



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:42 PM UTC

PDB ID : 4IMA / pdb_00004ima
Title : The structure of C436M-hLPYK in complex with Citrate/Mn/ATP/Fru-1,6-BP
Authors : Zhang, B.; Holyoak, T.; Fenton, A.W.; Tang, Q.L.; Prasannan, C.B.; Deng, J.P.
Deposited on : 2013-01-02
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 ⓘ](#)) 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

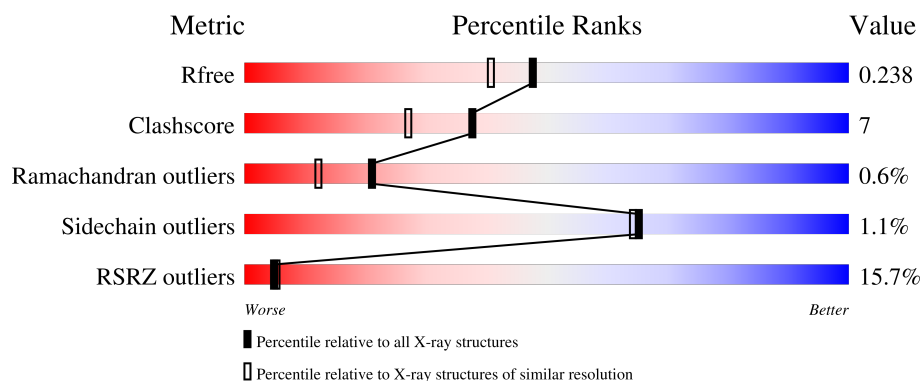
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

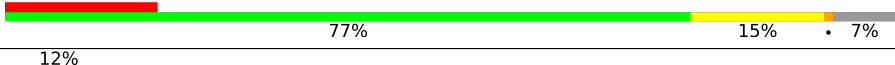
The reported resolution of this entry is 1.95 Å.

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	543	
1	B	543	
1	C	543	
1	D	543	

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
6	ADN	D	604	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16181 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	89	4	0
			3982	2506	715	742	19			
1	B	500	Total	C	N	O	S	127	2	0
			3800	2390	684	707	19			
1	C	505	Total	C	N	O	S	81	5	0
			3861	2432	693	718	18			
1	D	460	Total	C	N	O	S	87	3	0
			3520	2216	628	657	19			

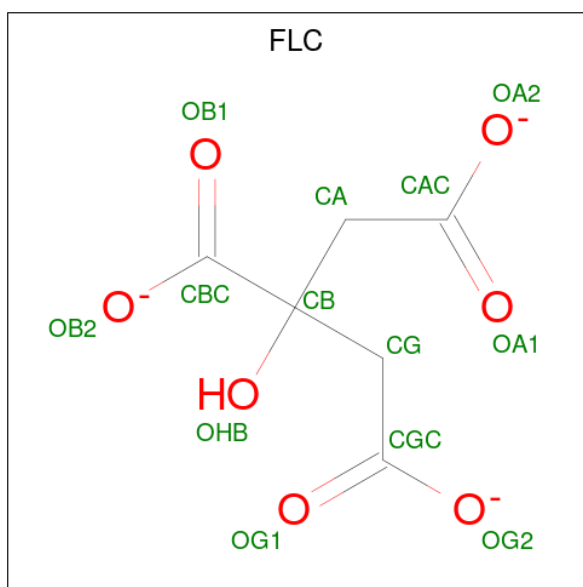
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	CYS	engineered mutation	UNP O75758
B	436	MET	CYS	engineered mutation	UNP O75758
C	436	MET	CYS	engineered mutation	UNP O75758
D	436	MET	CYS	engineered mutation	UNP O75758

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

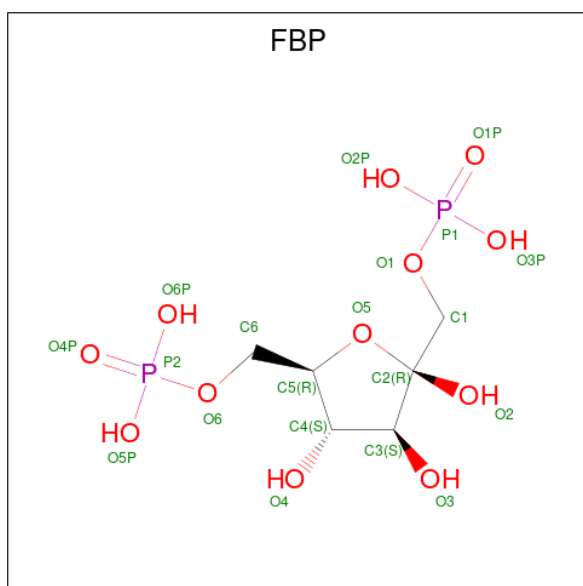
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



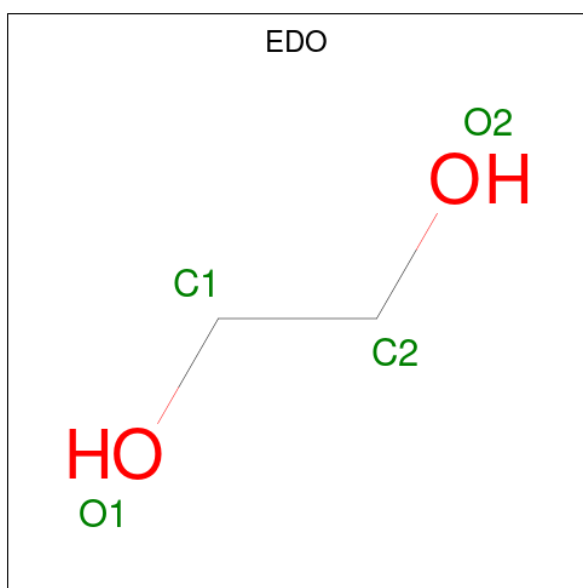
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	1	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	1	0
			13	6	7		

- Molecule 4 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



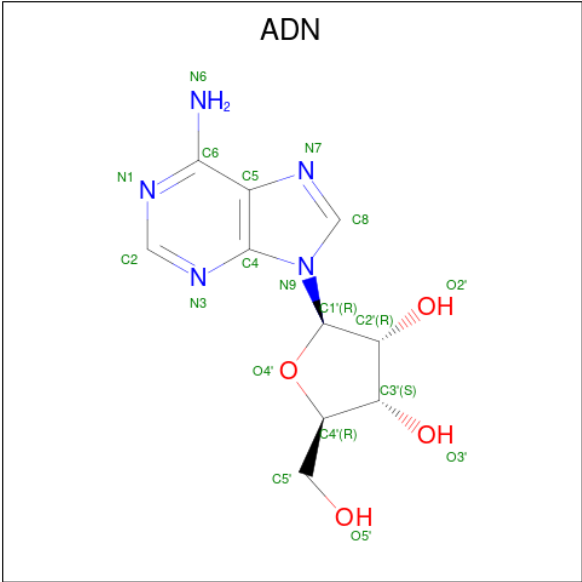
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			19	10	5	4		

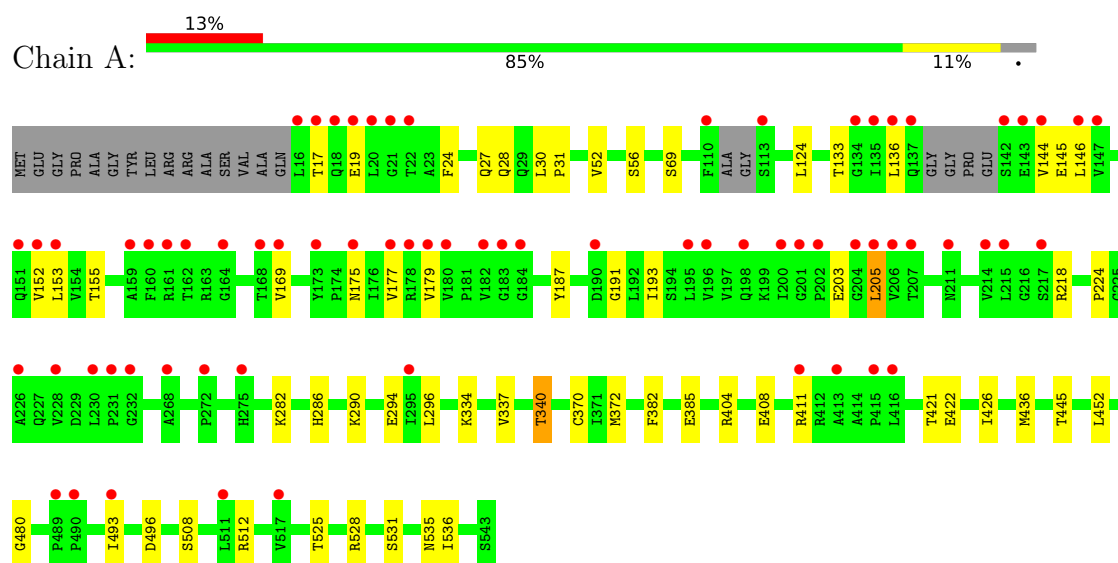
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		
7	B	223	Total	O	0	0
			223	223		
7	C	228	Total	O	0	0
			228	228		
7	D	199	Total	O	0	0
			199	199		

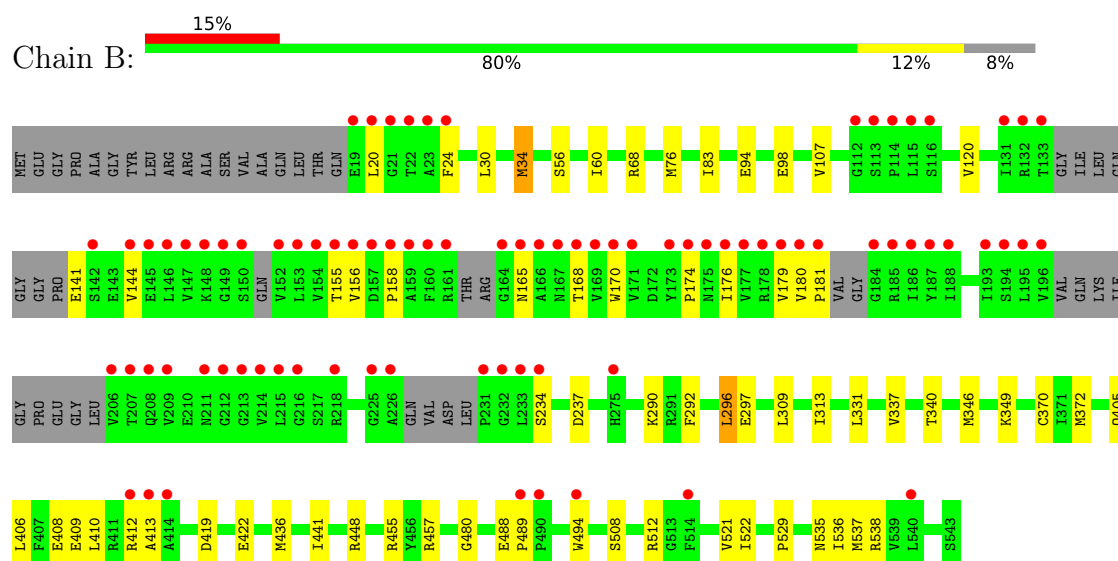
3 Residue-property plots [i](#)

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.

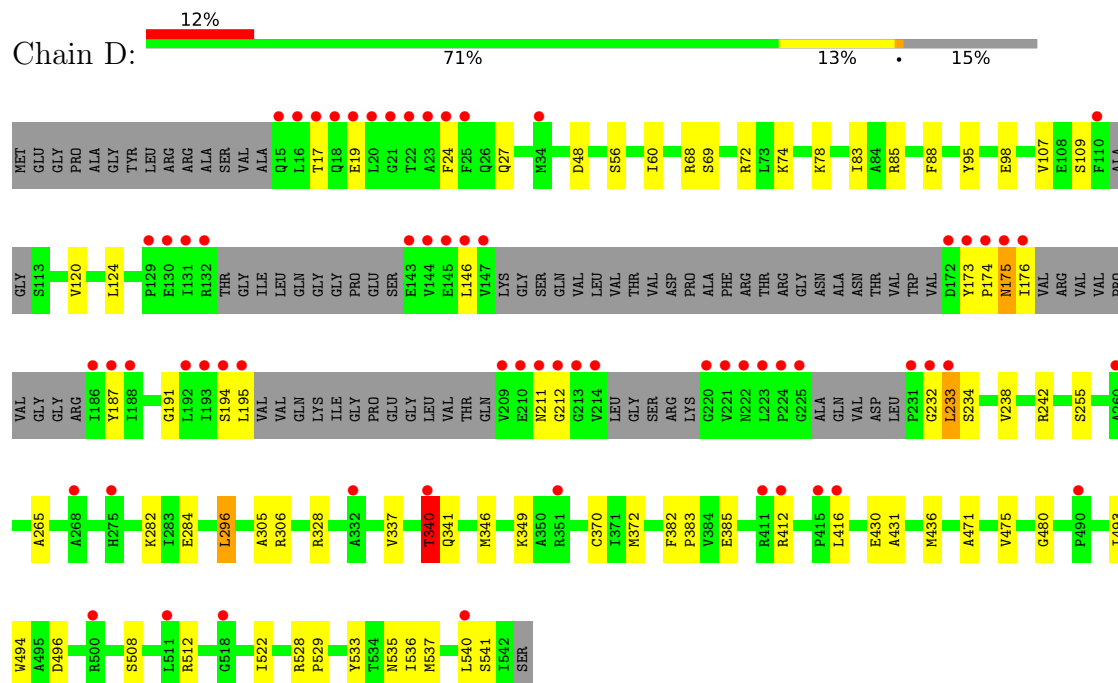
• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.75Å 204.73Å 86.53Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	38.89 – 1.95 38.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	87.3 (38.89-1.95) 97.4 (38.89-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.198 , 0.233 0.205 , 0.238	Depositor DCC
R_{free} test set	10106 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.088 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16181	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: ADN, MN, EDO, FLC, FBP

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	0.49	1/4056 (0.0%)	0.79	2/5491 (0.0%)
1	B	0.50	0/3862	0.78	1/5221 (0.0%)
1	C	0.51	0/3936	0.83	4/5326 (0.1%)
1	D	0.51	1/3580 (0.0%)	0.80	4/4835 (0.1%)
All	All	0.50	2/15434 (0.0%)	0.80	11/20873 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	341	GLN	C-O	-5.39	1.17	1.24
1	A	340	THR	C-O	-5.09	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	182	VAL	N-CA-CB	-12.40	90.17	110.14
1	C	181	PRO	CB-CA-C	8.95	126.32	111.56
1	D	340	THR	CA-C-N	-7.40	107.41	121.54
1	D	340	THR	C-N-CA	-7.40	107.41	121.54
1	B	181	PRO	N-CA-CB	6.91	110.60	103.00
1	D	306	ARG	N-CA-C	6.40	119.08	111.33
1	C	181	PRO	N-CA-C	-6.09	99.92	112.47
1	D	306	ARG	CB-CA-C	5.98	120.85	110.68
1	A	334	LYS	CA-C-N	5.91	125.84	119.76
1	A	334	LYS	C-N-CA	5.91	125.84	119.76
1	C	182	VAL	N-CA-C	5.71	117.67	109.51

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	3982	0	4071	43	0
1	B	3800	0	3863	48	0
1	C	3861	0	3946	65	0
1	D	3520	0	3572	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	4	2	0
3	B	13	0	4	1	0
3	C	13	0	4	1	0
3	D	13	0	4	3	0
4	A	20	0	10	0	0
4	B	20	0	10	0	0
4	C	20	0	10	0	0
4	D	20	0	10	0	0
5	B	4	0	6	0	0
6	D	19	0	13	0	0
7	A	209	0	0	3	0
7	B	223	0	0	2	0
7	C	228	0	0	5	0
7	D	199	0	0	3	0
All	All	16181	0	15527	208	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 7.

All (208) 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:173:TYR:CE1	1:C:230:LEU:HD21	1.85	1.11
1:C:173:TYR:CE1	1:C:230:LEU:CD2	2.44	0.99
1:B:156:VAL:HG21	1:B:174:PRO:HA	1.42	0.99
1:C:173:TYR:CD1	1:C:230:LEU:HD21	1.98	0.98
1:C:411[A]:ARG:HG3	1:C:426:ILE:HD11	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:ARG:NH1	1:D:533:TYR:CE1	2.45	0.84
1:D:194:SER:HB2	1:D:195:LEU:HB2	1.60	0.83
1:C:197:VAL:HA	1:C:207:THR:HG22	1.65	0.79
1:A:24:PHE:HZ	1:A:436:MET:HE2	1.52	0.75
1:A:24:PHE:CZ	1:A:436:MET:HE2	2.25	0.72
1:D:340:THR:O	7:D:724:HOH:O	2.09	0.70
1:B:522:ILE:HG23	1:B:537[A]:MET:HE3	1.75	0.69
1:C:156:VAL:HG11	1:C:174:PRO:HA	1.73	0.69
1:A:203:GLU:H	1:A:203:GLU:CD	2.01	0.68
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.75	0.67
1:C:68:ARG:NH2	1:C:98:GLU:HB2	2.09	0.67
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.76	0.66
1:D:296:LEU:HD12	1:D:296:LEU:O	1.96	0.66
1:D:173:TYR:CE1	1:D:175:ASN:HB3	2.31	0.65
1:A:177:VAL:HA	1:A:205:LEU:HD21	1.77	0.65
1:C:418:ARG:HD2	7:C:749:HOH:O	1.97	0.64
1:D:232:GLY:O	1:D:233:LEU:C	2.41	0.63
1:C:290:LYS:HE2	1:C:290:LYS:HA	1.79	0.63
1:B:290:LYS:HA	1:B:290:LYS:HE2	1.81	0.62
1:C:537:MET:HG3	1:D:537[A]:MET:HG2	1.81	0.62
1:C:284:GLU:HG2	1:C:305:ALA:HB3	1.80	0.62
1:C:68:ARG:HH21	1:C:98:GLU:HB2	1.64	0.62
1:B:508:SER:O	1:B:512:ARG:HG3	2.00	0.61
1:B:408:GLU:HG3	7:B:838:HOH:O	2.00	0.61
1:D:68:ARG:NH2	1:D:95:TYR:O	2.33	0.60
1:C:430:GLU:OE1	1:D:430:GLU:OE1	2.20	0.59
1:A:404:ARG:HG3	1:B:412:ARG:HH12	1.68	0.59
1:A:372:MET:HE1	3:A:602:FLC:OA1	2.02	0.59
1:C:331:LEU:HD11	1:C:413:ALA:CB	2.34	0.58
1:D:174:PRO:C	1:D:176:ILE:H	2.12	0.58
1:C:343:LEU:HD23	1:C:373:LEU:HD21	1.84	0.58
1:C:522:ILE:HG23	1:C:537:MET:HE3	1.85	0.58
1:B:296:LEU:HD12	1:B:296:LEU:O	2.06	0.56
1:D:528:ARG:NH1	1:D:533:TYR:HE1	1.99	0.56
1:B:179:VAL:HG13	1:B:180:VAL:HG23	1.87	0.56
1:D:372:MET:HE1	3:D:602:FLC:OA1	2.06	0.55
1:D:234:SER:O	1:D:238:VAL:HG23	2.06	0.55
1:C:173:TYR:CE1	1:C:230:LEU:HD22	2.39	0.55
1:C:229:ASP:OD2	1:C:229:ASP:N	2.30	0.55
1:A:187:TYR:HB3	1:A:191:GLY:HA2	1.87	0.55
1:D:233:LEU:CD2	1:D:265:ALA:HB1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:HD23	1:D:265:ALA:HB1	1.89	0.54
1:A:404:ARG:CG	1:B:412:ARG:HH12	2.21	0.54
1:D:17:THR:HA	1:D:19:GLU:OE1	2.08	0.54
1:D:74:LYS:HE3	1:D:109:SER:OG	2.07	0.54
1:A:282:LYS:HE3	3:A:602:FLC:OA2	2.08	0.54
1:A:144:VAL:HG22	1:A:145:GLU:N	2.23	0.54
1:B:337:VAL:HG22	1:B:370:CYS:HB2	1.91	0.53
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.89	0.53
1:B:68:ARG:NH2	1:B:98:GLU:HB2	2.23	0.53
1:D:493:ILE:HB	1:D:496:ASP:OD2	2.08	0.53
1:A:411:ARG:HG3	1:A:426:ILE:HD11	1.89	0.53
1:C:199:LYS:HB3	1:C:206:VAL:HB	1.91	0.53
1:C:258:ARG:HD2	7:C:868:HOH:O	2.07	0.53
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.90	0.53
1:C:331:LEU:HD11	1:C:413:ALA:HB1	1.90	0.53
1:D:27:GLN:HG2	7:D:716:HOH:O	2.09	0.52
1:A:177:VAL:HG12	1:A:205:LEU:HD22	1.91	0.52
1:D:69:SER:HB3	1:D:72:ARG:HB3	1.91	0.52
1:A:422:GLU:HG2	1:A:452:LEU:HD13	1.92	0.51
1:C:218:ARG:NH1	1:C:218:ARG:HB3	2.25	0.51
1:A:133:THR:O	1:A:218:ARG:HA	2.11	0.51
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.92	0.51
1:B:408:GLU:O	1:B:412:ARG:HG3	2.10	0.51
1:C:419:ASP:O	1:C:423:VAL:HG23	2.10	0.51
1:B:292:PHE:CZ	1:B:296:LEU:HD22	2.46	0.51
1:B:372:MET:HE1	3:B:602:FLC:OA2	2.11	0.51
1:A:493:ILE:O	1:A:496:ASP:HB2	2.11	0.50
1:C:339:ALA:HB1	1:C:372:MET:HE2	1.94	0.49
1:B:535:ASN:OD1	1:B:536:ILE:HG13	2.12	0.49
1:C:21:GLY:HA2	7:C:910:HOH:O	2.11	0.49
1:C:406:LEU:HD21	1:C:457:ARG:HG3	1.93	0.49
1:C:537:MET:HG3	1:D:537[A]:MET:CG	2.43	0.49
1:B:107:VAL:HG21	1:B:120:VAL:HB	1.93	0.49
1:A:445:THR:HB	1:A:531[B]:SER:OG	2.13	0.48
1:C:132:ARG:HD3	1:C:218:ARG:O	2.13	0.48
1:A:508:SER:O	1:A:512:ARG:HG3	2.13	0.48
1:A:144:VAL:HG22	1:A:145:GLU:H	1.78	0.48
1:A:296:LEU:HD13	1:A:296:LEU:C	2.39	0.48
1:B:155:THR:O	1:B:170:TRP:HA	2.14	0.48
1:D:508:SER:O	1:D:512:ARG:HG3	2.12	0.48
1:D:416:LEU:HD23	7:D:872:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:THR:O	1:C:170:TRP:HA	2.14	0.48
1:C:405:GLN:O	1:C:409:GLU:HG3	2.14	0.47
1:A:175:ASN:ND2	1:A:179:VAL:HG13	2.29	0.47
1:C:517:VAL:HG22	1:C:543:SER:O	2.14	0.47
1:D:173:TYR:CZ	1:D:175:ASN:HB3	2.49	0.47
1:C:218:ARG:HB3	1:C:218:ARG:HH11	1.78	0.47
1:D:88:PHE:CE1	1:D:124:LEU:HG	2.50	0.47
1:D:528:ARG:HD3	1:D:533:TYR:CE1	2.50	0.47
1:B:165:ASN:H	1:B:168:THR:HB	1.79	0.47
1:B:24:PHE:CZ	1:B:436:MET:HE2	2.50	0.47
1:D:24:PHE:CZ	1:D:436:MET:HE2	2.49	0.47
1:B:494:TRP:CD1	1:B:529:PRO:HG3	2.50	0.47
1:A:337:VAL:HG22	1:A:370:CYS:HB2	1.97	0.47
1:B:30:LEU:O	1:B:34:MET:HG2	2.15	0.47
1:C:115:LEU:HD23	1:C:504:PHE:CE1	2.50	0.47
1:C:422:GLU:HB3	7:C:706:HOH:O	2.15	0.46
1:B:156:VAL:HG22	1:B:156:VAL:O	2.15	0.46
1:D:284:GLU:HG2	1:D:305:ALA:HB3	1.96	0.46
1:D:382:PHE:HB3	1:D:385:GLU:HB2	1.97	0.46
1:C:420:PRO:HB2	7:C:703:HOH:O	2.15	0.46
1:C:508:SER:O	1:C:512:ARG:HG3	2.16	0.46
1:D:211:ASN:O	1:D:212:GLY:C	2.57	0.46
1:C:422:GLU:HG2	1:C:452:LEU:HD13	1.98	0.46
1:D:431:ALA:CB	1:D:537[A]:MET:HE1	2.45	0.46
1:D:471:ALA:O	1:D:475:VAL:HG13	2.16	0.46
1:B:331:LEU:O	1:B:455:ARG:NH2	2.49	0.46
1:C:229:ASP:O	1:C:230:LEU:C	2.59	0.46
1:C:343:LEU:HD23	1:C:373:LEU:CD2	2.45	0.46
1:D:195:LEU:C	1:D:195:LEU:HD23	2.41	0.46
1:D:194:SER:HB2	1:D:195:LEU:CB	2.37	0.45
1:D:187:TYR:HB3	1:D:191:GLY:HA2	1.97	0.45
1:C:195:LEU:HD23	1:C:209:VAL:HA	1.97	0.45
1:A:52:VAL:HG22	7:A:876:HOH:O	2.17	0.45
1:B:94:GLU:O	1:B:98:GLU:HG3	2.17	0.45
1:A:153:LEU:CD1	1:A:155:THR:HB	2.46	0.45
1:A:177:VAL:HG12	1:A:205:LEU:CD2	2.47	0.45
1:A:205:LEU:HD22	1:A:205:LEU:H	1.81	0.45
1:C:28:GLN:HG3	1:C:30:LEU:HG	1.98	0.45
1:C:173:TYR:CD2	1:C:176:ILE:HB	2.52	0.45
1:D:72:ARG:HH11	1:D:383:PRO:HG3	1.82	0.45
1:B:522:ILE:CG2	1:B:537[A]:MET:HE3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:GLY:O	1:D:234:SER:N	2.49	0.45
1:D:535:ASN:OD1	1:D:536:ILE:HG13	2.16	0.45
1:D:522:ILE:HG23	1:D:537[A]:MET:HE3	1.99	0.45
1:A:525:THR:HB	7:A:773:HOH:O	2.17	0.44
1:B:331:LEU:HD11	1:B:413:ALA:CB	2.47	0.44
1:A:153:LEU:HD22	1:A:205:LEU:O	2.17	0.44
1:C:89:SER:HA	1:C:127:LYS:HG3	1.99	0.44
1:C:177:VAL:HG22	1:C:177:VAL:O	2.17	0.44
1:D:255:SER:HA	1:D:282:LYS:HD3	1.99	0.44
1:A:27:GLN:HG2	7:A:823:HOH:O	2.17	0.44
1:A:382:PHE:HB3	1:A:385:GLU:HB2	1.99	0.44
1:B:331:LEU:HD11	1:B:413:ALA:HB1	2.00	0.44
1:D:346:MET:HA	1:D:349:LYS:O	2.16	0.44
1:A:205:LEU:HD22	1:A:205:LEU:N	2.32	0.44
1:B:156:VAL:HG21	1:B:174:PRO:CA	2.31	0.44
1:B:406:LEU:HD21	1:B:457:ARG:HG3	1.99	0.44
1:C:145:GLU:HA	1:C:214:VAL:HA	1.98	0.44
1:A:152:VAL:HG11	1:A:169:VAL:HG23	1.98	0.44
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.99	0.44
1:C:107:VAL:HG21	1:C:120:VAL:HB	1.99	0.44
1:D:436:MET:HE3	1:D:436:MET:HB3	1.90	0.44
1:A:28:GLN:HG3	1:A:30:LEU:HG	2.00	0.43
1:B:60:ILE:HG12	1:B:83:ILE:HB	2.00	0.43
1:B:419:ASP:OD2	1:B:448:ARG:NH2	2.49	0.43
1:C:410:LEU:HD13	1:C:455:ARG:O	2.18	0.43
1:C:30:LEU:O	1:C:34:MET:HG2	2.17	0.43
1:C:19[A]:GLU:H	1:C:19[A]:GLU:CD	2.26	0.43
1:C:185:ARG:HD3	1:C:210:GLU:OE1	2.19	0.43
1:B:176:ILE:HA	1:B:179:VAL:HG12	1.99	0.43
3:D:602:FLC:OHB	3:D:602:FLC:OG2	2.35	0.43
1:A:187:TYR:CE1	1:A:224:PRO:HG2	2.54	0.43
1:B:234:SER:HB2	1:B:237:ASP:H	1.84	0.43
1:B:290:LYS:HD2	1:D:48:ASP:OD2	2.19	0.43
1:D:233:LEU:HD22	1:D:265:ALA:CB	2.49	0.43
1:B:405:GLN:O	1:B:409:GLU:HG3	2.18	0.43
1:C:24:PHE:CE2	1:C:436:MET:HE2	2.54	0.43
1:D:85:ARG:NH2	3:D:602:FLC:OA1	2.52	0.43
1:C:124:LEU:C	1:C:124:LEU:HD23	2.44	0.42
1:D:107:VAL:HG21	1:D:120:VAL:HB	2.00	0.42
1:B:346:MET:HA	1:B:349:LYS:O	2.18	0.42
1:C:58[B]:SER:OG	1:C:370:CYS:SG	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:SER:CB	1:B:237:ASP:H	2.30	0.42
1:B:309:LEU:O	1:B:313:ILE:HG12	2.20	0.42
1:B:441:ILE:HD12	1:B:521:VAL:HG11	2.02	0.42
1:C:331:LEU:HD11	1:C:413:ALA:HB3	2.00	0.42
1:A:124:LEU:C	1:A:124:LEU:HD23	2.43	0.42
1:C:85:ARG:NH2	3:C:602:FLC:OA2	2.52	0.42
1:D:540:LEU:HD23	1:D:541:SER:O	2.20	0.42
1:A:56:SER:HB2	1:A:480:GLY:CA	2.50	0.42
1:D:528:ARG:NH1	1:D:529:PRO:O	2.52	0.42
1:D:494:TRP:CD1	1:D:529:PRO:HG3	2.55	0.42
1:B:56:SER:HB2	1:B:480:GLY:HA2	2.01	0.42
1:C:452:LEU:O	1:C:455:ARG:HG2	2.20	0.41
1:A:286:HIS:CE1	1:A:290:LYS:HG3	2.55	0.41
1:B:297:GLU:HG2	7:B:842:HOH:O	2.20	0.41
1:C:300:ASP:O	1:C:335:PRO:HD2	2.20	0.41
1:D:238:VAL:O	1:D:242:ARG:HG3	2.20	0.41
1:C:253:PHE:HD1	1:C:280:ILE:HB	1.85	0.41
1:D:174:PRO:C	1:D:176:ILE:N	2.78	0.41
1:C:404:ARG:HG3	1:D:412:ARG:HH12	1.84	0.41
1:C:537:MET:HE3	1:C:537:MET:HB2	1.90	0.41
1:B:410:LEU:HD13	1:B:455:ARG:O	2.20	0.41
1:A:30:LEU:N	1:A:31:PRO:CD	2.83	0.41
1:B:68:ARG:HH21	1:B:98:GLU:HB2	1.85	0.41
1:C:282:LYS:HE2	1:C:284:GLU:OE1	2.21	0.41
1:D:60:ILE:HG12	1:D:83:ILE:HB	2.03	0.41
1:D:337:VAL:HG22	1:D:370:CYS:HB2	2.03	0.41
1:A:187:TYR:HE1	1:A:224:PRO:HG2	1.85	0.40
1:B:488:GLU:OE1	1:B:489:PRO:HD2	2.21	0.40
1:D:56:SER:HB2	1:D:480:GLY:CA	2.51	0.40
1:D:175:ASN:O	1:D:176:ILE:C	2.64	0.40
1:C:535:ASN:OD1	1:C:536:ILE:HG13	2.21	0.40
1:A:146:LEU:HD12	1:A:193:ILE:HD13	2.02	0.40
1:B:24:PHE:CE2	1:B:436:MET:HE2	2.56	0.40
1:C:286:HIS:CE1	1:C:290:LYS:HG3	2.55	0.40
1:D:19:GLU:O	1:D:19:GLU:HG2	2.20	0.40
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.86	0.40
1:B:76:MET:HB2	1:B:76:MET:HE2	1.72	0.40
1:B:141:GLU:O	1:B:141:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	520/543 (96%)	504 (97%)	13 (2%)	3 (1%)	21	12
1	B	488/543 (90%)	470 (96%)	16 (3%)	2 (0%)	30	21
1	C	502/543 (92%)	484 (96%)	16 (3%)	2 (0%)	30	21
1	D	447/543 (82%)	427 (96%)	16 (4%)	4 (1%)	14	6
All	All	1957/2172 (90%)	1885 (96%)	61 (3%)	11 (1%)	21	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	D	340	THR
1	D	233	LEU
1	B	340	THR
1	D	175	ASN
1	A	340	THR
1	A	535	ASN
1	C	535	ASN
1	D	146	LEU
1	C	340	THR
1	B	158	PRO

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	424/432 (98%)	418 (99%)	6 (1%)	59	56
1	B	401/432 (93%)	396 (99%)	5 (1%)	63	61
1	C	410/432 (95%)	406 (99%)	4 (1%)	68	67
1	D	372/432 (86%)	369 (99%)	3 (1%)	73	74
All	All	1607/1728 (93%)	1589 (99%)	18 (1%)	65	64

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	69	SER
1	A	205	LEU
1	A	294	GLU
1	A	408	GLU
1	A	528	ARG
1	B	20	LEU
1	B	34	MET
1	B	144	VAL
1	B	296	LEU
1	B	422	GLU
1	C	34	MET
1	C	182	VAL
1	C	219	LYS
1	C	537	MET
1	D	78	LYS
1	D	296	LEU
1	D	328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	208	GLN
1	B	28	GLN
1	B	211	ASN
1	B	405	GLN
1	C	18	GLN
1	C	28	GLN
1	C	208	GLN
1	C	211	ASN

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Mol	Chain	Res	Type
1	C	222	ASN
1	C	247	HIS

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 14 ligands modelled in this entry, 4 are monoatomic - 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$
4	FBP	D	603	-	18,20,20	0.90	1 (5%)	21,32,32	0.83	1 (4%)
5	EDO	B	604	-	3,3,3	0.54	0	2,2,2	0.47	0
3	FLC	A	602	2	12,12,12	1.75	4 (33%)	17,17,17	1.37	1 (5%)
4	FBP	A	603	-	18,20,20	0.88	1 (5%)	21,32,32	0.78	1 (4%)
4	FBP	C	603	-	18,20,20	0.84	1 (5%)	21,32,32	0.80	0
6	ADN	D	604	-	21,21,21	1.32	3 (14%)	31,31,31	2.19	8 (25%)
3	FLC	B	602	2	12,12,12	2.12	4 (33%)	17,17,17	1.57	2 (11%)
3	FLC	C	602	2	12,12,12	2.11	4 (33%)	17,17,17	1.51	2 (11%)
4	FBP	B	603	-	18,20,20	0.90	1 (5%)	21,32,32	0.77	0
3	FLC	D	602	2	12,12,12	1.96	4 (33%)	17,17,17	1.42	2 (11%)

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
4	FBP	D	603	-	-	2/13/32/32	0/1/1/1
5	EDO	B	604	-	-	1/1/1/1	-
3	FLC	A	602	2	-	0/16/16/16	-
6	ADN	D	604	-	2/2/4/4	2/6/22/22	0/3/3/3
4	FBP	A	603	-	-	3/13/32/32	0/1/1/1
4	FBP	C	603	-	-	5/13/32/32	0/1/1/1
3	FLC	B	602	2	-	9/16/16/16	-
3	FLC	C	602	2	-	6/16/16/16	-
4	FBP	B	603	-	-	2/13/32/32	0/1/1/1
3	FLC	D	602	2	-	6/16/16/16	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	FLC	CB-CBC	-4.13	1.49	1.53
3	C	602	FLC	CB-CBC	-3.79	1.49	1.53
6	D	604	ADN	C6-N6	3.76	1.43	1.34
6	D	604	ADN	C5-N7	-3.44	1.32	1.39
3	D	602	FLC	CG-CB	-3.33	1.49	1.54
3	C	602	FLC	CG-CB	-3.32	1.49	1.54
3	C	602	FLC	CA-CB	-3.25	1.49	1.54
3	D	602	FLC	CA-CB	-3.20	1.50	1.54
3	B	602	FLC	CG-CB	-3.16	1.50	1.54
3	B	602	FLC	CA-CB	-3.14	1.50	1.54
3	D	602	FLC	CB-CBC	-3.04	1.50	1.53
3	C	602	FLC	OHB-CB	-2.77	1.38	1.43
4	B	603	FBP	O2-C2	2.70	1.45	1.40
4	D	603	FBP	O2-C2	2.67	1.45	1.40
3	A	602	FLC	CA-CB	-2.66	1.50	1.54
3	A	602	FLC	OHB-CB	-2.62	1.38	1.43
3	B	602	FLC	OHB-CB	-2.61	1.38	1.43
3	A	602	FLC	CG-CB	-2.58	1.50	1.54
4	A	603	FBP	O2-C2	2.47	1.45	1.40
3	D	602	FLC	OHB-CB	-2.44	1.38	1.43
3	A	602	FLC	CB-CBC	-2.42	1.51	1.53
4	C	603	FBP	O2-C2	2.34	1.44	1.40
6	D	604	ADN	C5-C4	2.26	1.43	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	604	ADN	C5-C4-N3	-6.12	118.29	126.72
6	D	604	ADN	N3-C4-N9	5.38	136.32	127.17
6	D	604	ADN	N3-C2-N1	-4.28	122.10	128.58
3	B	602	FLC	OB2-CBC-CB	4.18	121.16	113.14
3	C	602	FLC	OB2-CBC-CB	3.97	120.76	113.14
6	D	604	ADN	C2-N3-C4	3.86	121.26	111.83
6	D	604	ADN	C5-N7-C8	3.34	108.70	103.45
3	A	602	FLC	OB2-CBC-CB	3.27	119.42	113.14
3	D	602	FLC	OB2-CBC-CB	2.66	118.25	113.14
4	D	603	FBP	O6P-P2-O6	2.60	113.44	106.67
6	D	604	ADN	N9-C8-N7	-2.29	110.68	113.94
3	C	602	FLC	OG2-CGC-CG	2.25	121.48	114.35
3	D	602	FLC	OA2-CAC-CA	2.21	121.36	114.35
3	B	602	FLC	OG2-CGC-CG	2.21	121.34	114.35
6	D	604	ADN	C4-C5-N7	-2.16	108.12	110.58
4	A	603	FBP	O6P-P2-O6	2.16	112.29	106.67
6	D	604	ADN	C1'-N9-C8	-2.13	122.36	127.09

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	604	ADN	C1'
6	D	604	ADN	C3'

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	FLC	OHB-CB-CBC-OB1
4	C	603	FBP	C1-O1-P1-O2P
6	D	604	ADN	O4'-C4'-C5'-O5'
4	A	603	FBP	C4-C5-C6-O6
4	B	603	FBP	C4-C5-C6-O6
4	C	603	FBP	C4-C5-C6-O6
4	D	603	FBP	C4-C5-C6-O6
6	D	604	ADN	C3'-C4'-C5'-O5'
4	C	603	FBP	O5-C5-C6-O6
3	B	602	FLC	CA-CB-CBC-OB1
3	C	602	FLC	CA-CB-CBC-OB2
3	D	602	FLC	CA-CB-CBC-OB2
4	A	603	FBP	O5-C5-C6-O6
4	B	603	FBP	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	603	FBP	O5-C5-C6-O6
5	B	604	EDO	O1-C1-C2-O2
3	D	602	FLC	OHB-CB-CBC-OB2
3	B	602	FLC	CA-CB-CBC-OB2
3	C	602	FLC	CG-CB-CBC-OB2
3	D	602	FLC	CG-CB-CBC-OB2
4	C	603	FBP	C1-O1-P1-O1P
3	B	602	FLC	CA-CB-CG-CGC
3	C	602	FLC	OHB-CB-CBC-OB2
3	B	602	FLC	CG-CB-CBC-OB1
3	B	602	FLC	CG-CB-CBC-OB2
3	D	602	FLC	CB-CG-CGC-OG2
4	A	603	FBP	C1-O1-P1-O3P
4	C	603	FBP	C1-O1-P1-O3P
3	C	602	FLC	CB-CG-CGC-OG2
3	B	602	FLC	OHB-CB-CBC-OB2
3	B	602	FLC	CB-CG-CGC-OG1
3	C	602	FLC	CB-CG-CGC-OG1
3	B	602	FLC	CB-CG-CGC-OG2
3	D	602	FLC	CB-CG-CGC-OG1
3	C	602	FLC	CA-CB-CG-CGC
3	D	602	FLC	CA-CB-CG-CGC

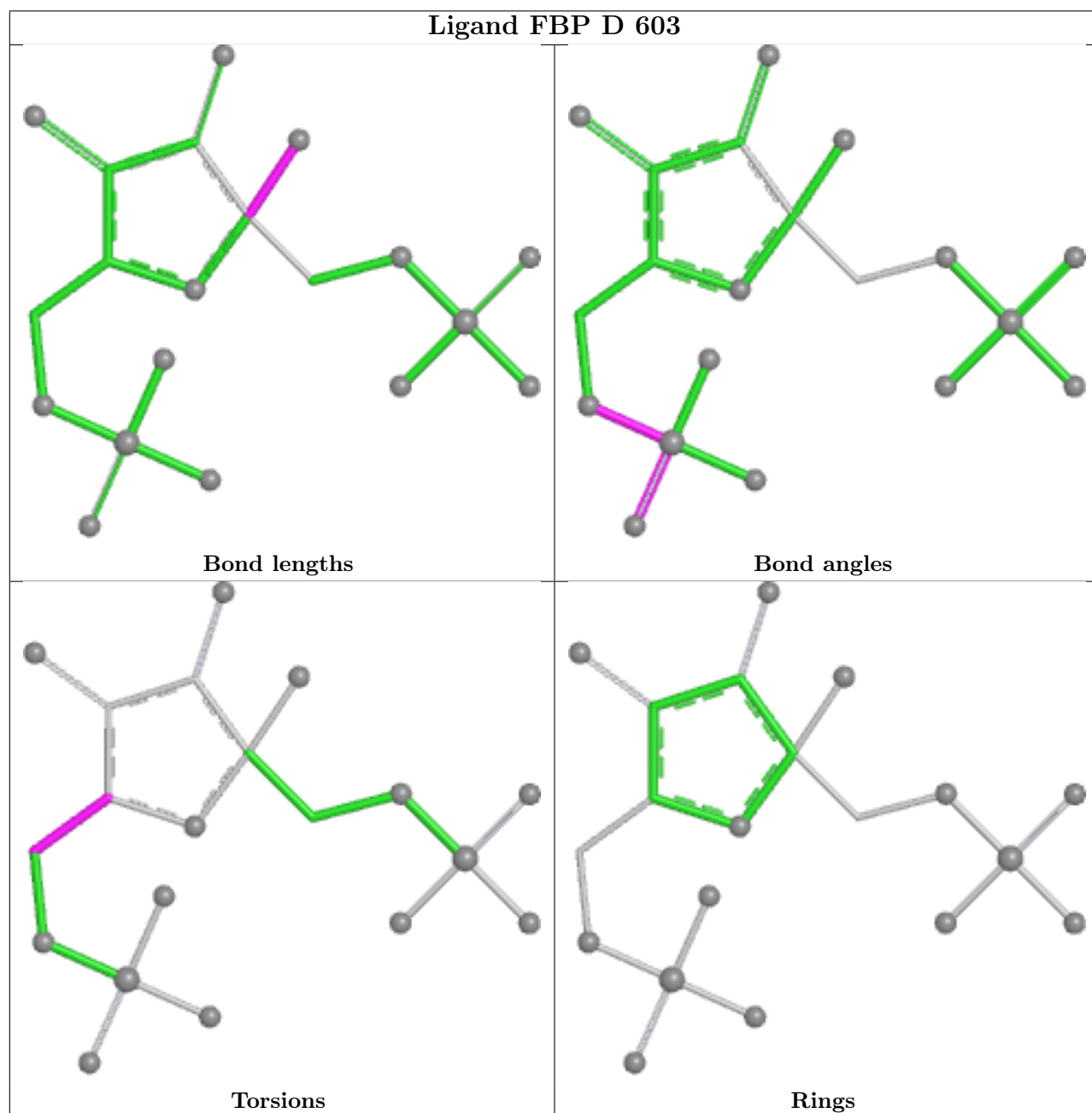
There are no ring outliers.

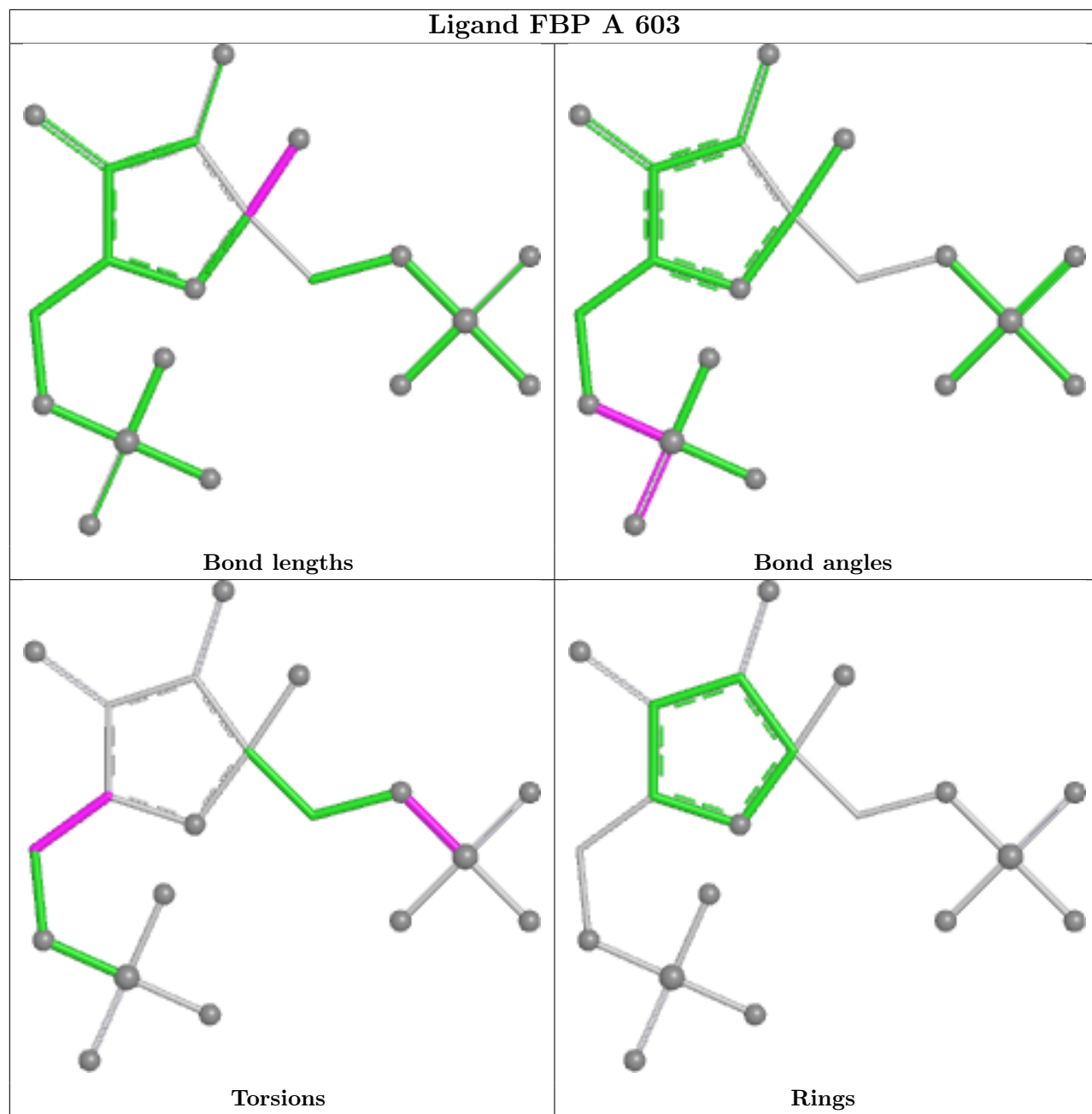
4 monomers are involved in 7 short contacts:

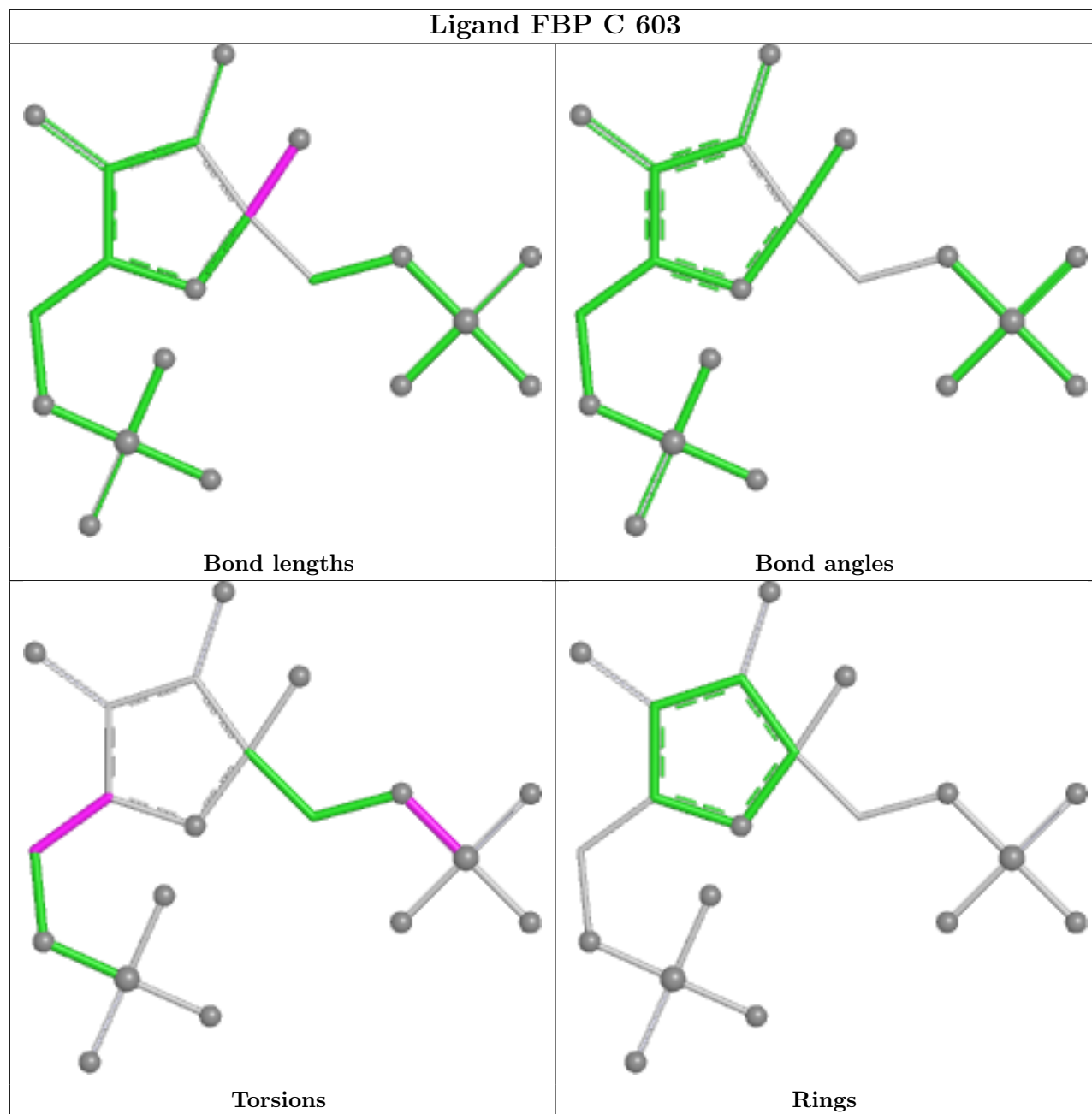
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	FLC	2	0
3	B	602	FLC	1	0
3	C	602	FLC	1	0
3	D	602	FLC	3	0

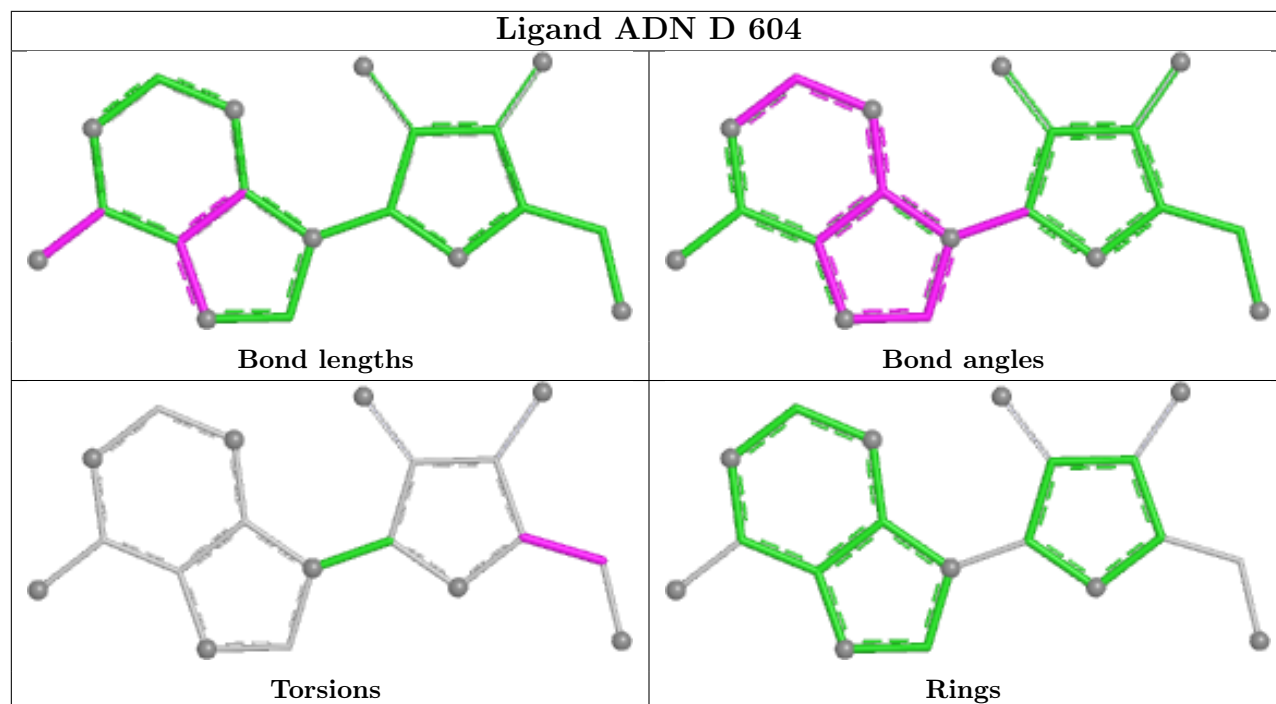
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

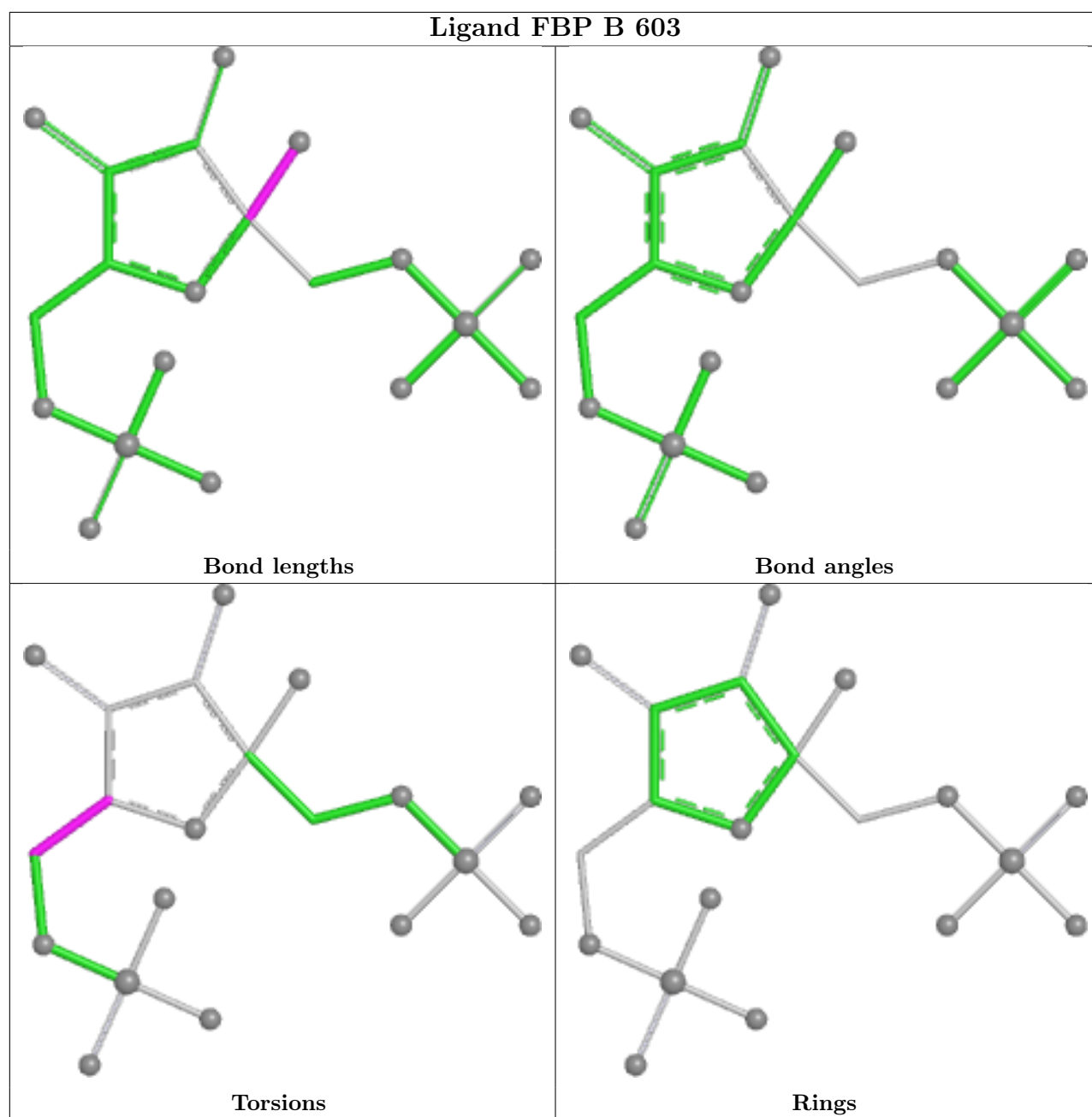
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	522/543 (96%)	0.80	70 (13%) 7 8	17, 34, 64, 76	33 (6%)
1	B	500/543 (92%)	0.90	84 (16%) 4 4	17, 34, 76, 97	43 (8%)
1	C	505/543 (93%)	0.95	93 (18%) 3 3	18, 34, 76, 99	37 (7%)
1	D	460/543 (84%)	0.86	64 (13%) 6 7	19, 34, 64, 93	30 (6%)
All	All	1987/2172 (91%)	0.88	311 (15%) 5 5	17, 34, 70, 99	143 (7%)

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	PRO	8.5
1	B	152	VAL	8.0
1	D	232	GLY	7.8
1	D	214	VAL	7.5
1	C	21	GLY	7.3
1	A	135	ILE	7.3
1	C	154	VAL	7.1
1	C	153	LEU	7.0
1	C	205	LEU	6.8
1	D	195	LEU	6.8
1	A	136	LEU	6.4
1	D	147	VAL	6.2
1	C	20	LEU	6.1
1	C	216	GLY	6.0
1	D	144	VAL	6.0
1	D	225	GLY	5.8
1	B	20	LEU	5.7
1	B	226	ALA	5.6
1	C	146	LEU	5.5
1	D	131	ILE	5.4
1	C	200	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	180	VAL	5.3
1	C	197	VAL	5.3
1	B	181	PRO	5.3
1	C	206	VAL	5.2
1	C	181	PRO	5.2
1	A	17	THR	5.1
1	B	177	VAL	5.1
1	B	166	ALA	5.1
1	D	212	GLY	5.1
1	D	233	LEU	5.1
1	B	154	VAL	5.1
1	C	209	VAL	5.0
1	A	16	LEU	5.0
1	C	229	ASP	5.0
1	B	215	LEU	4.9
1	B	206	VAL	4.9
1	C	196	VAL	4.9
1	C	152	VAL	4.8
1	B	160	PHE	4.8
1	C	177	VAL	4.8
1	D	174	PRO	4.8
1	C	215	LEU	4.8
1	C	170	TRP	4.7
1	B	153	LEU	4.7
1	C	19[A]	GLU	4.7
1	C	207	THR	4.7
1	C	144	VAL	4.6
1	D	17	THR	4.6
1	B	22	THR	4.6
1	B	196	VAL	4.6
1	C	183	GLY	4.6
1	A	162	THR	4.5
1	D	146	LEU	4.5
1	C	158	PRO	4.4
1	D	186	ILE	4.4
1	A	18	GLN	4.3
1	C	214	VAL	4.3
1	B	232	GLY	4.3
1	D	209	VAL	4.3
1	B	216	GLY	4.2
1	D	143	GLU	4.2
1	B	146	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	206	VAL	4.1
1	D	176	ILE	4.1
1	A	182	VAL	4.1
1	B	209	VAL	4.1
1	B	214	VAL	4.1
1	A	110	PHE	4.0
1	B	159	ALA	4.0
1	D	193	ILE	4.0
1	B	169	VAL	4.0
1	C	198	GLN	4.0
1	B	195	LEU	3.9
1	A	272	PRO	3.9
1	B	170	TRP	3.9
1	B	116	SER	3.9
1	C	230	LEU	3.9
1	C	176	ILE	3.9
1	A	137	GLN	3.8
1	D	223	LEU	3.8
1	B	231	PRO	3.8
1	C	184	GLY	3.8
1	C	226	ALA	3.8
1	A	214	VAL	3.8
1	B	19	GLU	3.8
1	A	232	GLY	3.7
1	C	151	GLN	3.7
1	B	144	VAL	3.7
1	C	171	VAL	3.7
1	B	207	THR	3.7
1	D	173	TYR	3.7
1	B	156	VAL	3.7
1	D	187	TYR	3.7
1	D	110	PHE	3.7
1	C	202	PRO	3.7
1	C	182	VAL	3.6
1	B	233	LEU	3.6
1	B	23	ALA	3.6
1	B	148	LYS	3.6
1	B	176	ILE	3.6
1	C	195	LEU	3.6
1	C	22	THR	3.5
1	C	156	VAL	3.5
1	D	211	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	133	THR	3.5
1	C	155	THR	3.5
1	B	114	PRO	3.5
1	D	22	THR	3.5
1	B	179	VAL	3.5
1	A	20	LEU	3.5
1	D	220	GLY	3.5
1	C	217	SER	3.4
1	B	21	GLY	3.4
1	B	208	GLN	3.4
1	B	167	ASN	3.4
1	D	172	ASP	3.3
1	D	21	GLY	3.3
1	B	161	ARG	3.3
1	D	194	SER	3.3
1	B	131	ILE	3.3
1	B	168	THR	3.3
1	A	142	SER	3.3
1	B	158	PRO	3.3
1	B	147	VAL	3.2
1	C	173	TYR	3.2
1	B	171	VAL	3.2
1	A	146	LEU	3.2
1	A	275	HIS	3.2
1	D	132	ARG	3.2
1	C	147	VAL	3.2
1	A	160	PHE	3.2
1	B	157	ASP	3.2
1	A	490	PRO	3.1
1	D	221	VAL	3.1
1	B	218	ARG	3.1
1	A	493	ILE	3.1
1	C	114	PRO	3.1
1	D	20	LEU	3.1
1	D	18	GLN	3.1
1	C	23	ALA	3.1
1	D	213	GLY	3.1
1	C	145	GLU	3.1
1	B	149	GLY	3.1
1	D	416	LEU	3.0
1	A	147	VAL	3.0
1	C	179	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	411[A]	ARG	3.0
1	B	150	SER	3.0
1	D	224	PRO	3.0
1	C	18	GLN	3.0
1	D	540	LEU	3.0
1	C	413	ALA	3.0
1	A	183	GLY	3.0
1	D	490	PRO	3.0
1	C	133	THR	2.9
1	A	200	ILE	2.9
1	B	115	LEU	2.9
1	B	178	ARG	2.9
1	B	164	GLY	2.9
1	B	194	SER	2.9
1	A	205	LEU	2.9
1	D	130	GLU	2.9
1	A	196	VAL	2.9
1	A	517	VAL	2.9
1	B	275	HIS	2.9
1	D	188	ILE	2.9
1	B	225	GLY	2.9
1	A	228	VAL	2.8
1	D	15	GLN	2.8
1	A	161	ARG	2.8
1	C	203	GLU	2.8
1	B	234	SER	2.8
1	C	113	SER	2.8
1	C	231	PRO	2.8
1	C	187	TYR	2.8
1	A	151	GLN	2.8
1	B	132	ARG	2.8
1	A	207	THR	2.8
1	C	115	LEU	2.8
1	A	144	VAL	2.8
1	C	228	VAL	2.8
1	C	227	GLN	2.7
1	D	175	ASN	2.7
1	B	145	GLU	2.7
1	C	149	GLY	2.7
1	B	193	ILE	2.7
1	C	199	LYS	2.7
1	D	340	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	16	LEU	2.7
1	A	217	SER	2.7
1	A	113	SER	2.7
1	A	19[A]	GLU	2.7
1	B	211	ASN	2.7
1	A	180	VAL	2.7
1	A	134	GLY	2.6
1	C	143	GLU	2.6
1	C	275	HIS	2.6
1	A	152	VAL	2.6
1	A	268	ALA	2.6
1	C	150	SER	2.6
1	B	412	ARG	2.6
1	C	218	ARG	2.6
1	A	21	GLY	2.6
1	C	204	GLY	2.6
1	C	208	GLN	2.6
1	B	113	SER	2.6
1	B	490	PRO	2.6
1	B	494	TRP	2.6
1	B	213	GLY	2.6
1	A	177	VAL	2.6
1	A	226	ALA	2.6
1	A	175	ASN	2.6
1	D	275	HIS	2.5
1	D	511	LEU	2.5
1	B	184	GLY	2.5
1	D	23	ALA	2.5
1	C	194	SER	2.5
1	B	540	LEU	2.5
1	A	143	GLU	2.5
1	B	173	TYR	2.5
1	A	416	LEU	2.5
1	C	232	GLY	2.5
1	D	192	LEU	2.5
1	D	412	ARG	2.5
1	C	494	TRP	2.5
1	A	190	ASP	2.5
1	A	204	GLY	2.4
1	B	112	GLY	2.4
1	B	165	ASN	2.4
1	A	195	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	511	LEU	2.4
1	B	514	PHE	2.4
1	A	168	THR	2.4
1	B	413	ALA	2.4
1	D	260	ALA	2.4
1	B	174	PRO	2.4
1	B	180	VAL	2.4
1	D	415	PRO	2.4
1	C	201	GLY	2.4
1	A	202	PRO	2.4
1	C	116	SER	2.4
1	A	22	THR	2.4
1	C	186	ILE	2.4
1	D	210	GLU	2.4
1	A	489	PRO	2.4
1	C	272	PRO	2.4
1	B	187	TYR	2.3
1	C	174	PRO	2.3
1	C	213	GLY	2.3
1	D	19	GLU	2.3
1	A	198	GLN	2.3
1	B	414	ALA	2.3
1	B	188	ILE	2.3
1	C	529	PRO	2.3
1	C	148	LYS	2.3
1	A	153	LEU	2.3
1	B	155	THR	2.3
1	D	25	PHE	2.3
1	C	493	ILE	2.3
1	D	500	ARG	2.3
1	D	518	GLY	2.3
1	A	230	LEU	2.3
1	B	186	ILE	2.2
1	C	193	ILE	2.2
1	D	34	MET	2.2
1	C	543	SER	2.2
1	A	211	ASN	2.2
1	C	415	PRO	2.2
1	D	268	ALA	2.2
1	D	351	ARG	2.2
1	A	215	LEU	2.2
1	C	270	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	530	GLY	2.2
1	A	159	ALA	2.2
1	A	413	ALA	2.2
1	D	332	ALA	2.2
1	A	178	ARG	2.2
1	D	222	ASN	2.1
1	A	173	TYR	2.1
1	C	188	ILE	2.1
1	A	184	GLY	2.1
1	A	201	GLY	2.1
1	C	224	PRO	2.1
1	C	412	ARG	2.1
1	C	414	ALA	2.1
1	D	24	PHE	2.1
1	C	157	ASP	2.1
1	A	164	GLY	2.1
1	C	185	ARG	2.1
1	A	231	PRO	2.1
1	C	490	PRO	2.1
1	B	175	ASN	2.1
1	A	295	ILE	2.1
1	A	411	ARG	2.1
1	B	142	SER	2.1
1	B	185	ARG	2.1
1	D	145	GLU	2.1
1	C	34	MET	2.1
1	A	169	VAL	2.1
1	D	129	PRO	2.1
1	C	511	LEU	2.1
1	C	350	ALA	2.1
1	C	519	ASP	2.1
1	C	131	ILE	2.0
1	A	179	VAL	2.0
1	A	415	PRO	2.0
1	B	24	PHE	2.0
1	B	212	GLY	2.0
1	B	489	PRO	2.0
1	D	411	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

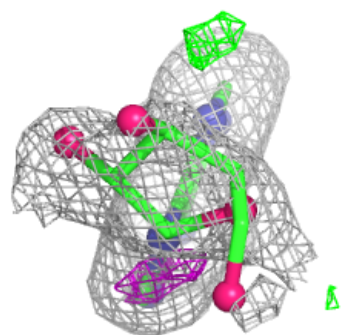
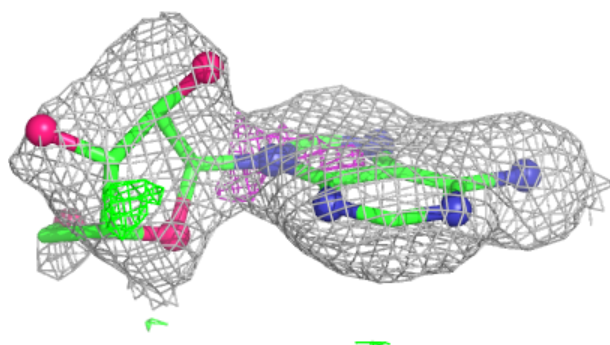
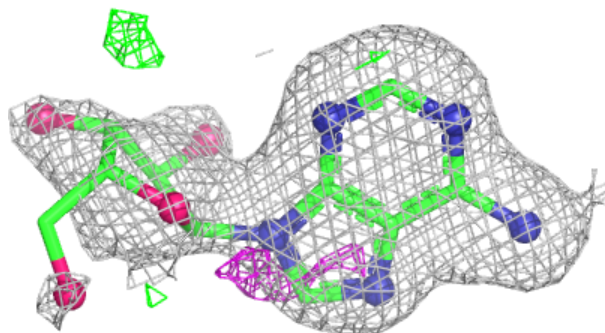
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	604	4/4	0.79	0.16	34,35,40,44	0
6	ADN	D	604	19/19	0.85	0.16	26,42,50,52	7
3	FLC	A	602	13/13	0.92	0.12	29,33,37,40	9
3	FLC	D	602	13/13	0.92	0.12	33,38,44,48	4
3	FLC	C	602	13/13	0.93	0.10	31,34,37,38	6
3	FLC	B	602	13/13	0.93	0.13	29,33,36,38	8
4	FBP	D	603	20/20	0.96	0.07	28,31,39,39	0
4	FBP	A	603	20/20	0.97	0.07	28,32,34,34	0
4	FBP	B	603	20/20	0.97	0.06	23,29,31,32	0
4	FBP	C	603	20/20	0.97	0.06	26,32,35,35	0
2	MN	C	601	1/1	0.99	0.04	36,36,36,36	0
2	MN	D	601	1/1	0.99	0.02	43,43,43,43	0
2	MN	A	601	1/1	0.99	0.03	37,37,37,37	0
2	MN	B	601	1/1	1.00	0.04	34,34,34,34	0

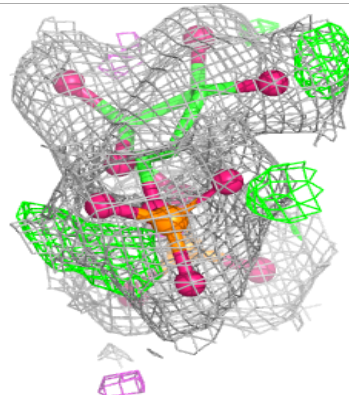
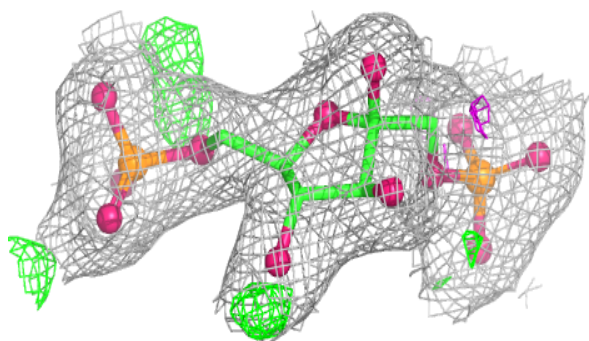
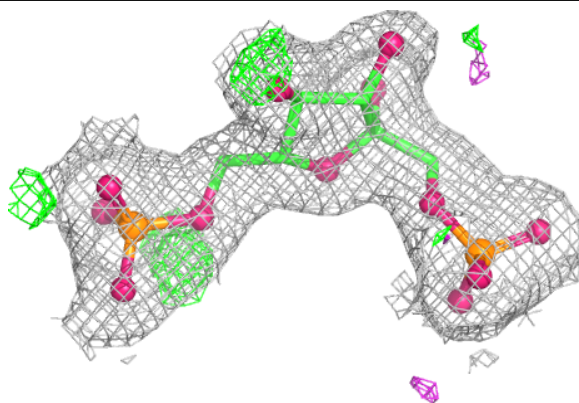
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN D 604:

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

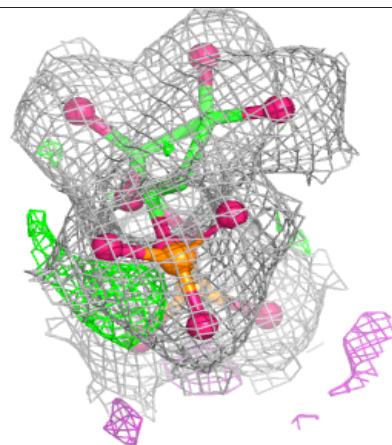
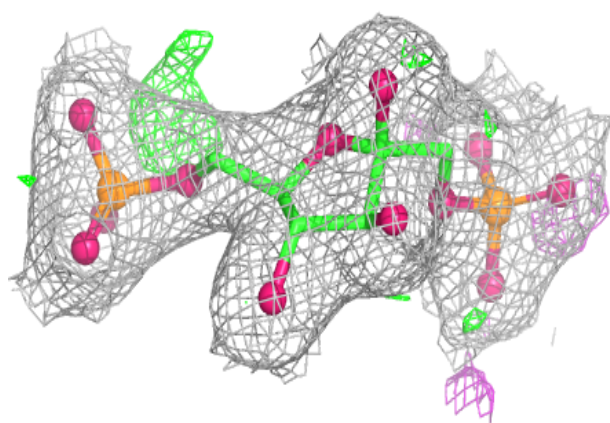
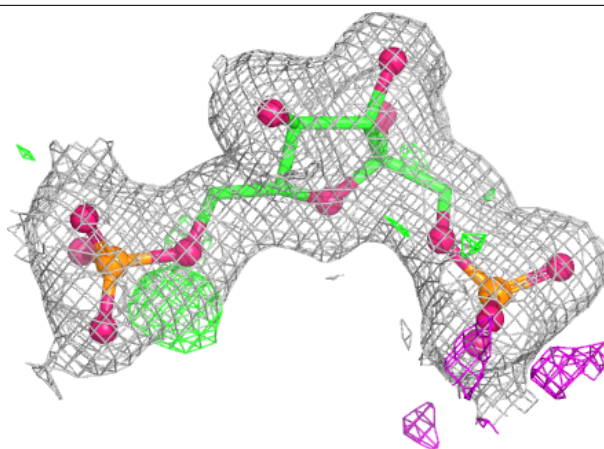
**Electron density around FBP D 603:**

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



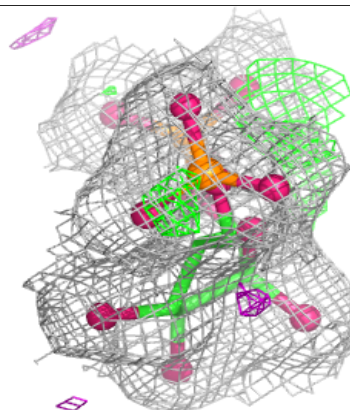
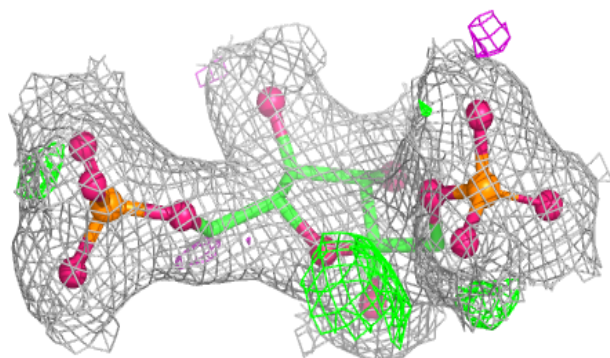
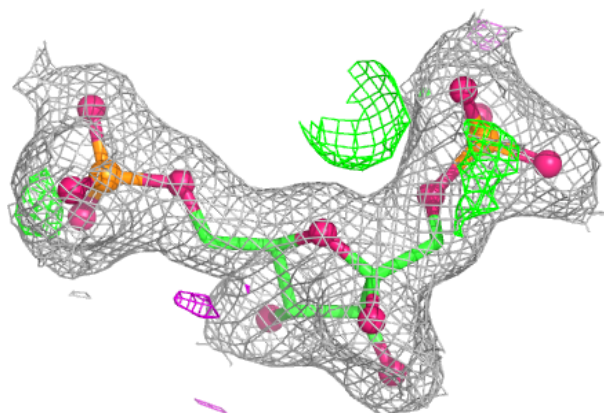
Electron density around FBP A 603:

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

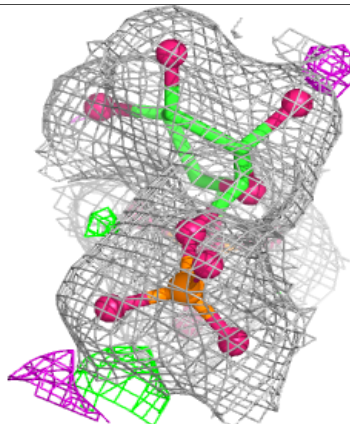
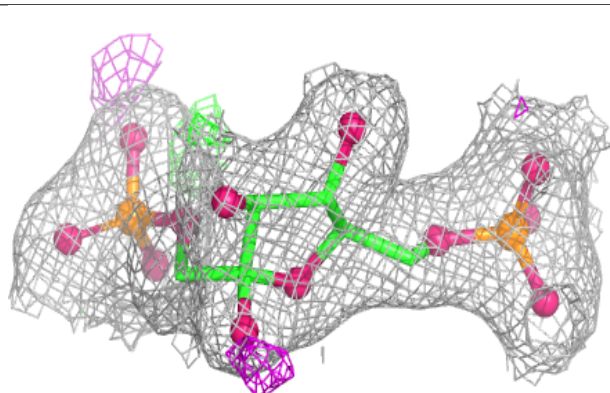
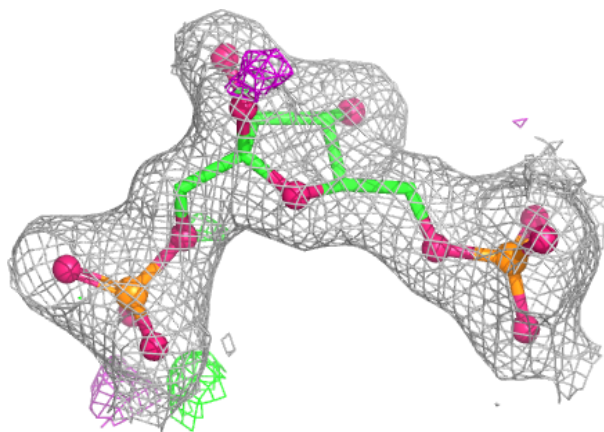


Electron density around FBP B 603:

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

**Electron density around FBP C 603:**

$2mF_o-DF_c$ (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.