Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 03:25 PM EDT

PDB ID	:	4IMA
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 (i) 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 (i)) were used in the production of this report:

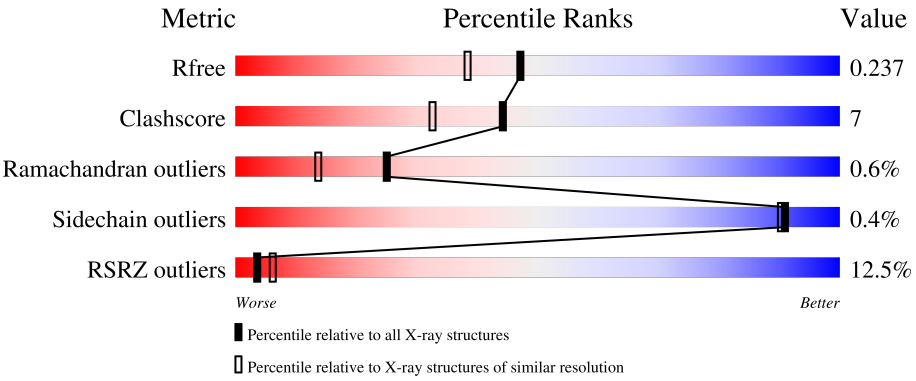
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 <=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	9% 86% 10% ·
1	B	543	13% 81% 11% 8%
1	C	543	12% 78% 14% · 7%
1	D	543	12% 71% 13% · 15%

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 (i)

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			

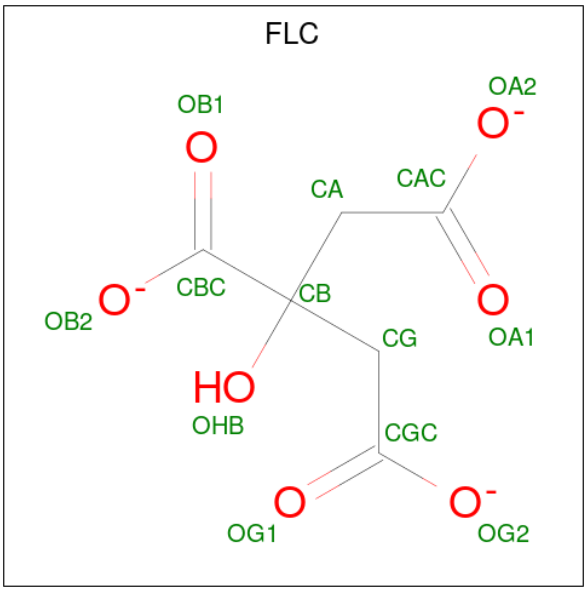
There are 4 discrepancies between the modelled and reference sequences:

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 (three-letter code: MN) (formula: Mn).

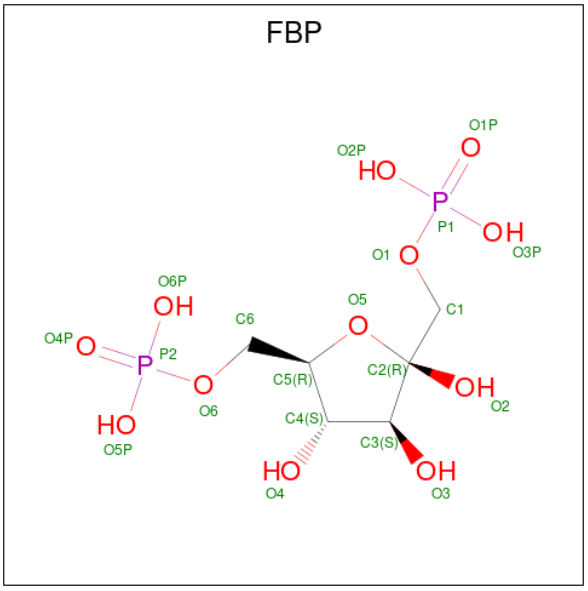
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



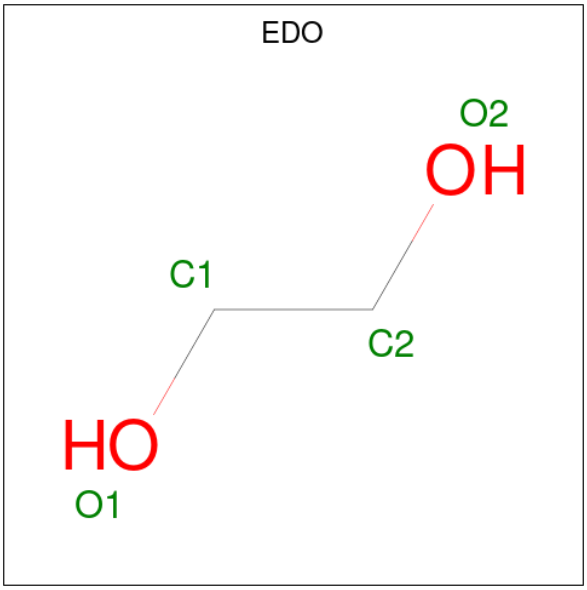
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	1	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	1	0

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



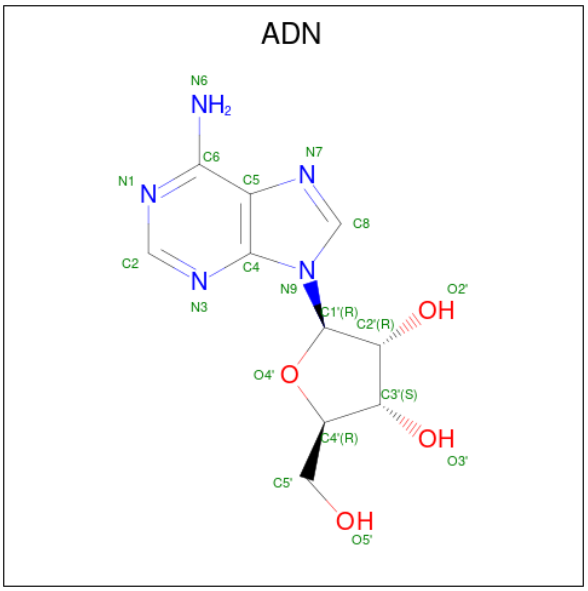
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: 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 (three-letter code: 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.

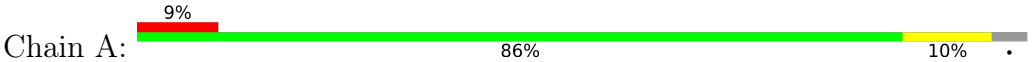
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		
7	B	223	Total	O	0	0
			223	223		
7	C	228	Total	O	0	0
			228	228		
7	D	199	Total	O	0	0
			199	199		

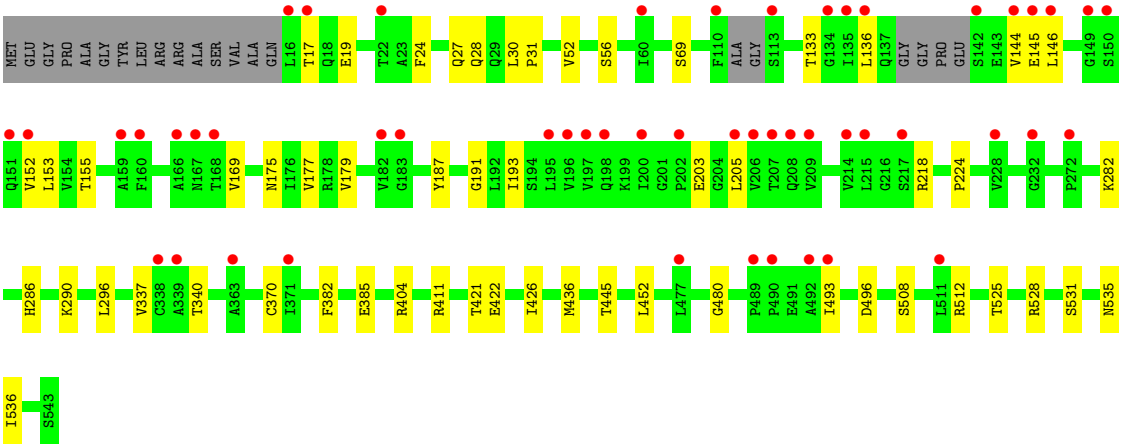
3 Residue-property plots

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

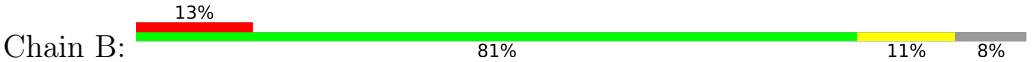
Chain A:

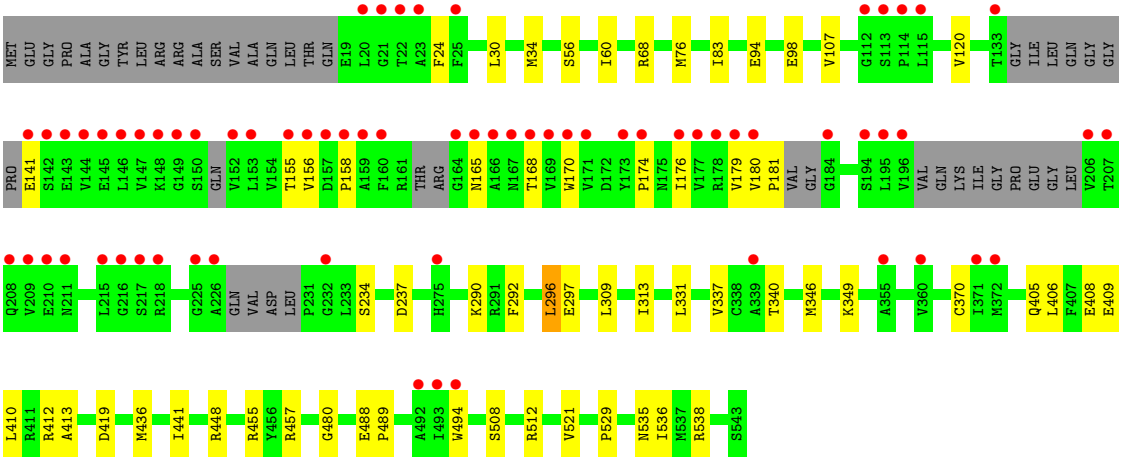




• Molecule 1: Pyruvate kinase

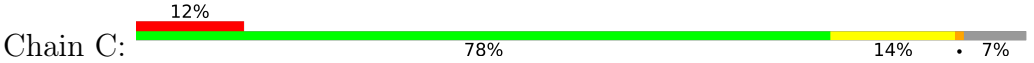
Chain B:

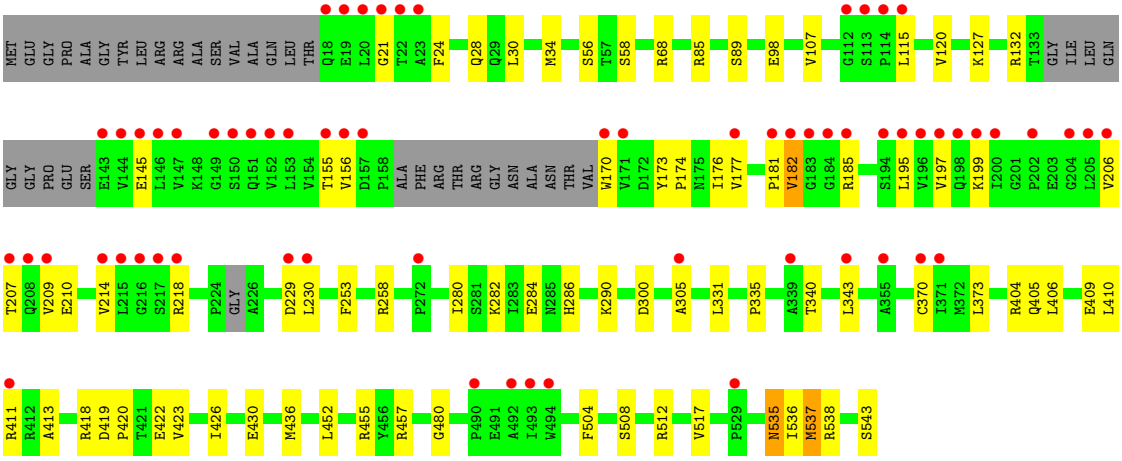




• Molecule 1: Pyruvate kinase

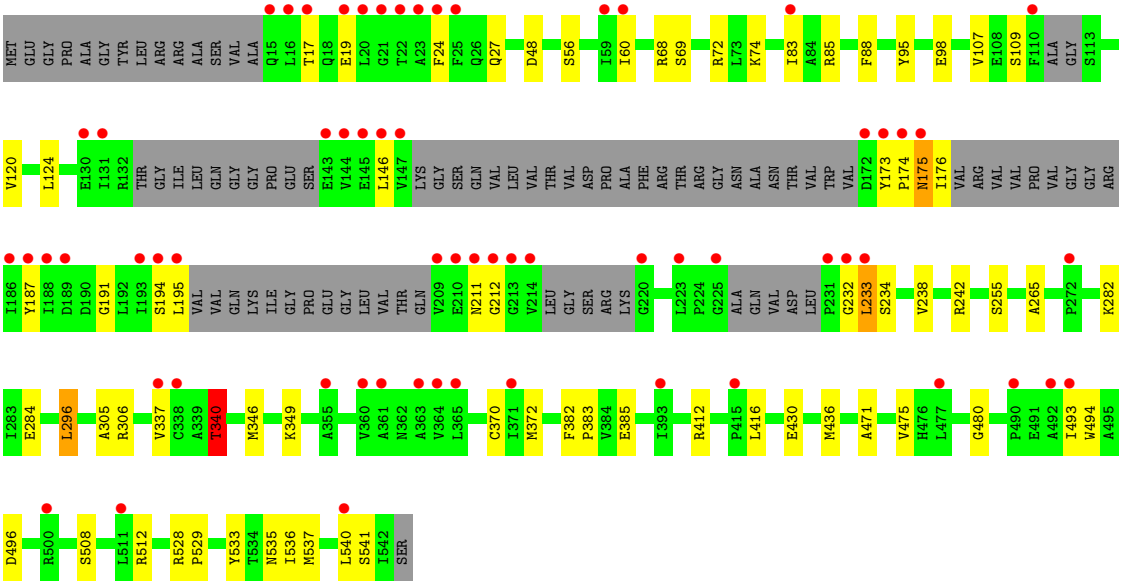
Chain C:





• Molecule 1: Pyruvate kinase

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 0.237	Depositor DCC
R_{free} test set	10100 reflections (5.04%)	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 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.088 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, MN, FBP, FLC, ADN

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	0.37	0/4056	0.51	0/5491
1	B	0.38	0/3862	0.51	1/5221 (0.0%)
1	C	0.39	0/3936	0.55	2/5326 (0.0%)
1	D	0.39	0/3580	0.54	2/4835 (0.0%)
All	All	0.38	0/15434	0.53	5/20873 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	182	VAL	N-CA-CB	-9.69	90.17	111.50
1	B	181	PRO	N-CA-CB	6.08	110.60	103.30
1	C	181	PRO	CB-CA-C	5.73	126.32	112.00
1	D	340	THR	C-N-CA	-5.72	107.41	121.70
1	D	306	ARG	CB-CA-C	5.22	120.85	110.40

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	41	0
1	B	3800	0	3863	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3861	0	3946	62	0
1	D	3520	0	3572	56	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	1	0
3	B	13	0	4	1	0
3	C	13	0	4	2	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	197	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 (197) 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
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:D:340:THR:O	7:D:724:HOH:O	2.09	0.70
1:C:156:VAL:HG11	1:C:174:PRO:HA	1.73	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:290:LYS:HE2	1:C:290:LYS:HA	1.79	0.63
1:A:203:GLU:H	1:A:203:GLU:CD	2.01	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:24:PHE:HZ	1:A:436:MET:HE2	1.68	0.59
1:D:232:GLY:O	1:D:233:LEU:C	2.41	0.59
1:C:331:LEU:HD11	1:C:413:ALA:CB	2.34	0.58
1:C:343:LEU:HD23	1:C:373:LEU:HD21	1.84	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: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
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:D:174:PRO:C	1:D:176:ILE:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:24:PHE:HZ	1:D:436:MET:HE2	1.75	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:A:493:ILE:O	1:A:496:ASP:HB2	2.11	0.50
1:B:24:PHE:HZ	1:B:436:MET:HE2	1.77	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
3:C:602:FLC:CAC	3:C:602:FLC:CGC	2.91	0.48
1:A:144:VAL:HG22	1:A:145:GLU:H	1.78	0.48
1:B:155:THR:O	1:B:170:TRP:HA	2.14	0.48
1:D:24:PHE:CZ	1:D:436:MET:HE2	2.48	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:436:MET:HE2	1:A:436:MET:HB3	1.71	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
3:B:602:FLC:CGC	3:B:602:FLC:CAC	2.94	0.46
1:C:422:GLU:HG2	1:C:452:LEU:HD13	1.98	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:343:LEU:HD23	1:C:373:LEU:CD2	2.45	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: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: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:372:MET:HE1	3:D:602:FLC:OA1	2.16	0.44
1:B:76:MET:HE2	1:B:76:MET:HB2	1.91	0.44
1:D:255:SER:HA	1:D:282:LYS:HD3	1.99	0.44
1:C:24:PHE:HZ	1:C:436:MET:HE3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:58[B]:SER:OG	1:C:370:CYS:SG	2.74	0.43
1:A:296:LEU:HD13	1:A:296:LEU:C	2.39	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:CZ	1:C:436:MET:HE3	2.53	0.43
1:D:85:ARG:NH2	3:D:602:FLC:OA1	2.52	0.43
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: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:C:85:ARG:NH2	3:C:602:FLC:OA2	2.52	0.42
1:D:211:ASN:O	1:D:212:GLY:C	2.57	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:C:537:MET:HE3	1:C:537:MET:HB2	1.83	0.41
1:D:238:VAL:O	1:D:242:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:PHE:HD1	1:C:280:ILE:HB	1.85	0.41
1:C:404:ARG:HG3	1:D:412:ARG:HH12	1.84	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:229:ASP:O	1:C:230:LEU:C	2.59	0.41
1:D:195:LEU:C	1:D:195:LEU:HD23	2.41	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: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: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:141:GLU:O	1:B:141:GLU:HG3	2.21	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	520/543 (96%)	504 (97%)	13 (2%)	3 (1%)	25	14
1	B	488/543 (90%)	470 (96%)	16 (3%)	2 (0%)	34	22
1	C	502/543 (92%)	484 (96%)	16 (3%)	2 (0%)	34	22
1	D	447/543 (82%)	427 (96%)	16 (4%)	4 (1%)	17	8
All	All	1957/2172 (90%)	1885 (96%)	61 (3%)	11 (1%)	25	14

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 (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	424/432 (98%)	421 (99%)	3 (1%)	84	82
1	B	401/432 (93%)	400 (100%)	1 (0%)	93	93
1	C	410/432 (95%)	408 (100%)	2 (0%)	88	88
1	D	372/432 (86%)	371 (100%)	1 (0%)	92	92
All	All	1607/1728 (93%)	1600 (100%)	7 (0%)	91	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	69	SER
1	A	528	ARG
1	B	296	LEU
1	C	182	VAL
1	C	537	MET
1	D	296	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	603	-	18,20,20	0.90	1 (5%)	23,32,32	0.77	0
4	FBP	A	603	-	18,20,20	0.87	1 (5%)	23,32,32	0.83	1 (4%)
4	FBP	D	603	-	18,20,20	0.90	1 (5%)	23,32,32	0.80	1 (4%)
3	FLC	B	602	2	12,12,12	2.06	4 (33%)	17,17,17	1.70	3 (17%)
3	FLC	D	602	2	12,12,12	1.90	4 (33%)	17,17,17	1.48	2 (11%)
4	FBP	C	603	-	18,20,20	0.84	1 (5%)	23,32,32	0.85	0
3	FLC	A	602	2	12,12,12	1.69	4 (33%)	17,17,17	1.44	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ADN	D	604	-	18,21,21	0.88	1 (5%)	18,31,31	1.46	4 (22%)
5	EDO	B	604	-	3,3,3	0.56	0	2,2,2	0.44	0
3	FLC	C	602	2	12,12,12	2.06	4 (33%)	17,17,17	1.64	3 (17%)

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	B	603	-	-	2/13/32/32	0/1/1/1
4	FBP	A	603	-	-	3/13/32/32	0/1/1/1
4	FBP	D	603	-	-	2/13/32/32	0/1/1/1
3	FLC	B	602	2	-	10/16/16/16	-
3	FLC	D	602	2	-	6/16/16/16	-
4	FBP	C	603	-	-	5/13/32/32	0/1/1/1
3	FLC	A	602	2	-	1/16/16/16	-
6	ADN	D	604	-	2/2/4/4	2/2/22/22	0/3/3/3
5	EDO	B	604	-	-	1/1/1/1	-
3	FLC	C	602	2	-	6/16/16/16	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	FLC	CB-CBC	-4.08	1.49	1.53
3	C	602	FLC	CB-CBC	-3.74	1.49	1.53
3	D	602	FLC	CG-CB	-3.20	1.49	1.53
3	C	602	FLC	CG-CB	-3.19	1.49	1.53
3	C	602	FLC	CA-CB	-3.12	1.49	1.53
3	D	602	FLC	CA-CB	-3.07	1.50	1.53
3	B	602	FLC	CG-CB	-3.03	1.50	1.53
3	B	602	FLC	CA-CB	-3.01	1.50	1.53
3	D	602	FLC	CB-CBC	-2.98	1.50	1.53
3	C	602	FLC	OHB-CB	-2.75	1.38	1.43
4	B	603	FBP	O2-C2	2.71	1.45	1.40
4	D	603	FBP	O2-C2	2.69	1.45	1.40
6	D	604	ADN	C6-N6	2.68	1.43	1.34
3	A	602	FLC	OHB-CB	-2.60	1.38	1.43
3	B	602	FLC	OHB-CB	-2.60	1.38	1.43
3	A	602	FLC	CA-CB	-2.54	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	FBP	O2-C2	2.48	1.45	1.40
3	A	602	FLC	CG-CB	-2.45	1.50	1.53
3	D	602	FLC	OHB-CB	-2.43	1.38	1.43
3	A	602	FLC	CB-CBC	-2.36	1.51	1.53
4	C	603	FBP	O2-C2	2.35	1.44	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	FLC	OB2-CBC-CB	4.67	121.16	113.05
3	C	602	FLC	OB2-CBC-CB	4.44	120.76	113.05
6	D	604	ADN	N3-C2-N1	-4.21	122.10	128.68
3	A	602	FLC	OB2-CBC-CB	3.67	119.42	113.05
3	D	602	FLC	OB2-CBC-CB	2.99	118.25	113.05
4	D	603	FBP	O6P-P2-O6	2.52	113.44	106.73
3	B	602	FLC	OB1-CBC-CB	-2.34	118.94	122.25
3	C	602	FLC	OG2-CGC-CG	2.22	121.48	114.35
3	D	602	FLC	OA2-CAC-CA	2.18	121.36	114.35
3	B	602	FLC	OG2-CGC-CG	2.18	121.34	114.35
3	C	602	FLC	OB1-CBC-CB	-2.17	119.18	122.25
6	D	604	ADN	C3'-C2'-C1'	2.16	104.22	100.98
4	A	603	FBP	O6P-P2-O6	2.09	112.29	106.73
6	D	604	ADN	C1'-N9-C4	2.08	130.30	126.64
6	D	604	ADN	N6-C6-N1	2.03	122.80	118.57

All (2) chirality outliers are listed below:

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

All (38) torsion outliers are listed below:

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

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

There are no ring outliers.

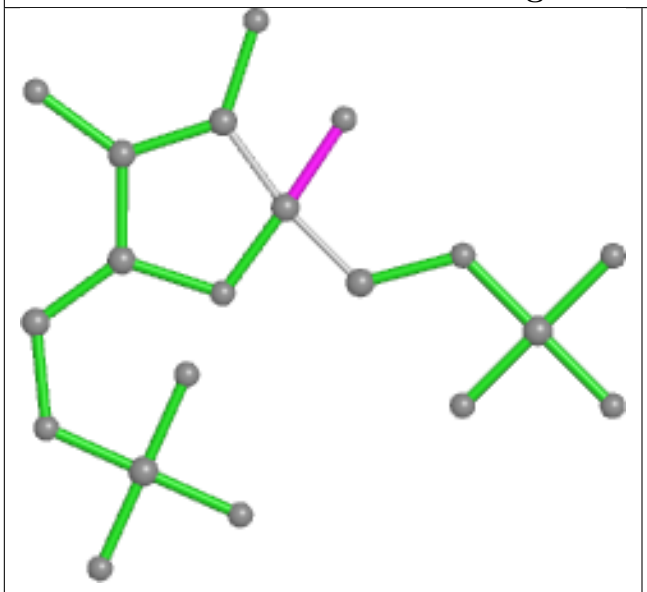
4 monomers are involved in 7 short contacts:

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

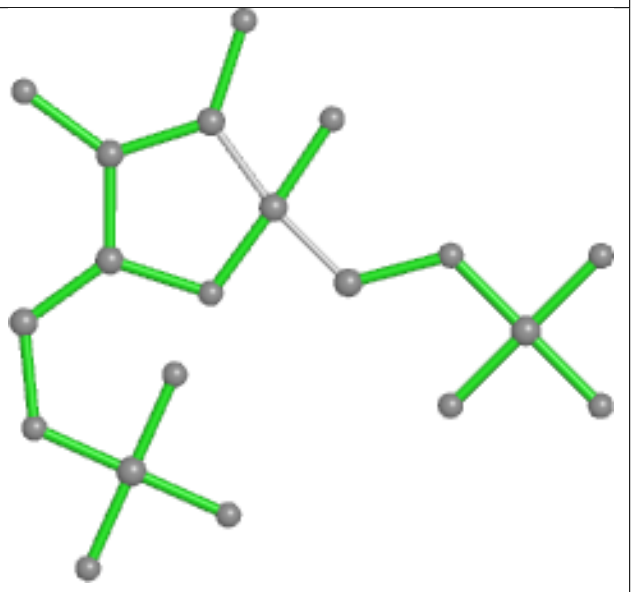
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

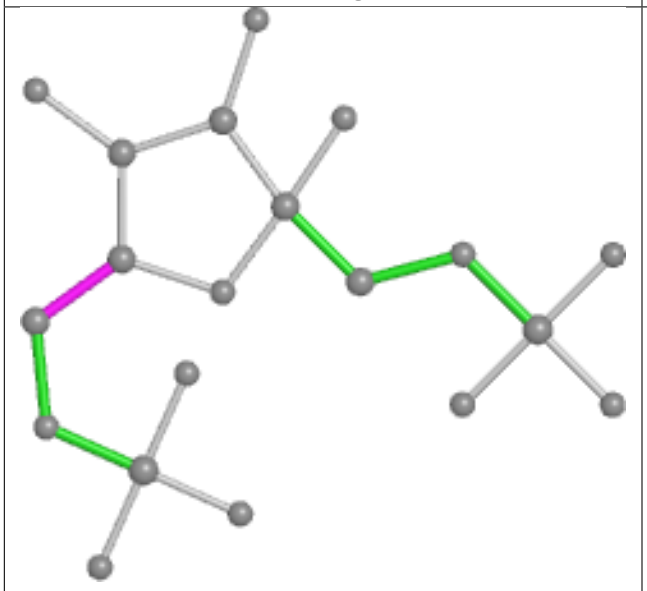
Ligand FBP B 603



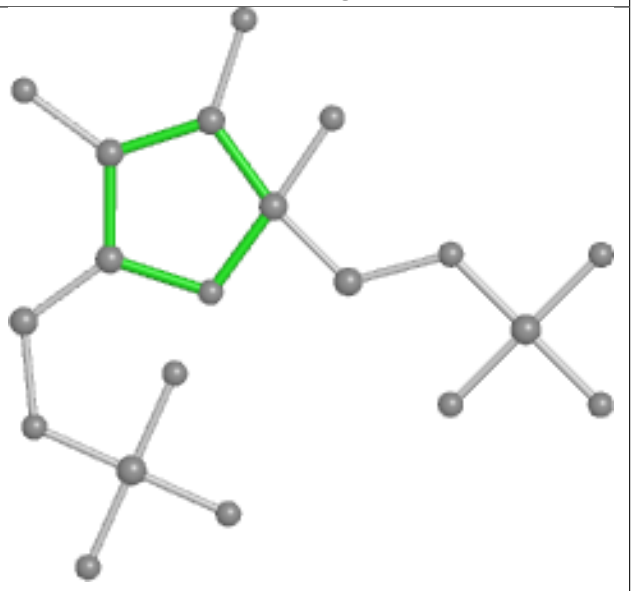
Bond lengths



Bond angles

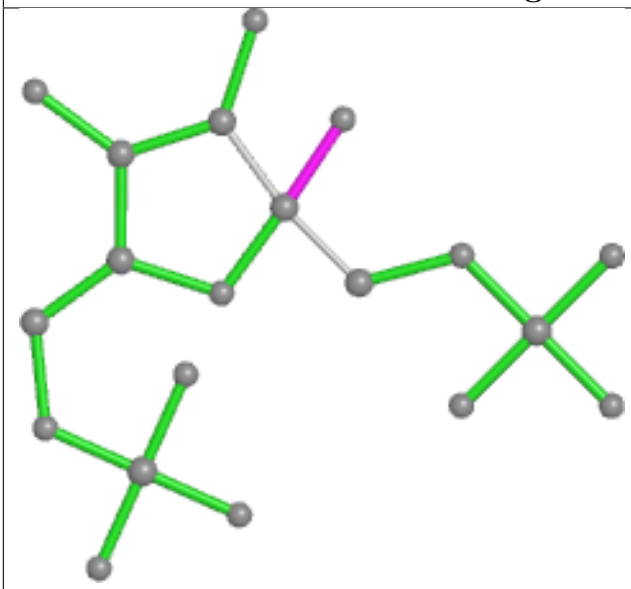


Torsions

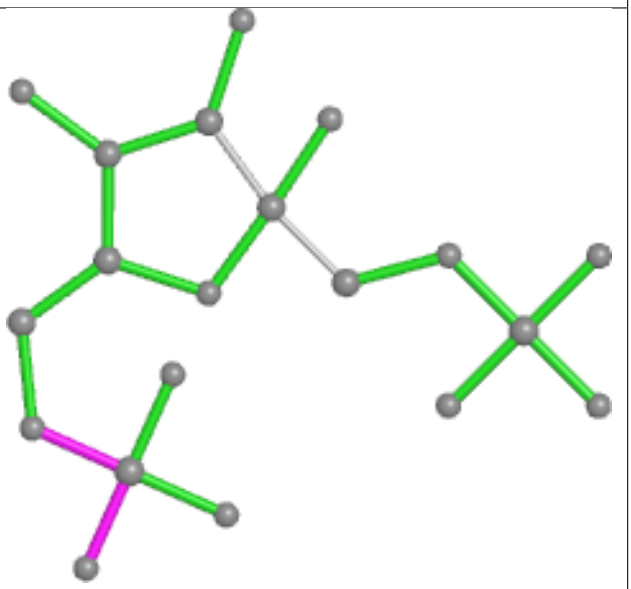


Rings

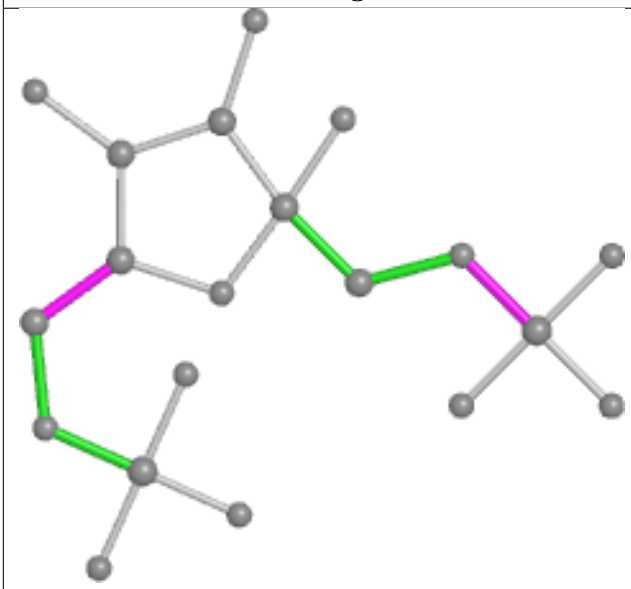
Ligand FBP A 603



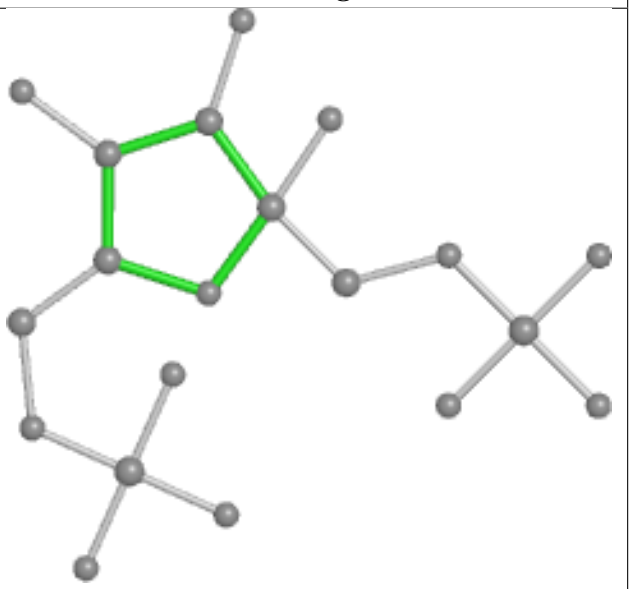
Bond lengths



Bond angles

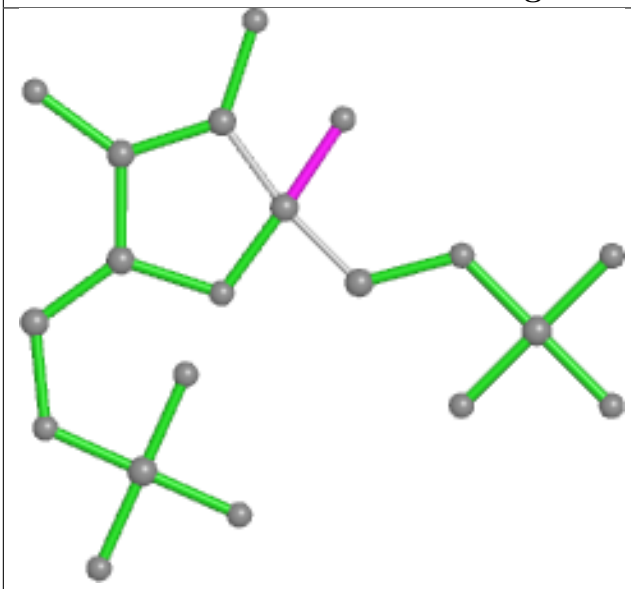


Torsions

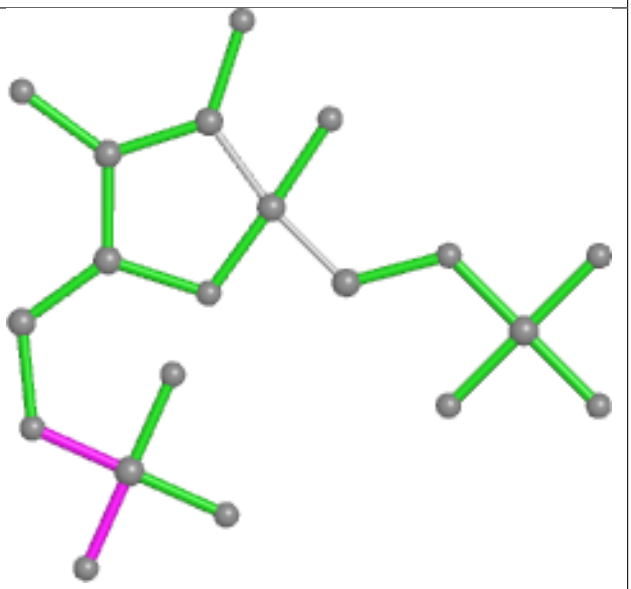


Rings

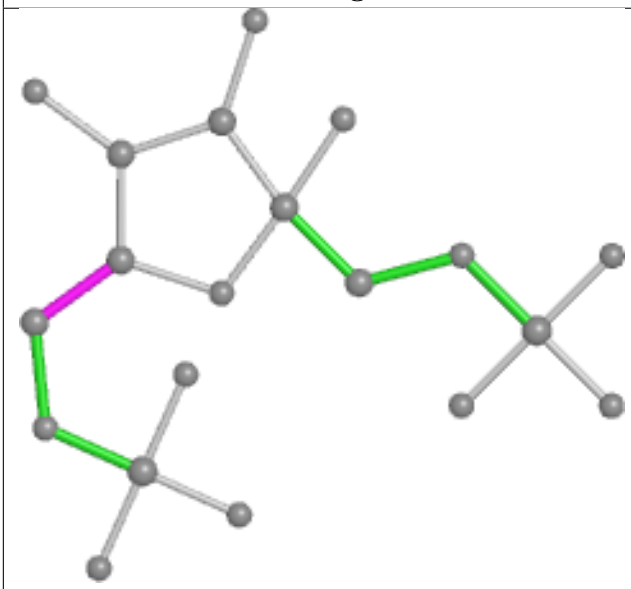
Ligand FBP D 603



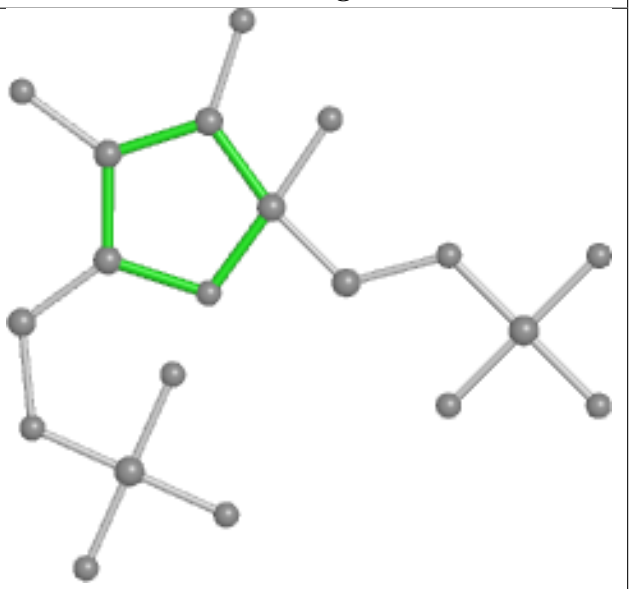
Bond lengths



Bond angles

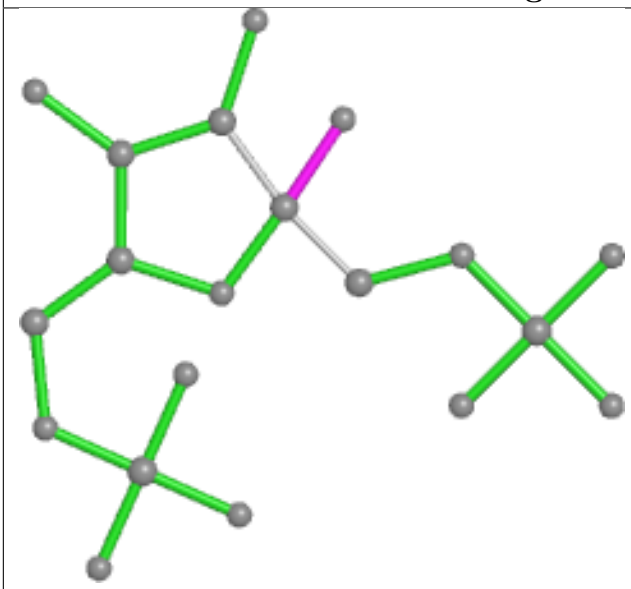


Torsions

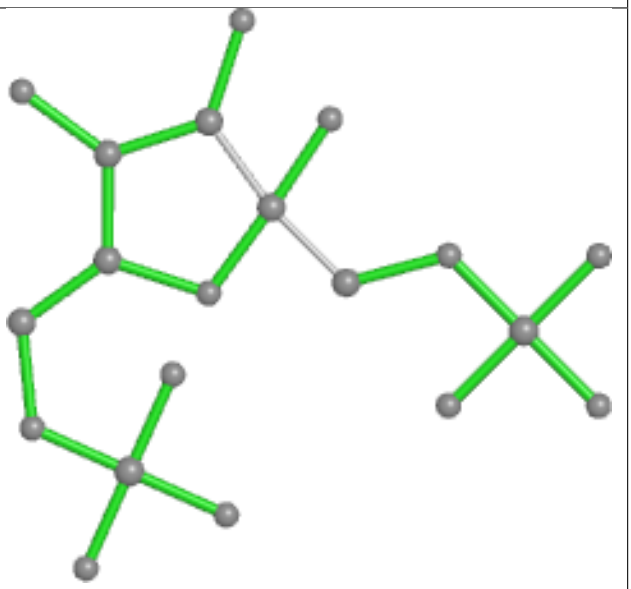


Rings

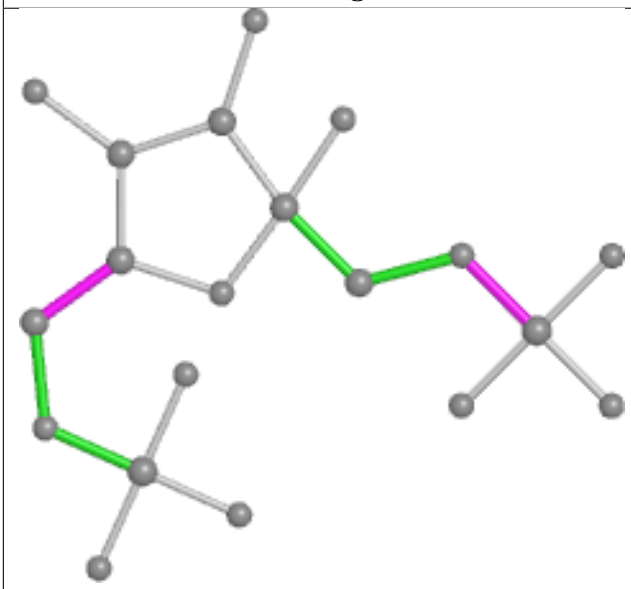
Ligand FBP C 603



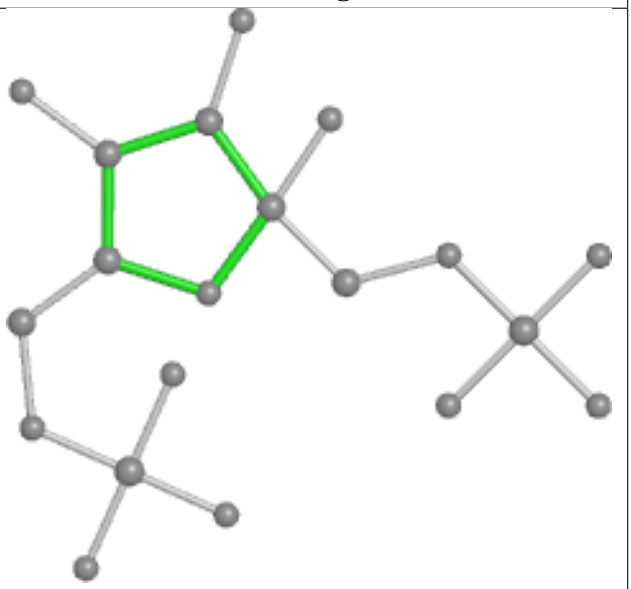
Bond lengths



Bond angles

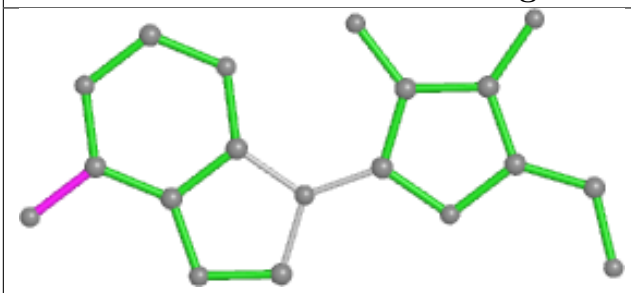


Torsions

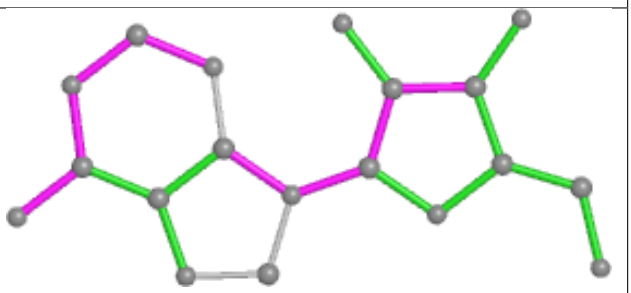


Rings

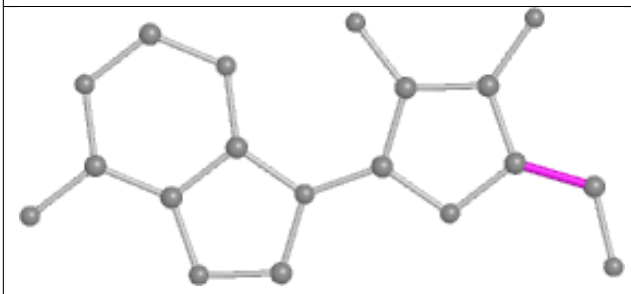
Ligand ADN D 604



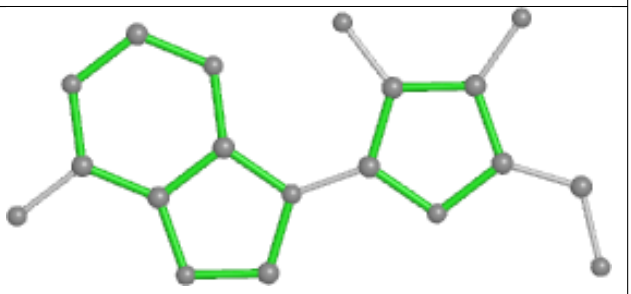
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.44	51 (9%) 7 12	22, 35, 67, 79	29 (5%)
1	B	500/543 (92%)	0.66	69 (13%) 2 4	21, 34, 82, 97	41 (8%)
1	C	505/543 (93%)	0.57	65 (12%) 3 5	23, 34, 84, 99	32 (6%)
1	D	460/543 (84%)	0.64	63 (13%) 3 4	23, 34, 79, 95	27 (5%)
All	All	1987/2172 (91%)	0.57	248 (12%) 3 6	21, 34, 78, 99	129 (6%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	144	VAL	8.9
1	B	196	VAL	7.8
1	D	146	LEU	7.8
1	D	195	LEU	7.4
1	D	147	VAL	7.0
1	D	231	PRO	6.9
1	D	232	GLY	6.9
1	C	21	GLY	6.8
1	B	168	THR	6.5
1	C	155	THR	6.4
1	B	170	TRP	6.3
1	D	214	VAL	6.3
1	B	159	ALA	6.0
1	B	142	SER	6.0
1	B	160	PHE	5.9
1	A	136	LEU	5.8
1	D	174	PRO	5.8
1	B	157	ASP	5.7
1	C	170	TRP	5.7
1	B	209	VAL	5.7
1	B	180	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	196	VAL	5.5
1	D	22	THR	5.5
1	D	220	GLY	5.4
1	C	200	ILE	5.3
1	B	206	VAL	5.3
1	C	146	LEU	5.3
1	B	21	GLY	5.2
1	A	182	VAL	5.2
1	B	144	VAL	5.2
1	D	209	VAL	5.2
1	B	171	VAL	5.2
1	B	146	LEU	5.0
1	D	16	LEU	5.0
1	D	194	SER	4.9
1	B	208	GLN	4.9
1	B	195	LEU	4.8
1	C	147	VAL	4.8
1	B	22	THR	4.7
1	B	156	VAL	4.7
1	C	207	THR	4.7
1	A	160	PHE	4.7
1	C	183	GLY	4.7
1	B	216	GLY	4.6
1	C	150	SER	4.6
1	A	206	VAL	4.6
1	B	184	GLY	4.6
1	B	225	GLY	4.5
1	D	193	ILE	4.5
1	B	164	GLY	4.5
1	D	145	GLU	4.5
1	D	212	GLY	4.5
1	A	135	ILE	4.5
1	C	195	LEU	4.5
1	C	208	GLN	4.5
1	B	149	GLY	4.5
1	C	182	VAL	4.4
1	B	158	PRO	4.4
1	C	145	GLU	4.4
1	B	152	VAL	4.3
1	C	184	GLY	4.3
1	C	217	SER	4.3
1	C	199	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	23	ALA	4.3
1	B	207	THR	4.3
1	B	215	LEU	4.2
1	D	211	ASN	4.2
1	C	215	LEU	4.2
1	A	493	ILE	4.2
1	D	493	ILE	4.2
1	C	214	VAL	4.2
1	C	229	ASP	4.1
1	B	167	ASN	4.1
1	A	183	GLY	4.1
1	A	196	VAL	4.1
1	C	209	VAL	4.1
1	C	152	VAL	4.1
1	B	165	ASN	4.0
1	C	171	VAL	4.0
1	C	114	PRO	4.0
1	D	173	TYR	3.9
1	A	272	PRO	3.9
1	C	156	VAL	3.9
1	C	216	GLY	3.9
1	B	226	ALA	3.8
1	B	115	LEU	3.8
1	D	143	GLU	3.8
1	C	230	LEU	3.8
1	B	145	GLU	3.8
1	D	17	THR	3.7
1	D	20	LEU	3.6
1	A	198	GLN	3.6
1	B	153	LEU	3.6
1	A	144	VAL	3.6
1	C	18	GLN	3.5
1	C	194	SER	3.5
1	C	218	ARG	3.5
1	C	22	THR	3.5
1	A	146	LEU	3.5
1	C	113	SER	3.5
1	B	210	GLU	3.4
1	B	113	SER	3.4
1	B	114	PRO	3.4
1	D	188	ILE	3.4
1	A	511	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	355	ALA	3.3
1	D	131	ILE	3.3
1	B	148	LYS	3.3
1	B	147	VAL	3.3
1	A	339	ALA	3.3
1	A	22	THR	3.3
1	C	181	PRO	3.3
1	B	150	SER	3.3
1	D	272	PRO	3.3
1	D	19	GLU	3.2
1	D	187	TYR	3.2
1	C	20	LEU	3.2
1	B	177	VAL	3.2
1	C	115	LEU	3.1
1	C	493	ILE	3.1
1	D	186	ILE	3.1
1	C	206	VAL	3.1
1	B	232	GLY	3.1
1	C	112	GLY	3.1
1	D	213	GLY	3.1
1	D	172	ASP	3.0
1	A	200	ILE	3.0
1	D	490	PRO	3.0
1	D	21	GLY	3.0
1	D	233	LEU	3.0
1	A	232	GLY	3.0
1	C	492	ALA	2.9
1	B	169	VAL	2.9
1	C	177	VAL	2.9
1	D	25	PHE	2.9
1	A	214	VAL	2.9
1	B	194	SER	2.9
1	A	228	VAL	2.9
1	D	24	PHE	2.9
1	C	204	GLY	2.9
1	A	208	GLN	2.8
1	C	198	GLN	2.8
1	C	157	ASP	2.8
1	B	493	ILE	2.8
1	C	197	VAL	2.8
1	B	166	ALA	2.8
1	B	133	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	185	ARG	2.8
1	B	179	VAL	2.8
1	B	155	THR	2.8
1	D	365	LEU	2.8
1	A	197	VAL	2.8
1	A	149	GLY	2.7
1	C	149	GLY	2.7
1	D	189	ASP	2.7
1	B	112	GLY	2.7
1	A	113	SER	2.7
1	A	207	THR	2.7
1	B	211	ASN	2.7
1	D	492	ALA	2.7
1	D	364	VAL	2.7
1	D	210	GLU	2.7
1	A	150	SER	2.6
1	D	393	ILE	2.6
1	A	205	LEU	2.6
1	D	511	LEU	2.6
1	D	60	ILE	2.6
1	A	17	THR	2.6
1	A	492	ALA	2.6
1	B	339	ALA	2.6
1	C	151	GLN	2.6
1	D	361	ALA	2.5
1	A	152	VAL	2.5
1	D	15	GLN	2.5
1	D	500	ARG	2.5
1	B	176	ILE	2.5
1	B	371	ILE	2.5
1	C	371	ILE	2.5
1	C	529	PRO	2.5
1	A	166	ALA	2.5
1	B	492	ALA	2.5
1	A	371	ILE	2.4
1	D	59	ILE	2.4
1	B	494	TRP	2.4
1	A	477	LEU	2.4
1	C	202	PRO	2.4
1	D	130	GLU	2.4
1	B	217	SER	2.4
1	D	338	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	343	LEU	2.4
1	D	477	LEU	2.4
1	A	110	PHE	2.4
1	A	217	SER	2.4
1	B	173	TYR	2.4
1	B	360	VAL	2.4
1	B	23	ALA	2.3
1	C	339	ALA	2.3
1	A	142	SER	2.3
1	C	205	LEU	2.3
1	B	275	HIS	2.3
1	A	134	GLY	2.3
1	D	225	GLY	2.3
1	A	159	ALA	2.3
1	B	178	ARG	2.3
1	A	195	LEU	2.3
1	C	411[A]	ARG	2.3
1	B	174	PRO	2.2
1	C	143	GLU	2.2
1	D	175	ASN	2.2
1	D	371	ILE	2.2
1	D	363	ALA	2.2
1	A	209	VAL	2.2
1	B	20	LEU	2.2
1	D	540	LEU	2.2
1	C	370	CYS	2.2
1	D	415	PRO	2.2
1	C	23	ALA	2.2
1	D	337	VAL	2.2
1	D	83	ILE	2.2
1	C	153	LEU	2.2
1	D	223	LEU	2.2
1	A	202	PRO	2.2
1	B	218	ARG	2.2
1	D	110	PHE	2.1
1	A	490	PRO	2.1
1	A	60	ILE	2.1
1	A	16	LEU	2.1
1	B	143	GLU	2.1
1	C	490	PRO	2.1
1	A	215	LEU	2.1
1	B	355	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	305	ALA	2.1
1	A	489	PRO	2.1
1	C	272	PRO	2.1
1	A	168	THR	2.1
1	C	144	VAL	2.1
1	A	151	GLN	2.1
1	C	19[A]	GLU	2.1
1	C	494	TRP	2.1
1	D	360	VAL	2.1
1	B	141	GLU	2.0
1	B	25	PHE	2.0
1	A	363	ALA	2.0
1	A	167	ASN	2.0
1	B	372	MET	2.0
1	C	355	ALA	2.0
1	A	338	CYS	2.0
1	A	145	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	EDO	B	604	4/4	0.85	0.18	34,35,40,44	0
6	ADN	D	604	19/19	0.89	0.23	26,42,50,52	7
3	FLC	A	602	13/13	0.94	0.15	29,33,37,40	9
3	FLC	D	602	13/13	0.94	0.12	33,38,44,48	4
4	FBP	D	603	20/20	0.96	0.08	28,31,39,39	0
3	FLC	C	602	13/13	0.96	0.10	31,34,37,38	6

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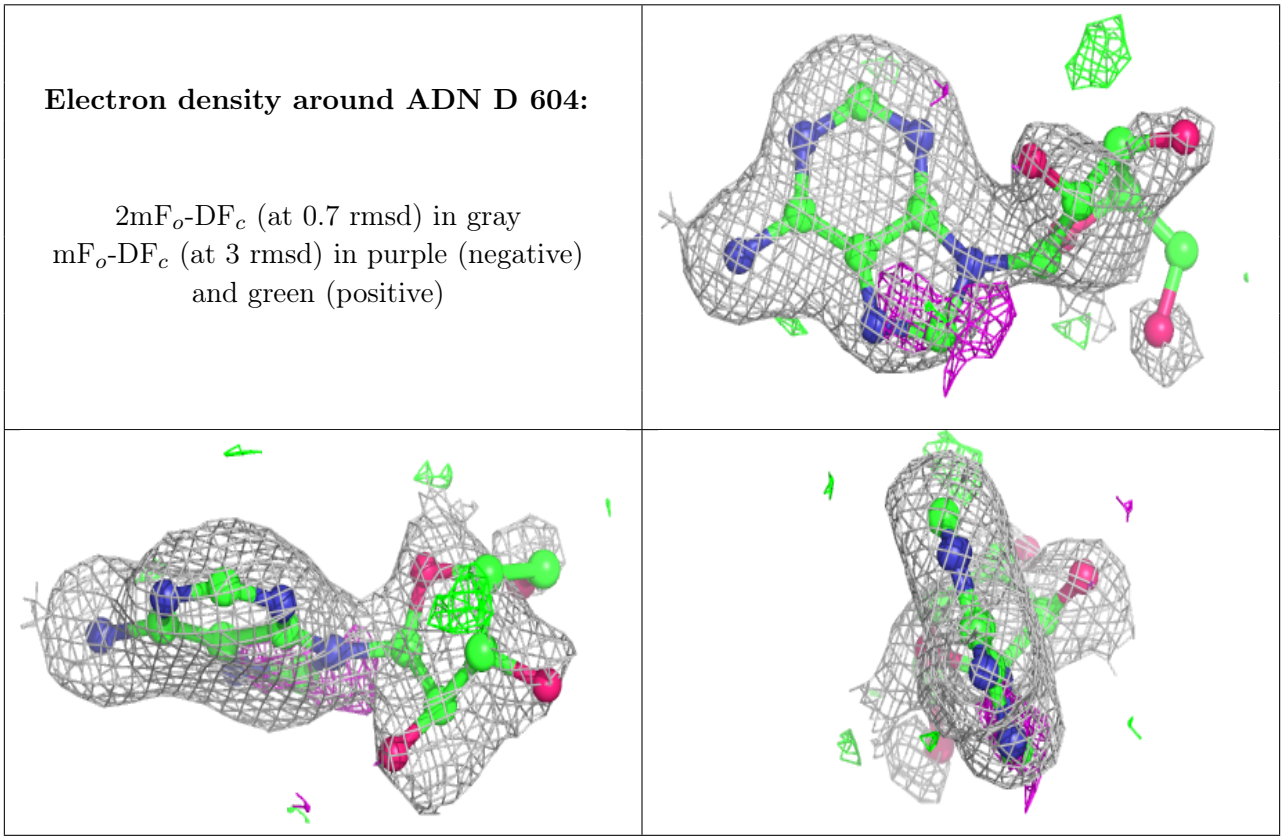
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FLC	B	602	13/13	0.96	0.20	29,33,36,38	8
4	FBP	A	603	20/20	0.97	0.09	28,32,34,34	0
4	FBP	B	603	20/20	0.97	0.08	23,29,31,32	0
4	FBP	C	603	20/20	0.97	0.08	26,32,35,35	0
2	MN	C	601	1/1	0.99	0.06	36,36,36,36	0
2	MN	D	601	1/1	0.99	0.07	43,43,43,43	0
2	MN	A	601	1/1	0.99	0.10	37,37,37,37	0
2	MN	B	601	1/1	1.00	0.05	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.

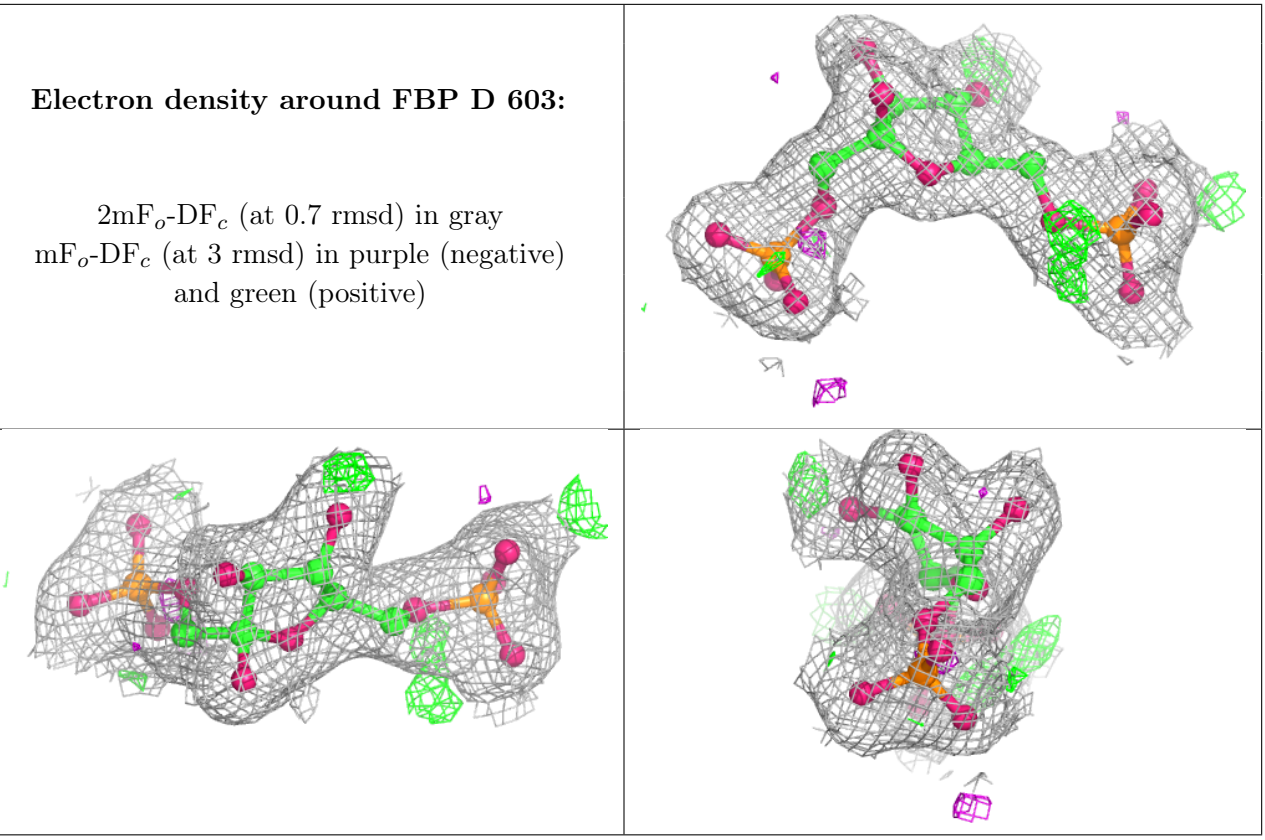
Electron density around ADN D 604:

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



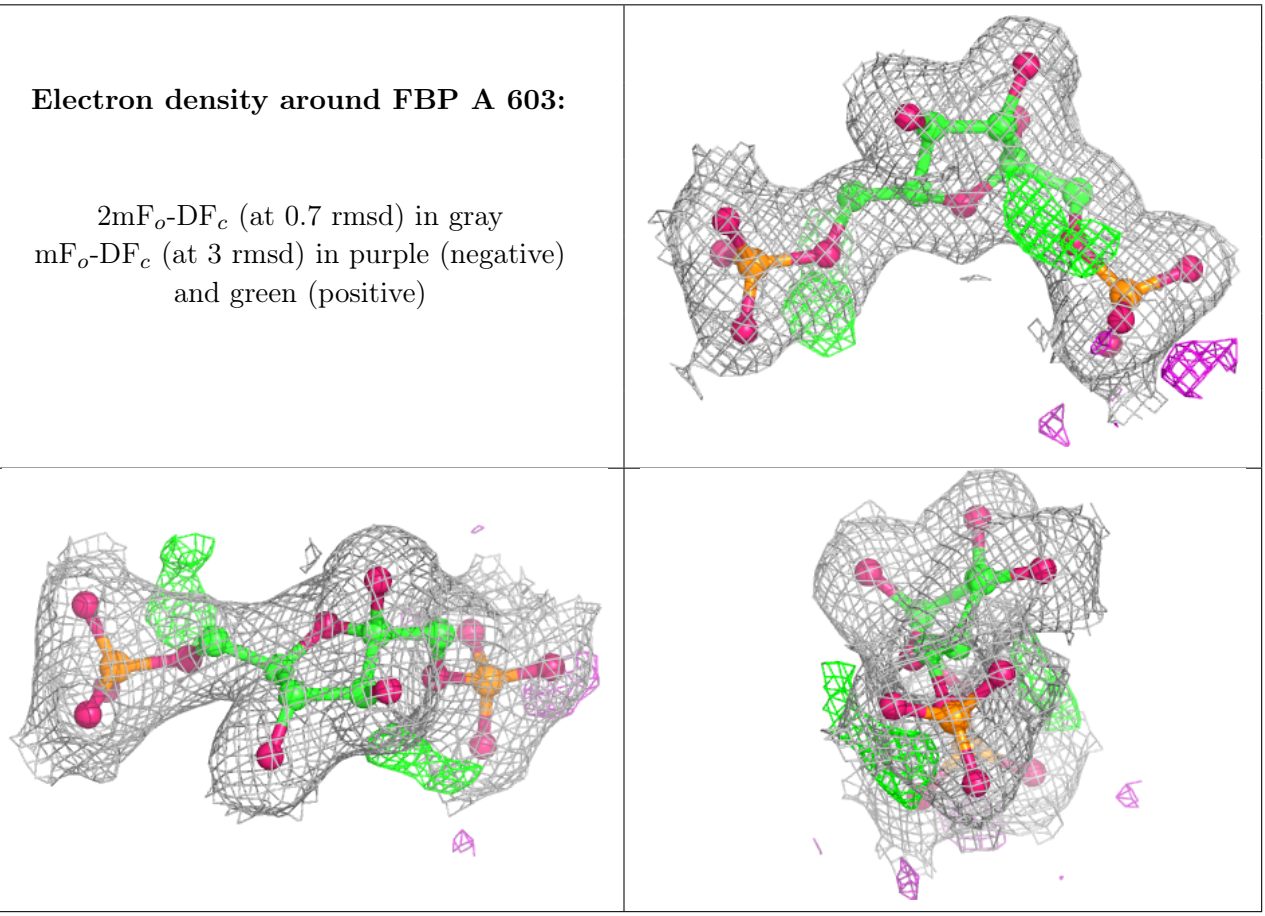
Electron density around FBP D 603:

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



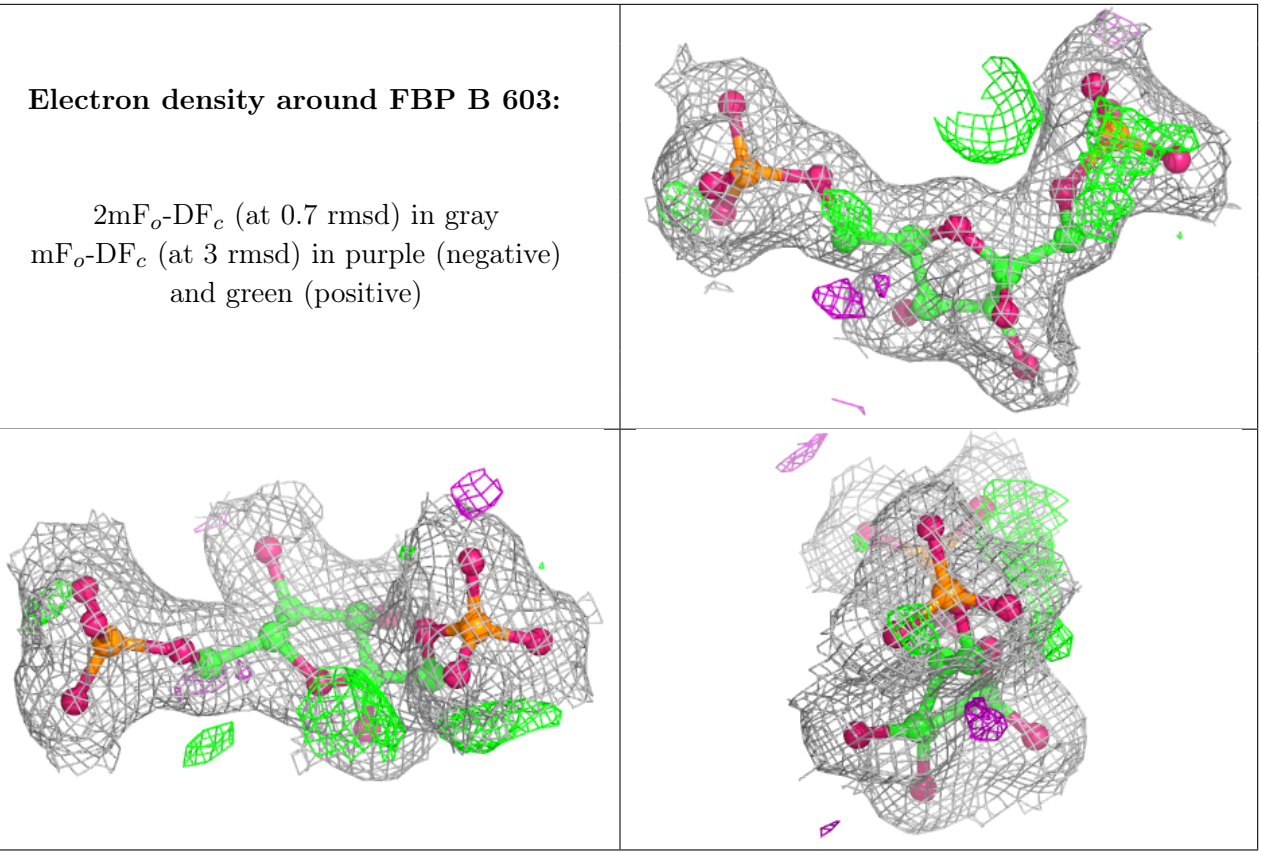
Electron density around FBP A 603:

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



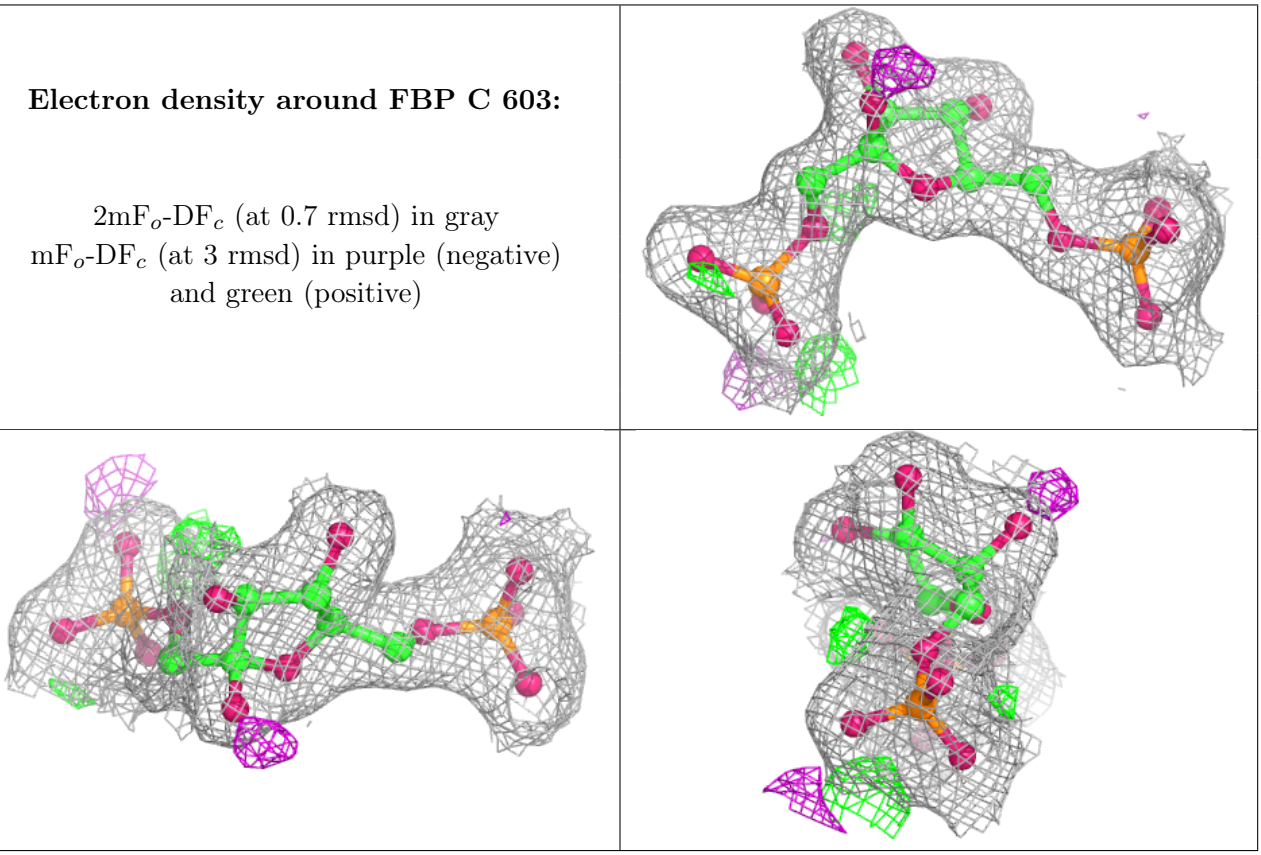
Electron density around FBP B 603:

$2mF_o$-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.