,9	1.40	1 (11%)	12,12,12	1.24	1 (8%)
2	FBP	B	541	-	18,20,20	0.87	1 (5%)	21,32,32	0.90	1 (4%)
2	FBP	D	541	-	18,20,20	0.97	1 (5%)	21,32,32	0.90	1 (4%)
3	TLA	C	534	-	9,9,9	1.55	2 (22%)	12,12,12	1.32	1 (8%)

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	TLA	B	538	-	-	0/12/12/12	-
3	TLA	D	542	-	-	0/12/12/12	-
6	ADP	A	538	-	-	4/12/28/32	0/1/1/3
3	TLA	C	542	-	-	0/12/12/12	-
3	TLA	D	543	-	-	1/12/12/12	-
2	FBP	A	541	-	-	2/13/32/32	0/1/1/1
2	FBP	C	541	-	-	1/1/3/32	-
4	DYY	D	550[B]	-	-	4/24/41/41	0/4/4/4
4	DYY	A	550[A]	-	-	5/24/41/41	0/4/4/4
4	DYY	A	550[B]	-	-	2/24/41/41	0/4/4/4
4	DYY	D	550[A]	-	-	3/24/41/41	0/4/4/4
3	TLA	A	542	-	-	0/12/12/12	-
3	TLA	B	542	-	-	0/12/12/12	-
2	FBP	B	541	-	-	2/13/32/32	0/1/1/1
2	FBP	D	541	-	-	2/13/32/32	0/1/1/1
3	TLA	C	534	-	-	0/12/12/12	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	550[B]	DYY	SAW-NAV	9.39	1.76	1.63
4	D	550[B]	DYY	SAW-NAV	8.66	1.75	1.63
4	A	550[B]	DYY	SAF-NAG	7.14	1.73	1.63
4	A	550[B]	DYY	OBD-SAW	6.76	1.50	1.43
4	D	550[A]	DYY	OBD-SAW	6.68	1.50	1.43
4	D	550[A]	DYY	SAW-NAV	6.62	1.72	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	550[A]	DYY	OAB-SAF	6.51	1.50	1.43
4	D	550[B]	DYY	OAS-SAF	6.50	1.50	1.43
4	A	550[A]	DYY	OAB-SAF	6.27	1.50	1.43
4	D	550[A]	DYY	OAJ-SAW	6.23	1.50	1.43
4	A	550[A]	DYY	OBD-SAW	6.17	1.50	1.43
4	D	550[A]	DYY	OAS-SAF	6.16	1.50	1.43
4	D	550[B]	DYY	OBD-SAW	6.15	1.50	1.43
4	A	550[B]	DYY	OAS-SAF	6.12	1.50	1.43
4	D	550[B]	DYY	SAF-NAG	6.03	1.71	1.63
4	A	550[B]	DYY	OAB-SAF	5.96	1.49	1.43
4	D	550[B]	DYY	OAB-SAF	5.92	1.49	1.43
4	A	550[B]	DYY	OAJ-SAW	5.66	1.49	1.43
4	A	550[A]	DYY	OAS-SAF	5.61	1.49	1.43
4	A	550[A]	DYY	SAW-NAV	5.53	1.71	1.63
4	A	550[A]	DYY	OAJ-SAW	5.46	1.49	1.43
4	D	550[B]	DYY	OAJ-SAW	5.35	1.49	1.43
4	A	550[A]	DYY	SAF-NAG	4.23	1.69	1.63
4	D	550[A]	DYY	SAF-NAG	4.21	1.69	1.63
6	A	538	ADP	PA-O3A	3.99	1.63	1.59
2	A	541	FBP	O2-C2	3.24	1.46	1.40
2	D	541	FBP	O2-C2	2.75	1.45	1.40
2	B	541	FBP	O2-C2	2.74	1.45	1.40
3	C	534	TLA	C3-C4	-2.62	1.48	1.52
2	C	541	FBP	P2-O6	2.59	1.64	1.59
4	A	550[B]	DYY	CAH-NAG	2.08	1.50	1.47
3	C	534	TLA	O4-C4	2.06	1.28	1.22
3	D	542	TLA	O41-C4	-2.05	1.24	1.30
3	B	542	TLA	O41-C4	-2.04	1.24	1.30

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	550[B]	DYY	CAX-SAW-NAV	8.19	117.17	107.28
4	D	550[B]	DYY	CAX-SAW-NAV	7.87	116.78	107.28
4	A	550[A]	DYY	OAJ-SAW-OBD	-7.41	108.03	119.59
4	D	550[A]	DYY	CAX-SAW-NAV	7.18	115.95	107.28
4	A	550[A]	DYY	CAX-SAW-NAV	6.99	115.72	107.28
4	A	550[B]	DYY	OAJ-SAW-OBD	-6.81	108.96	119.59
4	A	550[B]	DYY	OAB-SAF-OAS	-6.70	109.13	119.59
4	D	550[B]	DYY	OAJ-SAW-OBD	-6.67	109.17	119.59
4	D	550[B]	DYY	OAB-SAF-OAS	-6.59	109.30	119.59
4	D	550[A]	DYY	OAJ-SAW-OBD	-6.26	109.83	119.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	550[A]	DYY	OAB-SAF-OAS	-6.15	110.00	119.59
4	A	550[A]	DYY	OAB-SAF-OAS	-6.08	110.11	119.59
4	A	550[B]	DYY	CAE-SAF-NAG	5.59	117.59	103.63
4	D	550[B]	DYY	CAE-SAF-NAG	4.93	115.94	103.63
4	A	550[A]	DYY	CAE-SAF-NAG	4.88	115.81	103.63
4	D	550[A]	DYY	CAE-SAF-NAG	4.46	114.77	103.63
4	D	550[B]	DYY	OBD-SAW-NAV	4.21	110.65	106.69
4	D	550[B]	DYY	CAU-NAV-SAW	-3.84	109.91	117.06
4	D	550[B]	DYY	CAH-NAG-CAT	-3.78	107.77	112.12
4	D	550[B]	DYY	OAB-SAF-NAG	3.72	110.19	106.69
6	A	538	ADP	O5'-PA-O1A	-3.61	94.64	108.94
4	A	550[B]	DYY	OBD-SAW-NAV	3.46	109.95	106.69
6	A	538	ADP	O5'-C5'-C4'	3.41	120.59	108.99
6	A	538	ADP	O2A-PA-O5'	3.38	122.89	107.57
4	A	550[B]	DYY	CAH-NAG-CAT	-3.23	108.41	112.12
4	A	550[B]	DYY	OAB-SAF-NAG	3.05	109.56	106.69
4	D	550[B]	DYY	CAC-CAD-CAE	-3.02	118.78	123.50
4	A	550[B]	DYY	CAT-NAG-SAF	-2.97	111.52	117.06
4	A	550[B]	DYY	CAI-NAV-CAU	-2.96	108.72	112.12
4	D	550[A]	DYY	OAS-SAF-NAG	2.93	109.45	106.69
4	D	550[A]	DYY	CAH-NAG-CAT	-2.89	108.80	112.12
4	A	550[B]	DYY	CAU-NAV-SAW	-2.87	111.72	117.06
4	A	550[A]	DYY	OAJ-SAW-NAV	2.87	109.39	106.69
6	A	538	ADP	PA-O5'-C5'	-2.87	104.92	121.35
4	D	550[A]	DYY	CAC-CAD-CAE	-2.79	119.14	123.50
4	A	550[B]	DYY	CAC-CAD-CAE	-2.76	119.19	123.50
4	A	550[A]	DYY	CAH-NAG-CAT	-2.61	109.11	112.12
4	A	550[A]	DYY	CAC-CAD-CAE	-2.59	119.45	123.50
3	A	542	TLA	O41-C4-C3	2.57	120.46	113.31
3	D	543	TLA	O11-C1-C2	2.47	120.16	113.31
4	D	550[B]	DYY	OAJ-SAW-NAV	-2.45	104.38	106.69
4	D	550[B]	DYY	CAI-NAV-CAU	-2.40	109.36	112.12
2	B	541	FBP	O6-P2-O4P	2.40	112.93	106.44
3	B	542	TLA	O11-C1-C2	2.39	119.96	113.31
6	A	538	ADP	C3'-C2'-C1'	2.36	105.92	101.46
4	A	550[A]	DYY	CAU-NAV-SAW	-2.36	112.67	117.06
4	D	550[A]	DYY	CAR-CAE-CAD	2.36	120.05	115.00
4	A	550[A]	DYY	OAB-SAF-NAG	2.31	108.86	106.69
3	D	542	TLA	O41-C4-C3	2.22	119.48	113.31
4	A	550[A]	DYY	CAR-CAE-CAD	2.20	119.72	115.00
4	D	550[B]	DYY	CAR-CAE-CAD	2.17	119.65	115.00
4	A	550[B]	DYY	CAR-CAE-CAD	2.16	119.63	115.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	550[A]	DYY	CAI-NAV-CAU	-2.16	109.64	112.12
2	D	541	FBP	O4-C4-C3	2.15	118.61	112.16
3	C	534	TLA	O4-C4-C3	-2.13	115.94	121.62
3	B	538	TLA	O41-C4-C3	2.10	119.16	113.31
4	D	550[A]	DYY	CAQ-CAR-CAE	-2.10	120.22	123.50
4	D	550[A]	DYY	OAB-SAF-NAG	2.09	108.66	106.69
3	D	543	TLA	O41-C4-C3	2.08	119.10	113.31
4	D	550[B]	DYY	FAA-CAD-CAE	2.03	121.61	118.93
4	D	550[A]	DYY	CAU-NAV-SAW	-2.03	113.29	117.06
2	A	541	FBP	O6P-P2-O5P	2.01	115.34	107.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

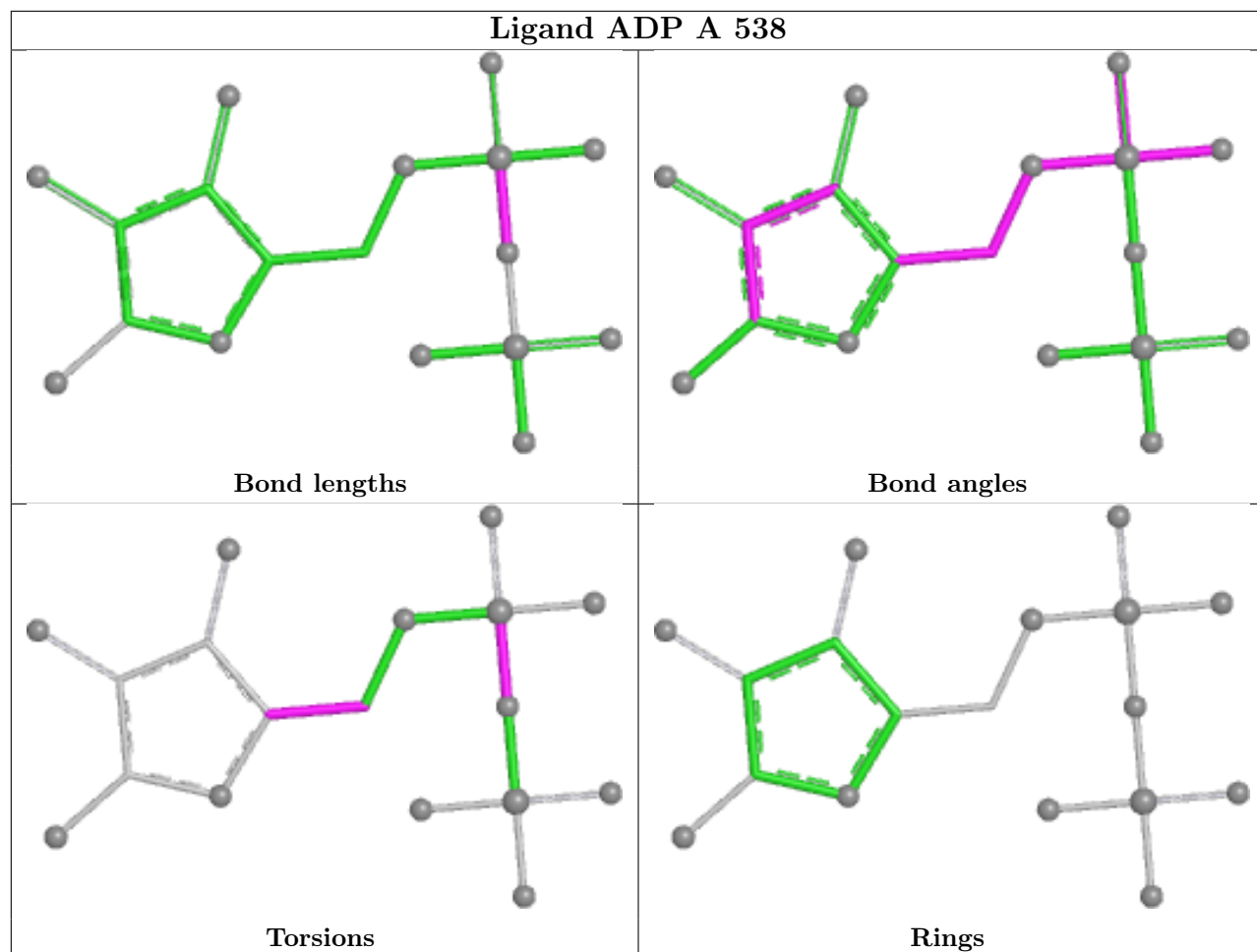
Mol	Chain	Res	Type	Atoms
4	D	550[B]	DYY	CAI-NAV-SAW-OB
2	A	541	FBP	C4-C5-C6-O6
2	B	541	FBP	C4-C5-C6-O6
6	A	538	ADP	O4'-C4'-C5'-O5'
6	A	538	ADP	C3'-C4'-C5'-O5'
4	A	550[B]	DYY	CAI-NAV-SAW-OB
4	D	550[B]	DYY	CAI-NAV-SAW-CAX
4	A	550[A]	DYY	CAI-NAV-SAW-OB
4	D	550[A]	DYY	CAI-NAV-SAW-OB
2	D	541	FBP	C4-C5-C6-O6
4	A	550[B]	DYY	CAH-NAG-SAF-OAB
2	C	541	FBP	C6-O6-P2-O4P
2	A	541	FBP	O5-C5-C6-O6
2	B	541	FBP	O5-C5-C6-O6
4	A	550[A]	DYY	CAT-NAG-SAF-OAS
4	D	550[B]	DYY	CAU-NAV-SAW-OB
2	D	541	FBP	O5-C5-C6-O6
6	A	538	ADP	PB-O3A-PA-O2A
4	D	550[A]	DYY	CAR-CAE-SAF-OAB
4	D	550[A]	DYY	CAT-NAG-SAF-OAS
4	A	550[A]	DYY	CAI-NAV-SAW-CAX
6	A	538	ADP	PB-O3A-PA-O1A
3	D	543	TLA	C2-C3-C4-O4
4	A	550[A]	DYY	CAR-CAE-SAF-OAS
4	A	550[A]	DYY	CAD-CAE-SAF-OAB
4	D	550[B]	DYY	CAR-CAE-SAF-OAS

There are no ring outliers.

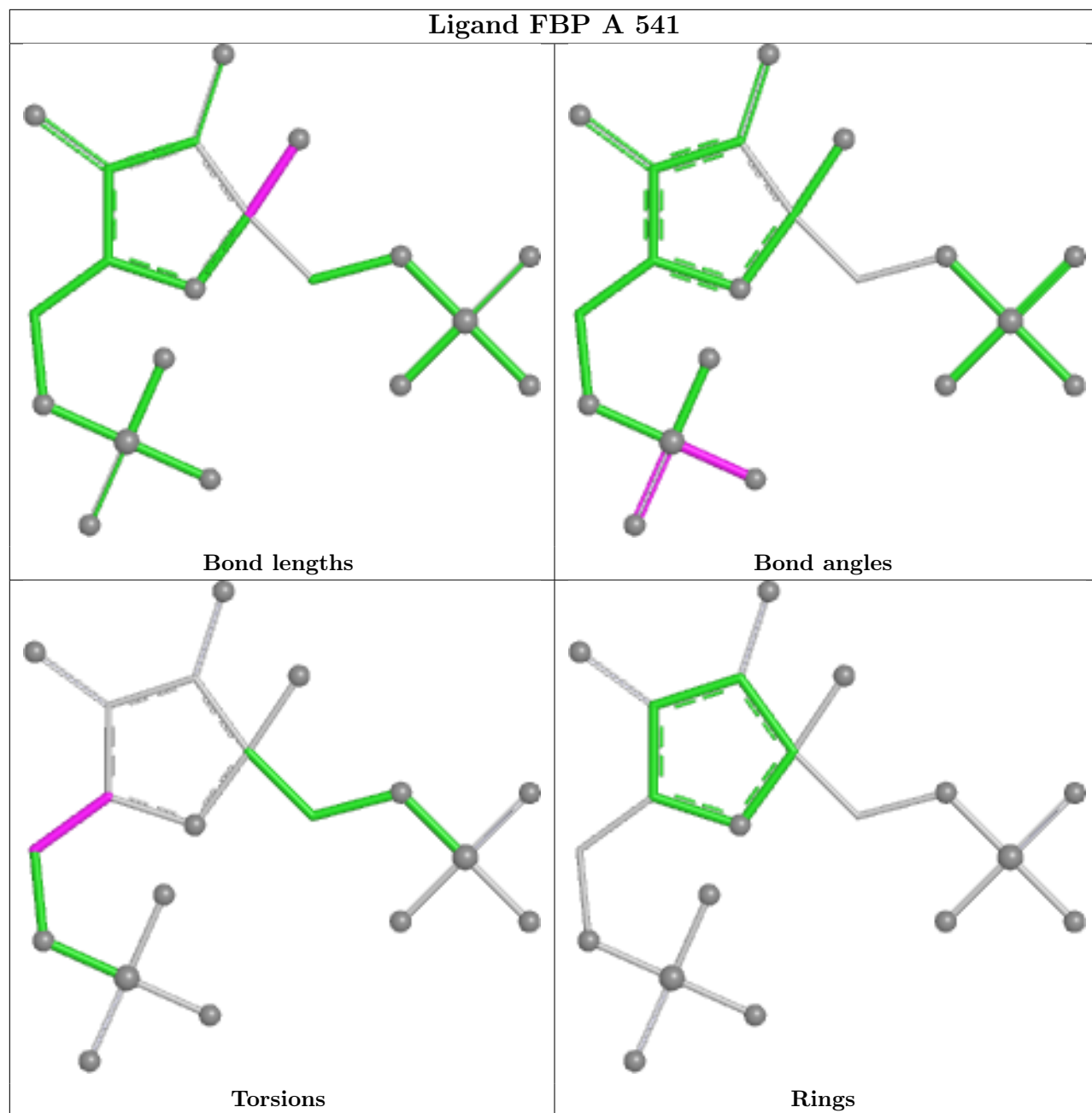
4 monomers are involved in 17 short contacts:

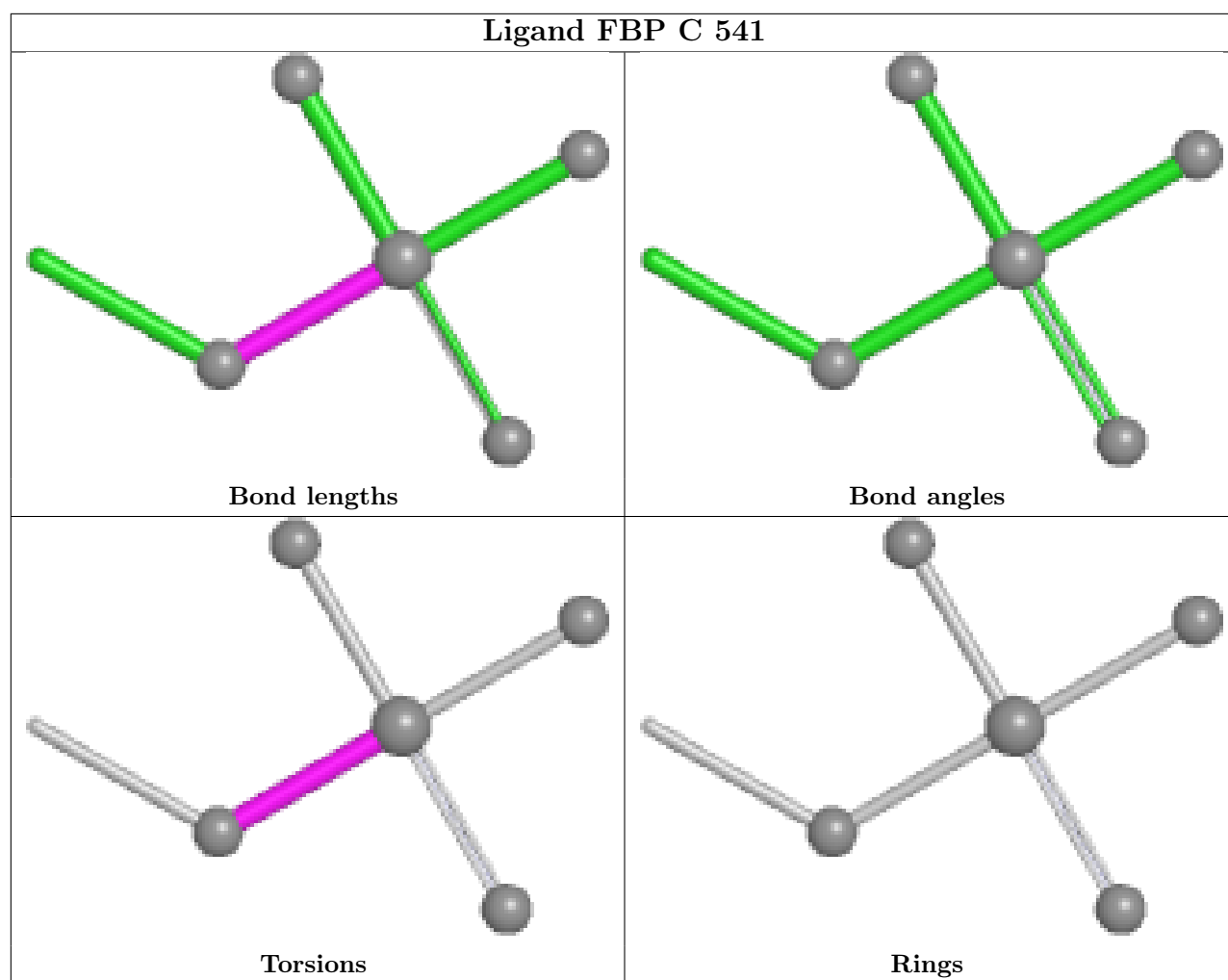
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	550[B]	DYY	4	0
4	A	550[A]	DYY	4	0
4	A	550[B]	DYY	5	0
4	D	550[A]	DYY	4	0

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.

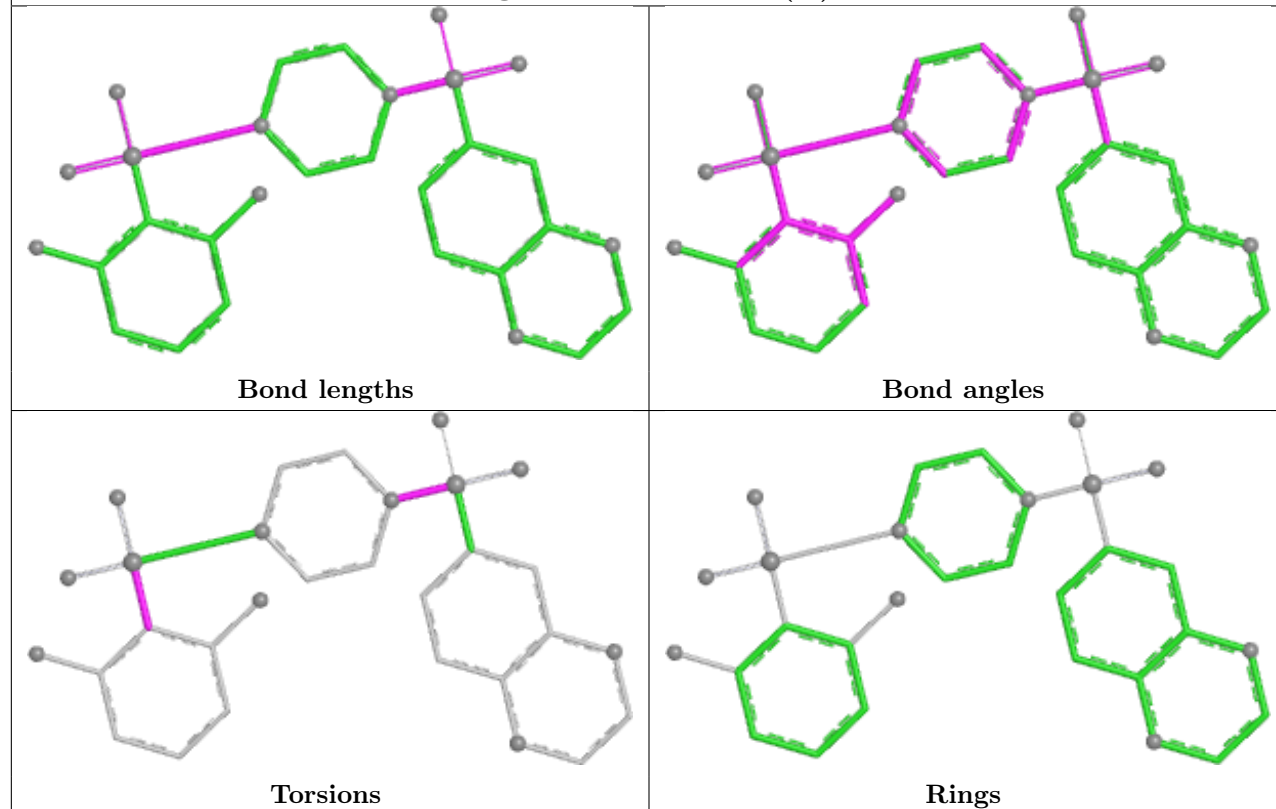


Ligand FBP A 541

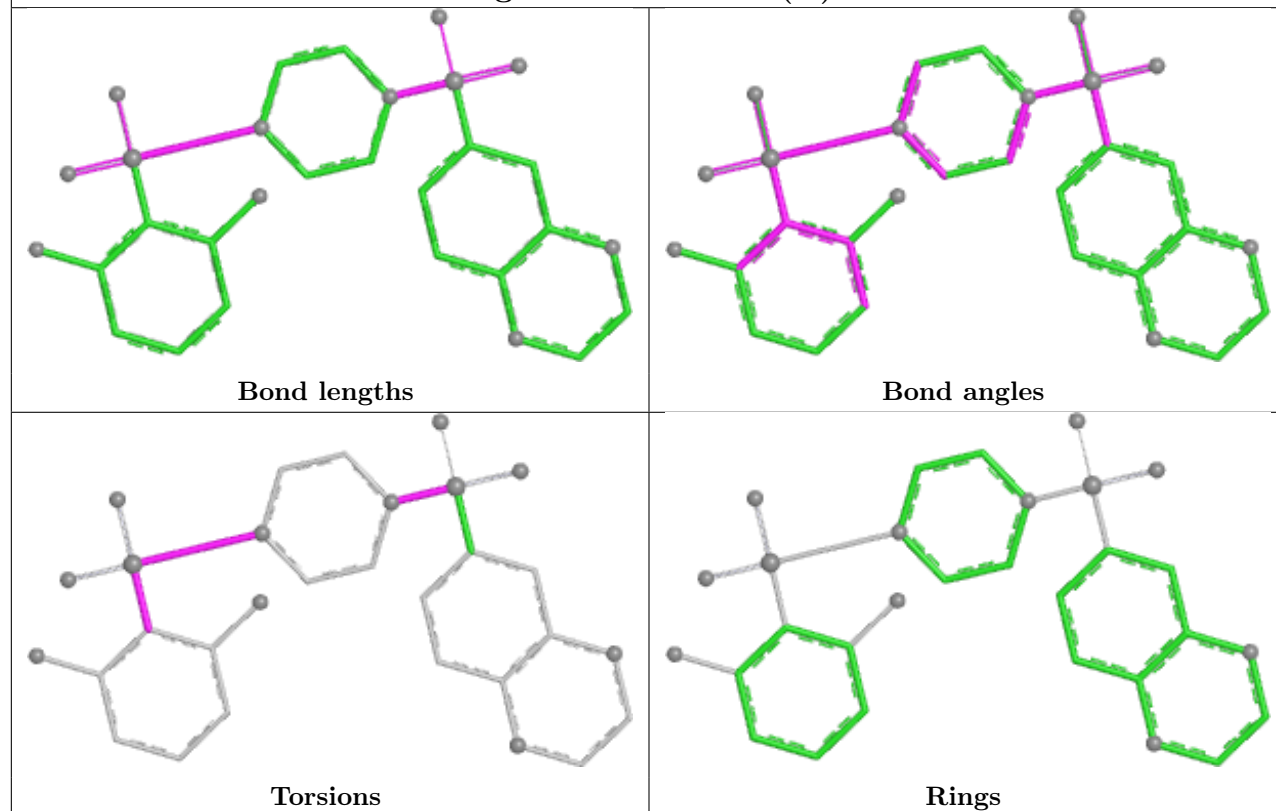




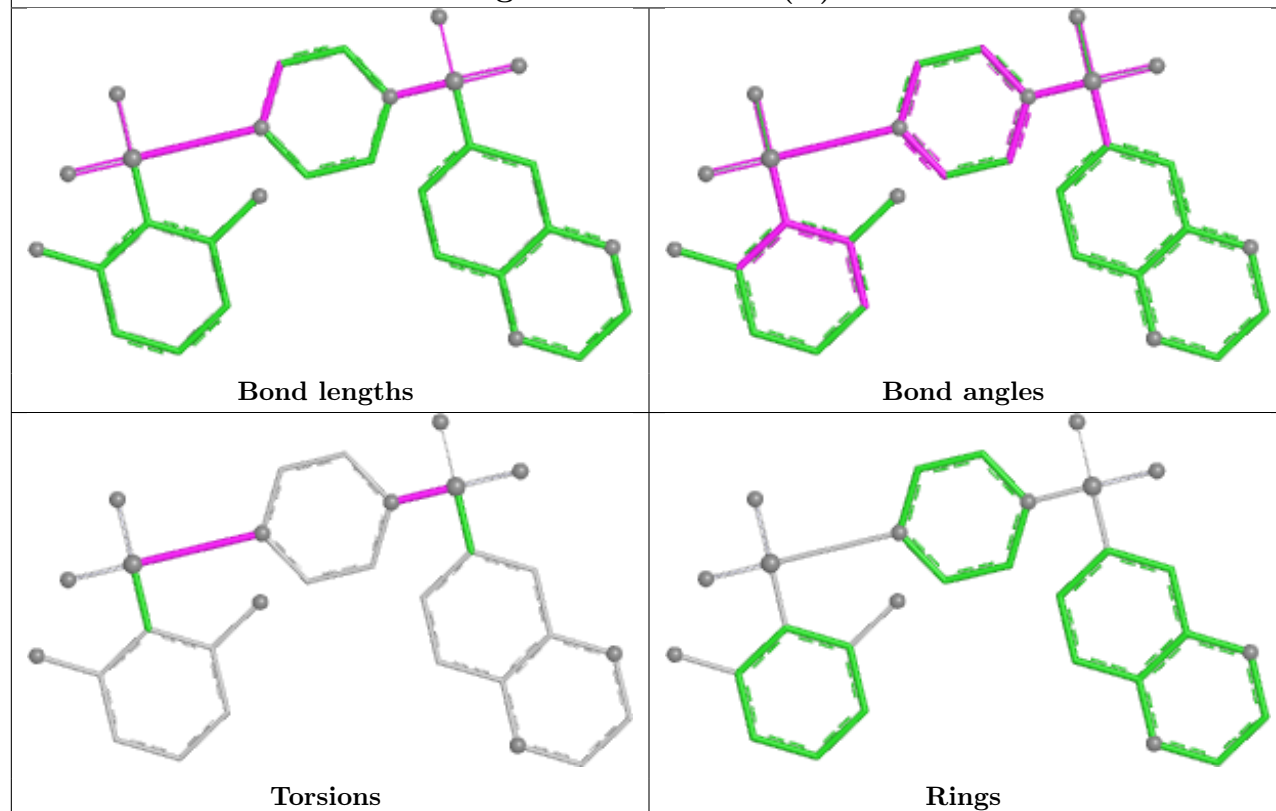
Ligand DYY D 550 (B)



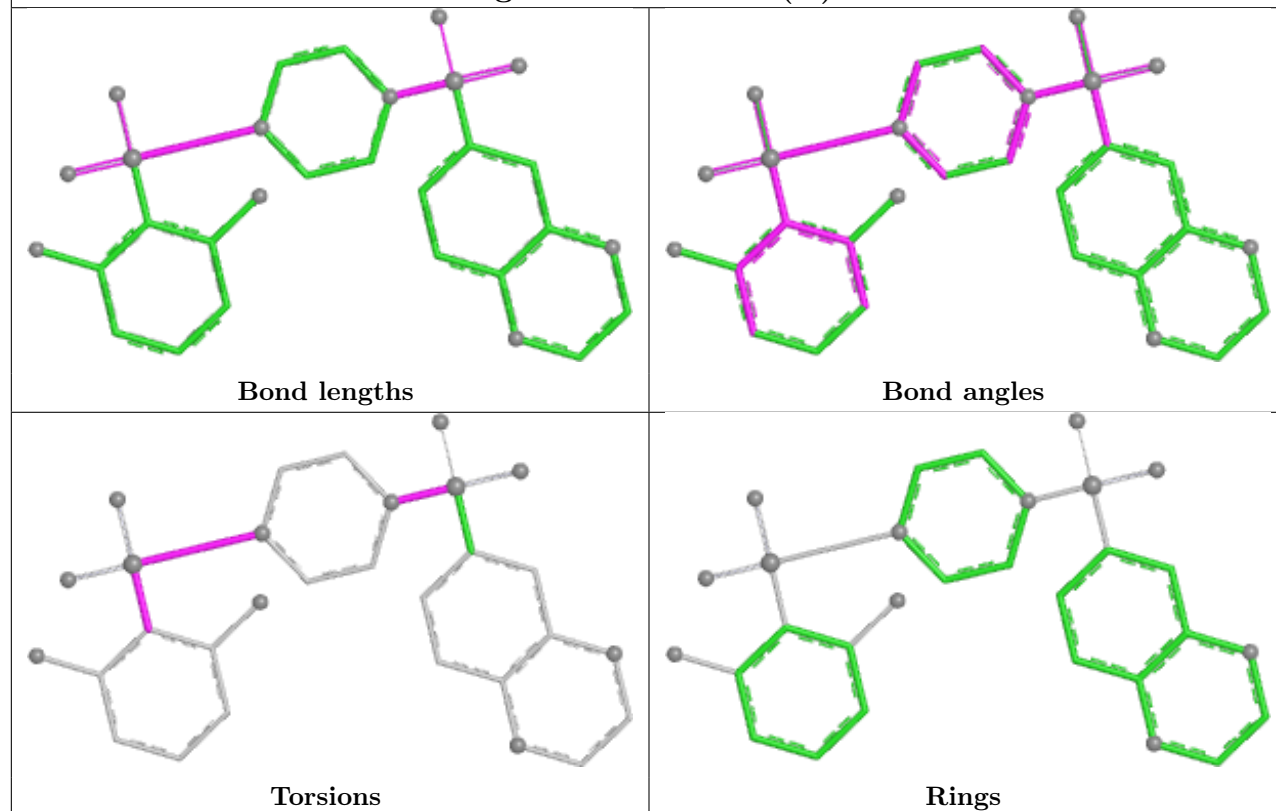
Ligand DYY A 550 (A)

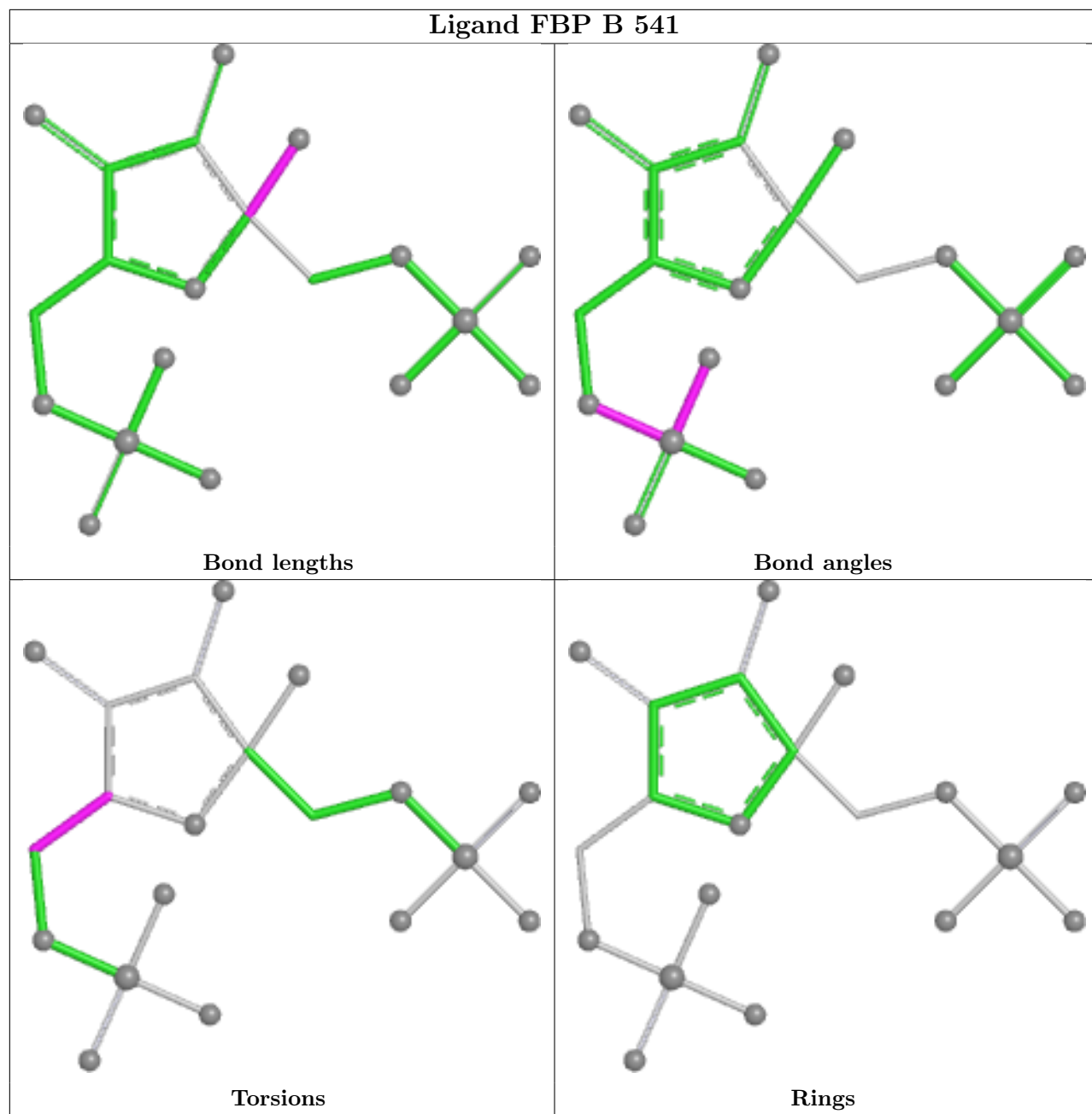


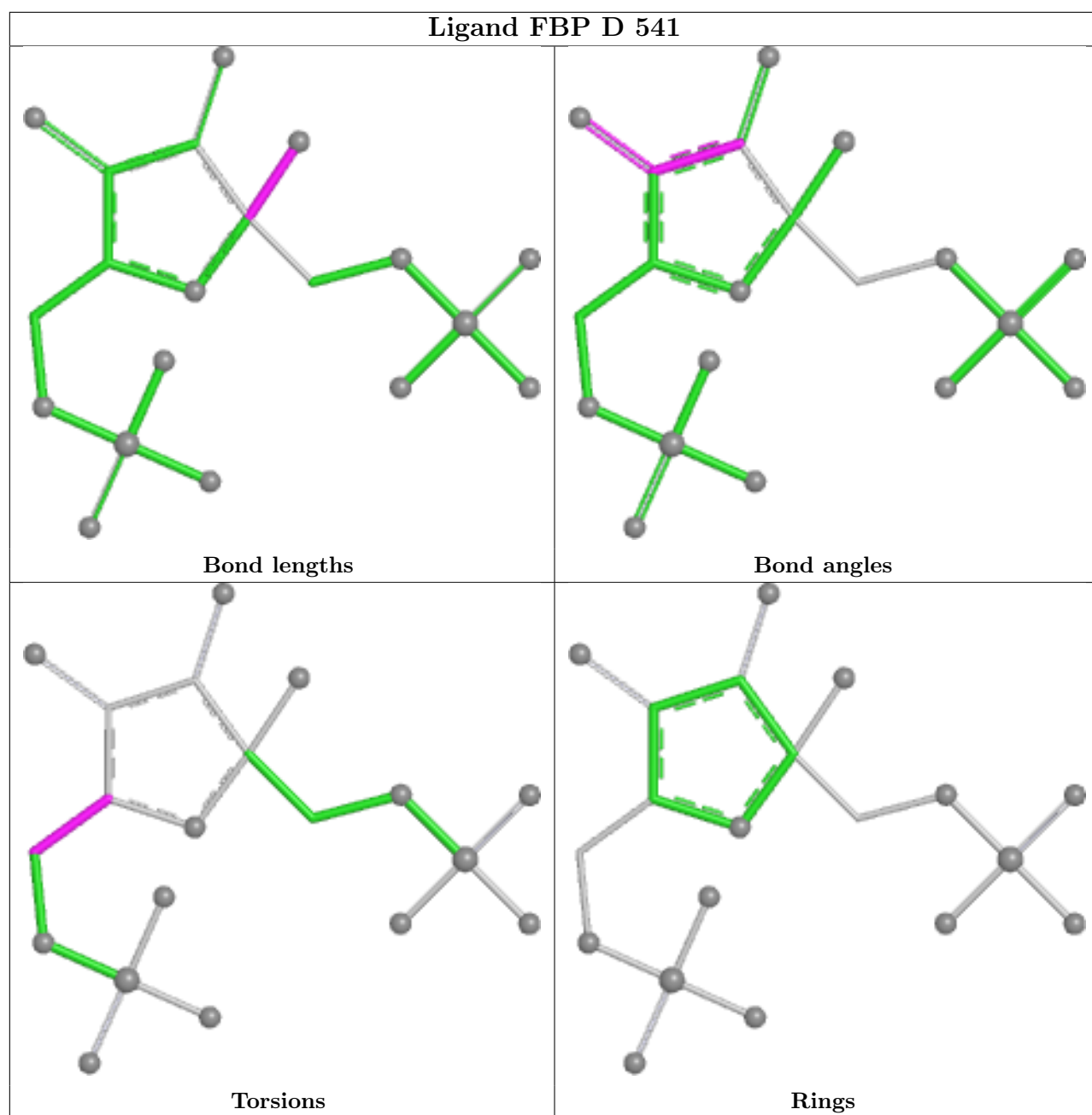
Ligand DYY A 550 (B)



Ligand DYY D 550 (A)







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	519/550 (94%)	0.46	54 (10%)	11 11	12, 23, 48, 60	2 (0%)
1	B	505/550 (91%)	0.48	69 (13%)	6 6	10, 23, 59, 81	3 (0%)
1	C	515/550 (93%)	0.19	22 (4%)	40 41	13, 22, 40, 62	4 (0%)
1	D	509/550 (92%)	0.41	47 (9%)	14 14	10, 23, 46, 65	4 (0%)
All	All	2048/2200 (93%)	0.38	192 (9%)	14 14	10, 23, 49, 81	13 (0%)

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	8.5
1	C	404	ILE	7.9
1	B	132	VAL	7.3
1	D	144	LEU	6.1
1	A	404	ILE	6.0
1	C	515	TRP	5.7
1	D	191	ASP	5.4
1	B	142	ILE	5.3
1	A	192	PHE	5.0
1	B	185	VAL	5.0
1	B	14	GLN	5.0
1	B	156	ILE	4.9
1	B	194	VAL	4.8
1	A	405	THR	4.8
1	D	156	ILE	4.6
1	C	403	PRO	4.6
1	C	517	PRO	4.6
1	A	217	ASP	4.5
1	B	123	LEU	4.5
1	B	124	ILE	4.5
1	A	13	ILE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	403	PRO	4.4
1	B	138	ALA	4.4
1	D	204	GLY	4.3
1	B	148	TYR	4.3
1	B	143	THR	4.2
1	B	170	VAL	4.2
1	B	159	LEU	4.2
1	B	197	VAL	4.2
1	B	192	PHE	4.1
1	D	147	ALA	4.0
1	D	192	PHE	4.0
1	B	183	LEU	3.9
1	B	199	ASN	3.9
1	A	134	LEU	3.8
1	C	213	GLY	3.8
1	B	133	GLU	3.8
1	D	159	LEU	3.8
1	B	402	ALA	3.8
1	A	138	ALA	3.8
1	A	200	GLY	3.7
1	D	132	VAL	3.7
1	B	40	ILE	3.6
1	D	124	ILE	3.6
1	D	14	GLN	3.6
1	A	132	VAL	3.5
1	B	478	VAL	3.5
1	D	404	ILE	3.5
1	A	14	GLN	3.5
1	A	170	VAL	3.5
1	B	146	ASN	3.5
1	A	190	ALA	3.4
1	D	122	GLY	3.4
1	D	402	ALA	3.4
1	A	197	VAL	3.4
1	A	482	TRP	3.4
1	B	140	LEU	3.4
1	C	14	GLN	3.4
1	A	171	GLY	3.4
1	C	402	ALA	3.3
1	C	405	THR	3.3
1	D	123	LEU	3.3
1	B	147	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	195	THR	3.3
1	B	193	LEU	3.2
1	B	152	CYS	3.2
1	B	424	CYS	3.2
1	B	41	THR	3.2
1	B	155	ASN	3.2
1	C	424	CYS	3.2
1	C	521	PHE	3.2
1	B	181	ILE	3.1
1	B	172	SER	3.1
1	B	180	LEU	3.1
1	D	143	THR	3.1
1	D	158	TRP	3.1
1	A	168	VAL	3.1
1	D	145	ASP	3.0
1	D	139	THR	3.0
1	D	401	LEU	3.0
1	A	137	GLY	3.0
1	D	146	ASN	2.9
1	A	189	GLY	2.9
1	A	40	ILE	2.9
1	D	193	LEU	2.8
1	A	135	LYS	2.8
1	B	139	THR	2.8
1	C	406	SER	2.8
1	D	148	TYR	2.8
1	A	185	VAL	2.7
1	B	191	ASP	2.7
1	D	154	GLU	2.7
1	B	18	LEU	2.7
1	C	165	CYS	2.7
1	D	202	SER	2.7
1	B	404	ILE	2.7
1	B	145	ASP	2.7
1	A	193	LEU	2.7
1	B	144	LEU	2.7
1	B	221	VAL	2.7
1	D	152	CYS	2.7
1	B	175	TYR	2.7
1	D	138	ALA	2.7
1	B	406	SER	2.6
1	B	168	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	40	ILE	2.6
1	A	402	ALA	2.6
1	A	202	SER	2.6
1	A	133	GLU	2.6
1	A	144	LEU	2.6
1	A	196	GLU	2.6
1	D	175	TYR	2.6
1	B	157	LEU	2.6
1	B	401	LEU	2.6
1	D	170	VAL	2.6
1	A	136	LYS	2.6
1	C	190	ALA	2.6
1	D	403	PRO	2.6
1	A	201	GLY	2.5
1	A	156	ILE	2.5
1	A	408	PRO	2.5
1	A	406	SER	2.5
1	D	134	LEU	2.5
1	A	142	ILE	2.5
1	A	129	THR	2.5
1	A	139	THR	2.5
1	A	194	VAL	2.5
1	D	150	GLU	2.5
1	B	103	ILE	2.4
1	B	125	LYS	2.4
1	D	203	LEU	2.4
1	D	205	SER	2.4
1	A	148	TYR	2.4
1	B	164	ILE	2.4
1	D	142	ILE	2.4
1	D	149	MET	2.4
1	B	165	CYS	2.4
1	D	424	CYS	2.4
1	B	154	GLU	2.4
1	B	131	GLU	2.3
1	B	205	SER	2.3
1	B	196	GLU	2.3
1	A	488	LEU	2.3
1	B	203	LEU	2.3
1	A	470[A]	PHE	2.3
1	B	158	TRP	2.3
1	B	24	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	2.3
1	B	23	ALA	2.3
1	C	401	LEU	2.3
1	D	163	ASN	2.3
1	A	178	ASP	2.3
1	C	156	ILE	2.3
1	A	528	VAL	2.3
1	C	170	VAL	2.3
1	D	22	MET	2.3
1	C	408	PRO	2.2
1	A	199	ASN	2.2
1	A	186	LYS	2.2
1	B	171	GLY	2.2
1	B	201	GLY	2.2
1	A	22	MET	2.2
1	A	401	LEU	2.2
1	B	403	PRO	2.2
1	D	199	ASN	2.2
1	B	42	ALA	2.2
1	B	200	GLY	2.2
1	A	191	ASP	2.1
1	B	198	GLU	2.1
1	D	178	ASP	2.1
1	B	184	GLN	2.1
1	A	500[A]	ARG	2.1
1	A	424	CYS	2.1
1	C	522	THR	2.1
1	C	192	PHE	2.1
1	D	194	VAL	2.1
1	B	163	ASN	2.1
1	A	182	SER	2.1
1	B	182	SER	2.1
1	D	219	PRO	2.1
1	A	124	ILE	2.1
1	D	201	GLY	2.0
1	A	407	ASP	2.0
1	C	167	VAL	2.0
1	C	168	VAL	2.0
1	D	180	LEU	2.0
1	D	405	THR	2.0
1	B	174	ILE	2.0
1	D	161	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	214	ALA	2.0
1	C	214	ALA	2.0
1	B	151	LYS	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	C	533	1/1	-0.39	1.66	2,2,2,2	1
5	UNX	B	534	1/1	-0.25	1.23	2,2,2,2	1
5	UNX	D	533	1/1	-0.05	1.33	2,2,2,2	1
5	UNX	A	536	1/1	0.12	1.25	2,2,2,2	1
5	UNX	A	537	1/1	0.14	1.37	2,2,2,2	1
5	UNX	D	532	1/1	0.16	1.30	2,2,2,2	1
5	UNX	A	533	1/1	0.24	1.15	2,2,2,2	1
5	UNX	B	537	1/1	0.25	1.44	2,2,2,2	1
5	UNX	D	535	1/1	0.30	1.33	2,2,2,2	1
5	UNX	B	536	1/1	0.34	1.23	2,2,2,2	1
5	UNX	C	532	1/1	0.34	1.18	2,2,2,2	1
5	UNX	A	534	1/1	0.45	1.16	2,2,2,2	1
5	UNX	A	535	1/1	0.51	1.23	2,2,2,2	1
5	UNX	D	534	1/1	0.52	1.30	2,2,2,2	1
5	UNX	A	532	1/1	0.54	1.20	2,2,2,2	1
5	UNX	B	533	1/1	0.61	1.20	2,2,2,2	1
5	UNX	B	535	1/1	0.69	1.32	2,2,2,2	1
4	DYY	D	550[B]	30/30	0.74	0.17	29,36,40,41	30
4	DYY	D	550[A]	30/30	0.74	0.17	30,38,44,45	30

Continued on next page...

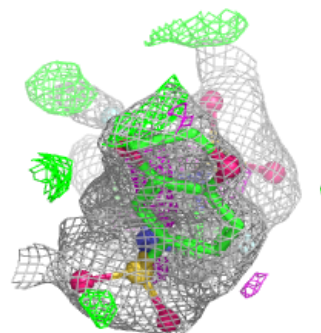
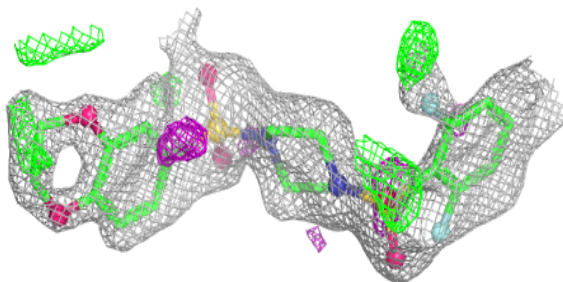
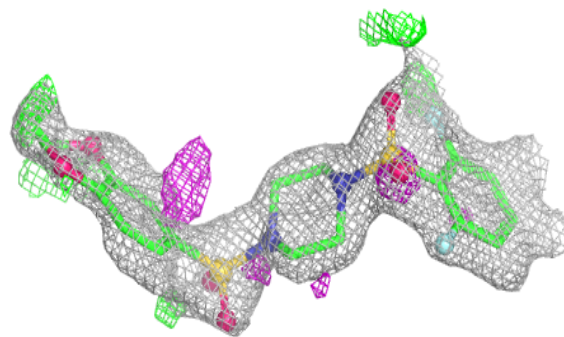
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	C	541	6/20	0.78	0.15	42,45,47,48	0
6	ADP	A	538	18/27	0.81	0.18	19,25,26,28	18
3	TLA	D	543	10/10	0.82	0.11	46,48,51,52	0
3	TLA	C	542	10/10	0.87	0.11	23,32,37,39	0
4	DYY	A	550[B]	30/30	0.88	0.13	32,38,43,44	30
3	TLA	D	542	10/10	0.88	0.09	32,34,36,36	0
4	DYY	A	550[A]	30/30	0.88	0.13	24,35,38,39	30
3	TLA	B	538	10/10	0.89	0.08	34,35,36,36	0
5	UNX	B	532	1/1	0.90	1.24	3,3,3,3	1
3	TLA	B	542	10/10	0.91	0.08	26,30,30,31	0
3	TLA	C	534	10/10	0.91	0.08	22,24,28,29	0
3	TLA	A	542	10/10	0.91	0.08	22,26,28,30	0
2	FBP	A	541	20/20	0.93	0.09	21,29,33,35	0
2	FBP	B	541	20/20	0.98	0.05	15,19,24,24	0
2	FBP	D	541	20/20	0.98	0.04	13,15,17,18	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.

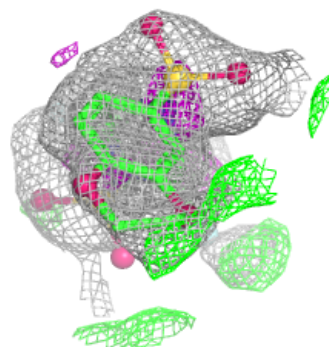
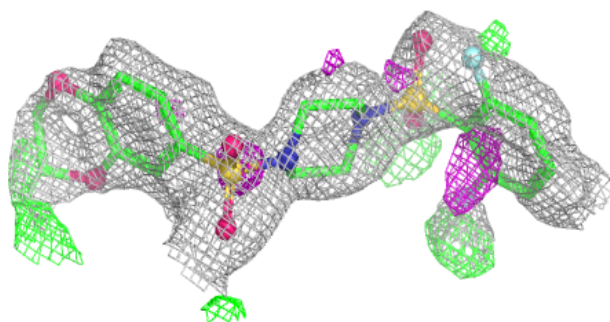
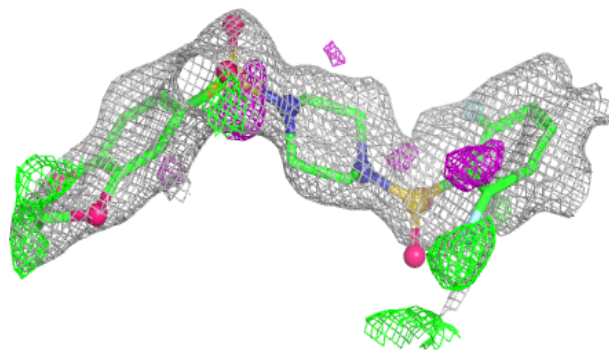
Electron density around DYY D 550 (B):

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

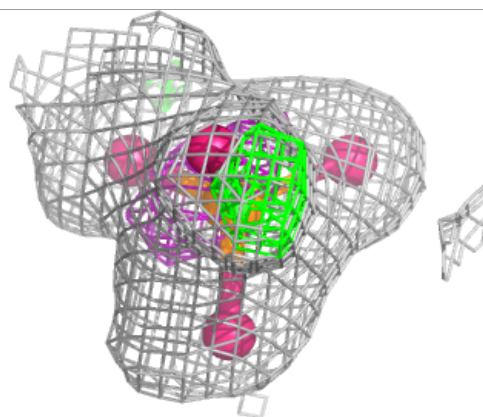
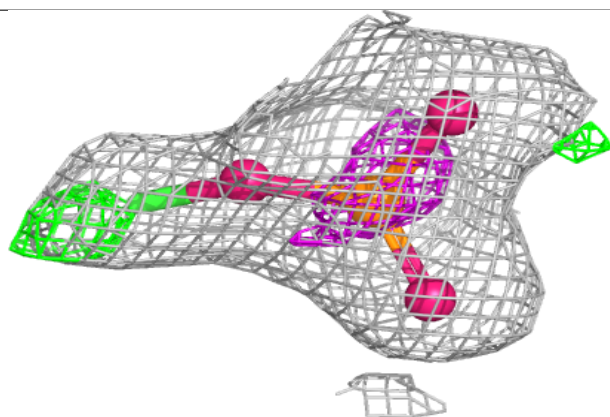
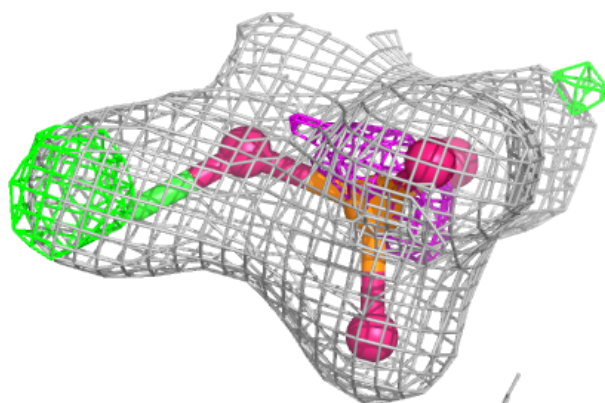


Electron density around DYY D 550 (A):

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

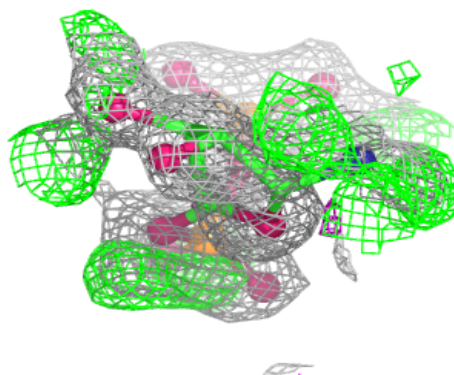
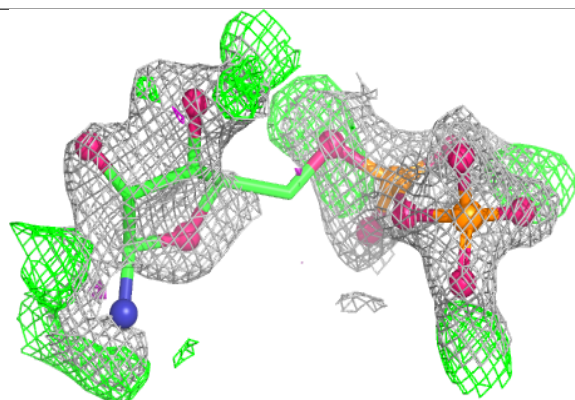
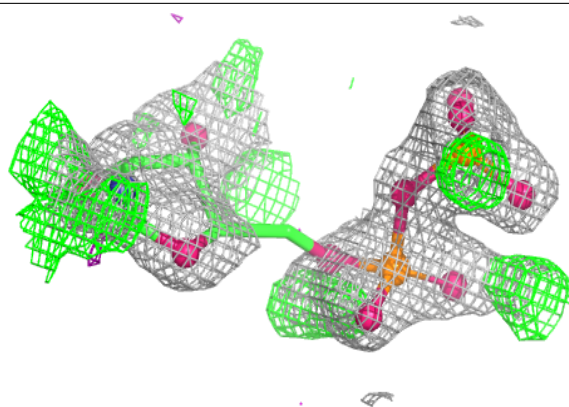
**Electron density around FBP C 541:**

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

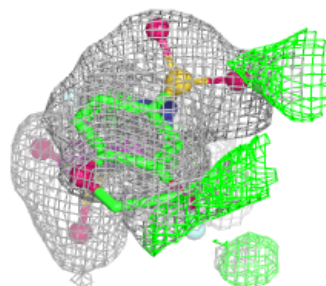
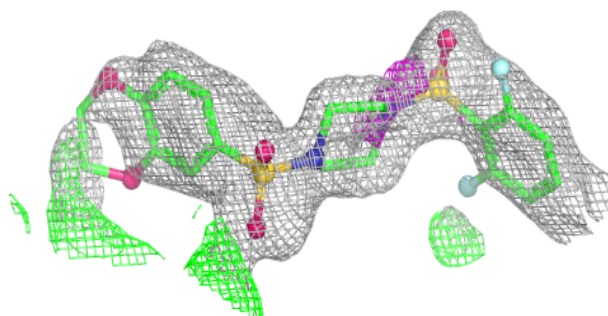
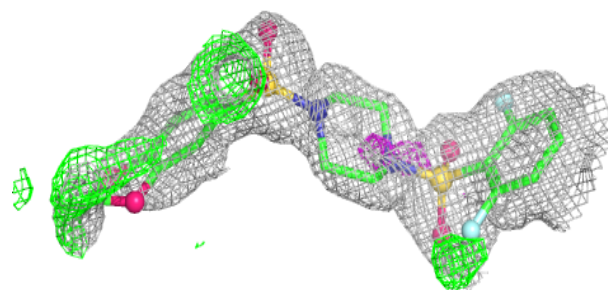


Electron density around ADP A 538:

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

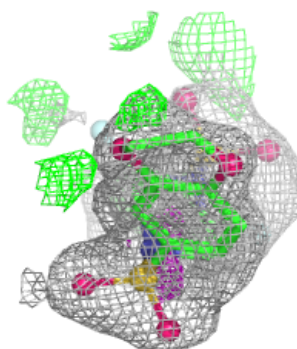
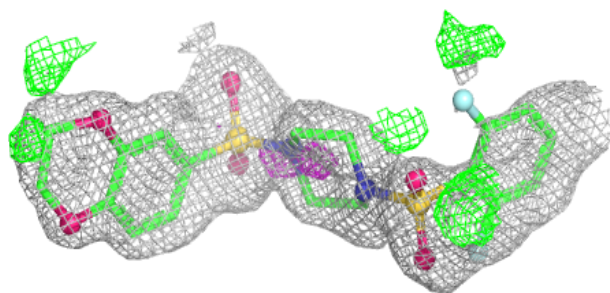
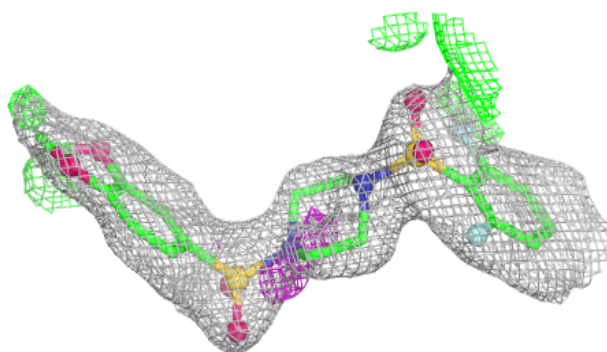
**Electron density around DYY A 550 (B):**

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

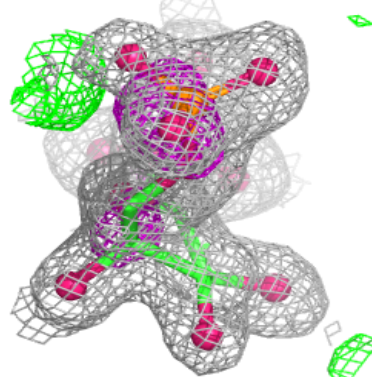
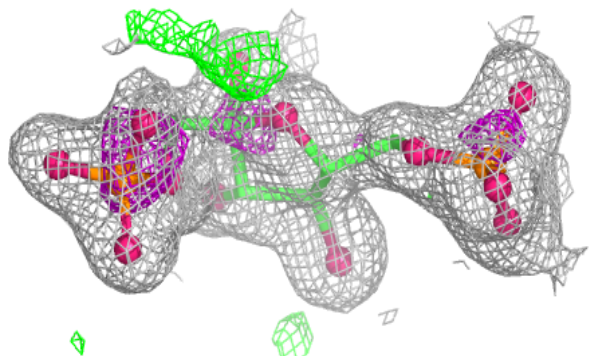
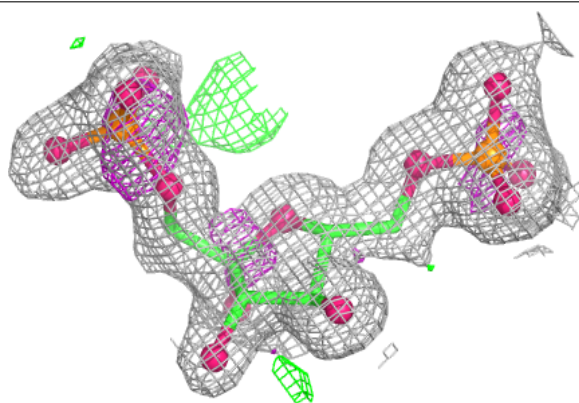


Electron density around DYY A 550 (A):

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

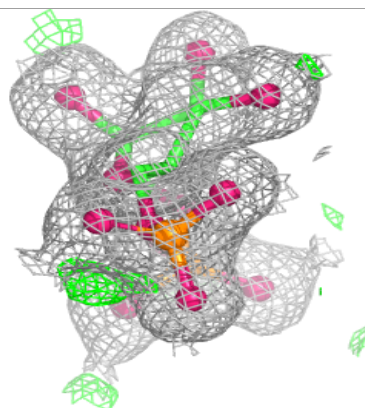
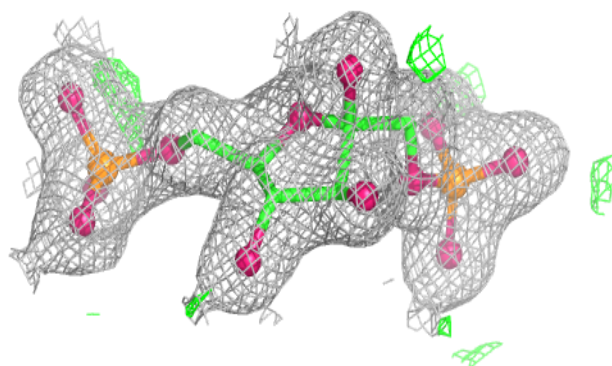
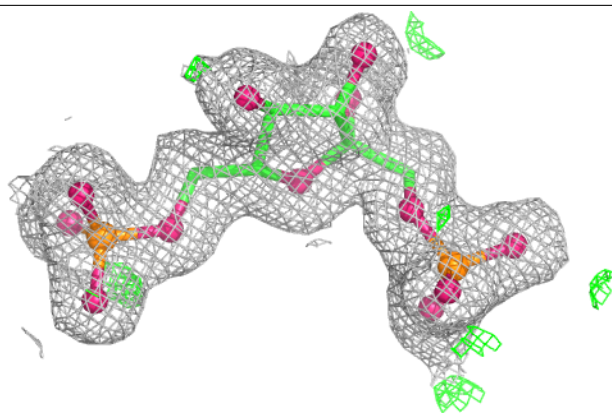
**Electron density around FBP A 541:**

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

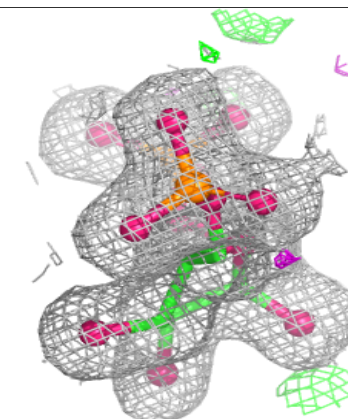
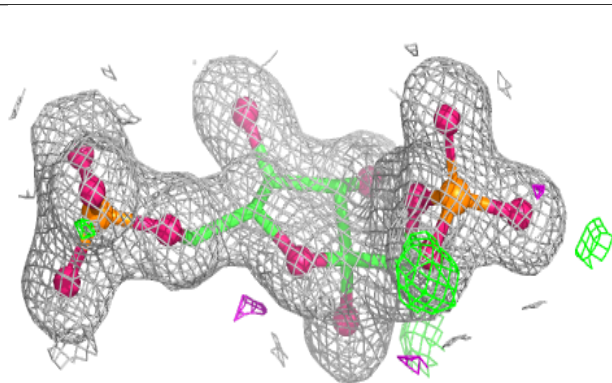
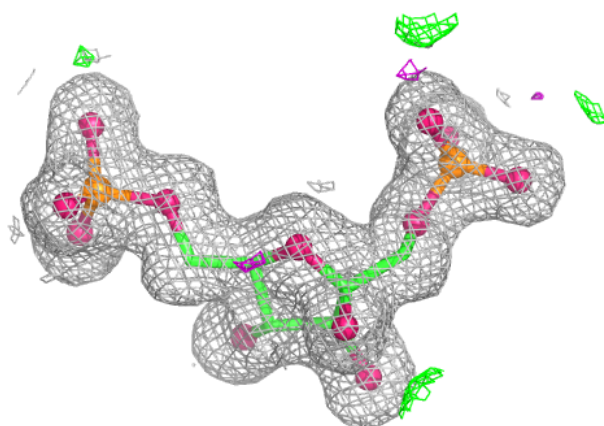


Electron density around FBP B 541:

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

**Electron density around FBP D 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.