Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2024 – 04:58 PM JST

PDB ID	:	8XFD
Title	:	Crystal structure of pyruvate kinase tetramer in complex with allosteric activator, Mitapivat (MTPV, AG-348)
Authors	:	Sun, R.; Achour, A.
Deposited on	:	2023-12-13
Resolution	:	2.10 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:

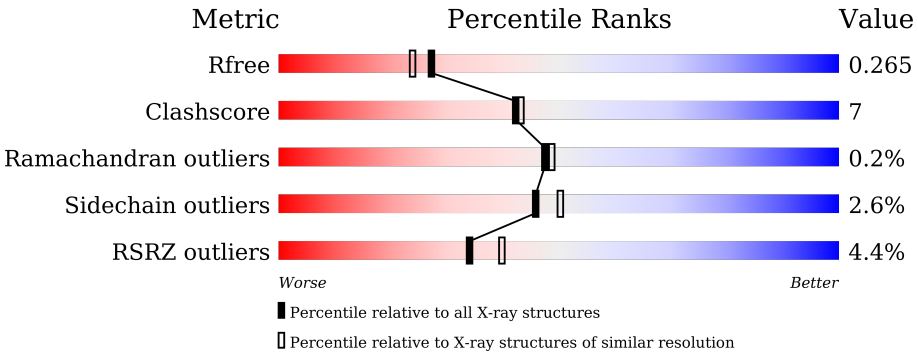
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	2% 82% 12% • 5%
1	B	543	3% 77% 17% • 5%
1	C	543	7% 76% 17% •• 6%
1	D	543	4% 81% 14% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16621 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.

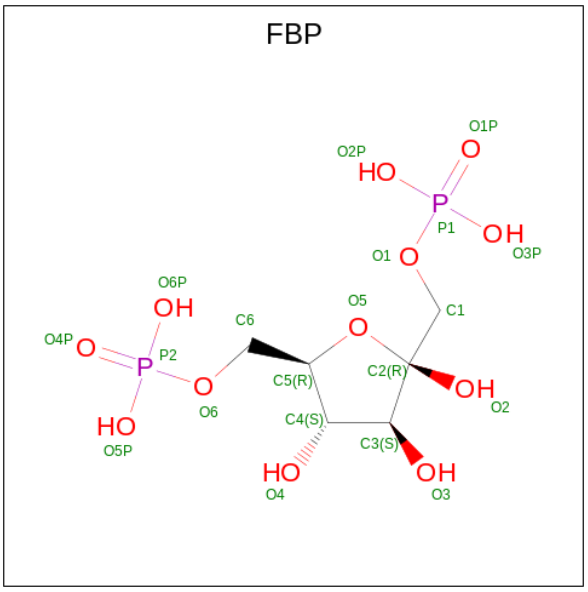
- Molecule 1 is a protein called Isoform L-type of Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3895	2448	705	724	18			
1	B	517	Total	C	N	O	S	0	0	0
			3908	2455	709	726	18			
1	C	511	Total	C	N	O	S	0	0	0
			3872	2433	702	719	18			
1	D	517	Total	C	N	O	S	0	0	0
			3912	2457	709	728	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

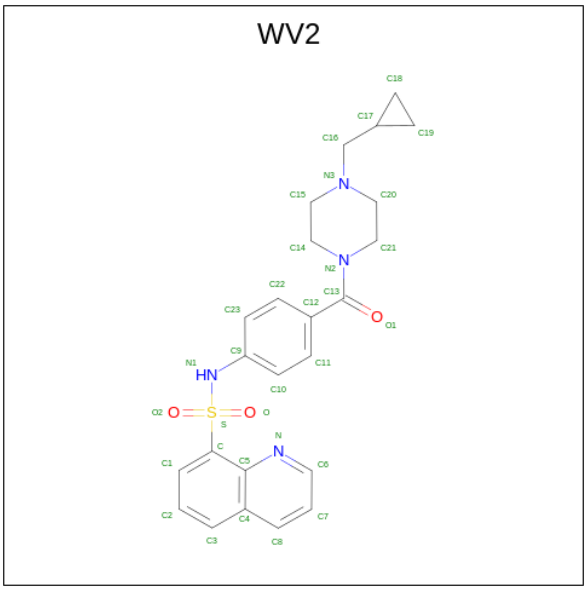
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 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
3	A	1	Total C O P 20 6 12 2	0	0
3	B	1	Total C O P 20 6 12 2	0	0
3	C	1	Total C O P 20 6 12 2	0	0
3	D	1	Total C O P 20 6 12 2	0	0

- Molecule 4 is mitapivat (three-letter code: WV2) (formula: $C_{24}H_{26}N_4O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			32	24	4	3	1		
4	D	1	Total	C	N	O	S	0	0
			32	24	4	3	1		

- Molecule 5 is water.

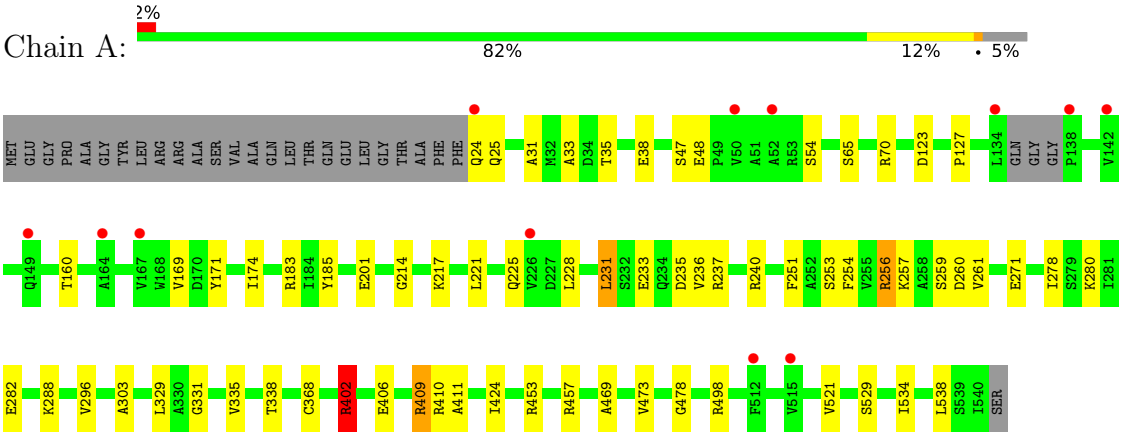
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	256	Total	O	0	0
			256	256		
5	B	213	Total	O	0	0
			213	213		
5	C	156	Total	O	0	0
			156	156		
5	D	261	Total	O	0	0
			261	261		

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.

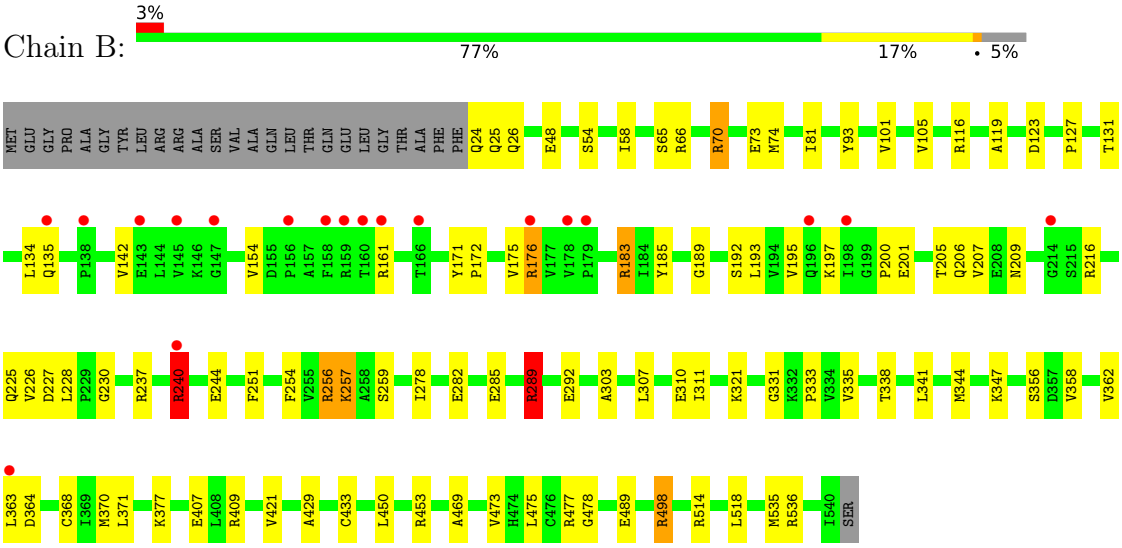
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

Chain A:



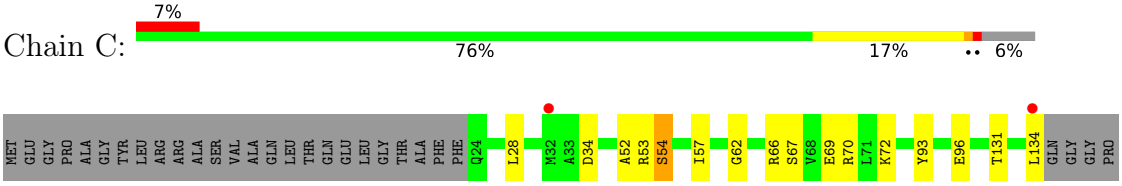
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

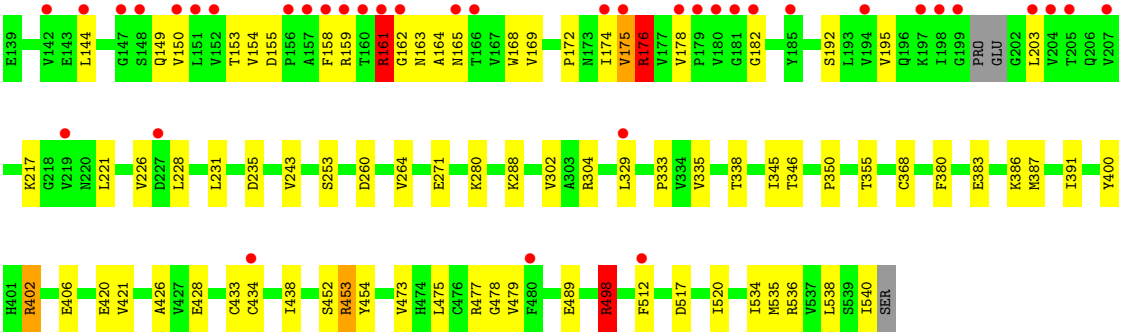
Chain B:



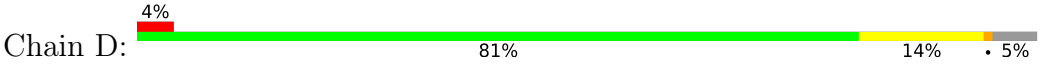
• Molecule 1: Isoform L-type of Pyruvate kinase PKLR

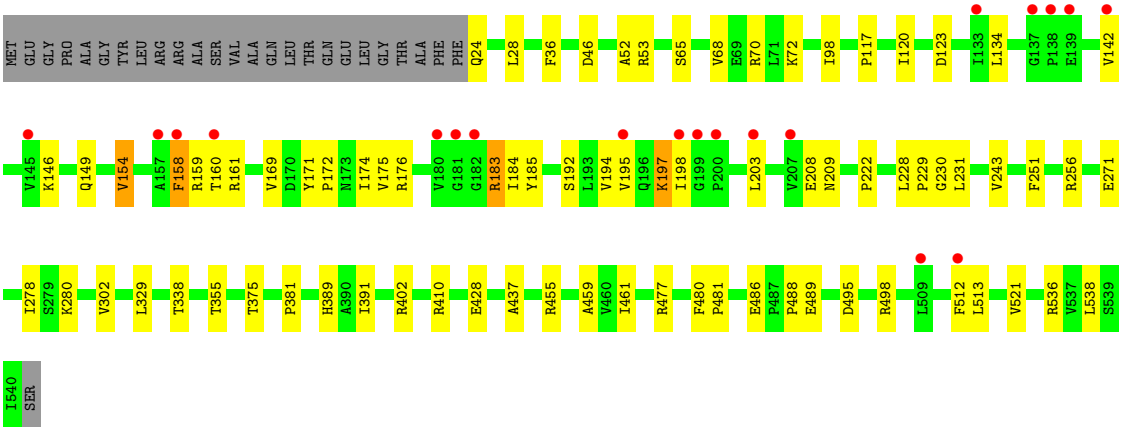
Chain C:





• Molecule 1: Isoform L-type of Pyruvate kinase PKLR





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.93Å 86.96Å 91.55Å 76.78° 66.88° 80.22°	Depositor
Resolution (Å)	54.43 – 2.10 54.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.5 (54.43-2.10) 96.5 (54.43-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.39 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.232 , 0.265 0.231 , 0.265	Depositor DCC
R_{free} test set	6502 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16621	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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: FBP, MG, WV2

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	0.43	0/3958	0.62	0/5364
1	B	0.46	1/3972 (0.0%)	0.72	9/5385 (0.2%)
1	C	0.42	1/3932 (0.0%)	0.66	7/5326 (0.1%)
1	D	0.43	0/3976	0.67	1/5390 (0.0%)
All	All	0.43	2/15838 (0.0%)	0.67	17/21465 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ARG	CG-CD	-7.06	1.34	1.51
1	C	402	ARG	CG-CD	-5.51	1.38	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	154	VAL	CG1-CB-CG2	-17.44	82.99	110.90
1	B	176	ARG	CG-CD-NE	12.89	138.88	111.80
1	B	176	ARG	CA-CB-CG	-10.45	90.41	113.40
1	B	176	ARG	CB-CG-CD	10.30	138.38	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	240	ARG	CB-CG-CD	7.69	131.60	111.60
1	C	161	ARG	CG-CD-NE	7.39	127.31	111.80
1	C	176	ARG	CG-CD-NE	7.39	127.31	111.80
1	C	402	ARG	CG-CD-NE	7.10	126.72	111.80
1	B	240	ARG	CG-CD-NE	6.57	125.60	111.80
1	C	161	ARG	CA-CB-CG	6.57	127.84	113.40
1	B	257	LYS	CD-CE-NZ	-6.43	96.92	111.70
1	C	161	ARG	CB-CG-CD	-6.37	95.05	111.60
1	B	289	ARG	CB-CG-CD	5.83	126.75	111.60
1	B	240	ARG	CA-CB-CG	5.80	126.16	113.40
1	B	289	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	161	ARG	CD-NE-CZ	5.15	130.81	123.60
1	C	175	VAL	C-N-CA	-5.04	109.11	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	ARG	Sidechain
1	A	409	ARG	Sidechain
1	B	183	ARG	Sidechain
1	B	289	ARG	Sidechain
1	C	161	ARG	Sidechain
1	C	176	ARG	Sidechain
1	C	498	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3895	0	3978	44	0
1	B	3908	0	3988	71	0
1	C	3872	0	3956	68	0
1	D	3912	0	3992	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
3	A	20	0	10	0	0
3	B	20	0	10	0	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	B	32	0	0	2	0
4	D	32	0	0	0	0
5	A	256	0	0	2	0
5	B	213	0	0	2	0
5	C	156	0	0	1	0
5	D	261	0	0	0	0
All	All	16621	0	15954	220	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 (220) 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:257:LYS:HG2	1:B:289:ARG:HH22	0.90	1.03
1:B:257:LYS:HG2	1:B:289:ARG:NH2	1.73	1.03
1:B:175:VAL:HG23	1:B:176:ARG:HD3	1.41	1.02
1:B:257:LYS:CG	1:B:289:ARG:HH22	1.75	1.00
1:C:400:TYR:OH	1:C:402:ARG:NH1	2.00	0.94
1:D:52:ALA:HB2	1:D:512:PHE:CE2	2.10	0.86
1:C:288:LYS:NZ	5:C:701:HOH:O	2.11	0.83
1:B:289:ARG:NH1	1:B:292:GLU:OE1	2.13	0.81
1:C:66:ARG:HH22	1:C:96:GLU:HG3	1.43	0.81
1:D:154:VAL:HG21	1:D:172:PRO:HA	1.65	0.79
1:B:257:LYS:HA	1:B:289:ARG:NH2	1.98	0.79
1:B:135:GLN:HG2	1:B:161:ARG:HA	1.69	0.75
1:C:175:VAL:HA	1:C:203:LEU:HD11	1.70	0.73
1:B:175:VAL:C	1:B:176:ARG:HG2	1.97	0.72
1:D:154:VAL:HG23	1:D:154:VAL:O	1.91	0.70
1:D:154:VAL:O	1:D:154:VAL:CG2	2.40	0.70
1:D:175:VAL:HA	1:D:203:LEU:HD21	1.73	0.69
1:A:406:GLU:OE1	1:A:409:ARG:NH1	2.26	0.68
1:A:402:ARG:NH2	1:D:410:ARG:HD3	2.09	0.66
1:C:231:LEU:HD11	1:C:264:VAL:HA	1.77	0.66
1:C:155:ASP:HB3	1:C:158:PHE:HD2	1.60	0.66
1:C:131:THR:HG22	1:C:217:LYS:H	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LYS:HD3	1:D:198:ILE:H	1.62	0.65
1:D:158:PHE:HD1	1:D:161:ARG:HB2	1.62	0.65
1:C:231:LEU:HD21	1:C:264:VAL:HG22	1.78	0.65
1:B:321:LYS:NZ	1:B:364:ASP:OD1	2.31	0.64
1:A:25:GLN:HA	1:A:47:SER:OG	1.98	0.64
1:C:163:ASN:OD1	1:C:164:ALA:N	2.31	0.64
1:D:65:SER:HA	1:D:70:ARG:HG2	1.80	0.63
1:B:256:ARG:O	1:B:289:ARG:NH2	2.31	0.62
1:C:66:ARG:NH2	1:C:93:TYR:O	2.32	0.62
1:C:175:VAL:HG23	1:C:176:ARG:HD2	1.82	0.62
1:C:34:ASP:C	1:C:402:ARG:NH1	2.54	0.61
1:A:25:GLN:HB3	1:A:48:GLU:O	2.00	0.61
1:B:154:VAL:HG11	1:B:172:PRO:HA	1.83	0.61
1:A:409:ARG:HG3	1:A:424:ILE:HD11	1.83	0.61
1:D:134:LEU:HD13	1:D:142:VAL:HG23	1.81	0.61
1:A:335:VAL:HG22	1:A:368:CYS:HB2	1.83	0.60
1:A:236:VAL:O	1:A:240:ARG:HG2	2.01	0.60
1:D:159:ARG:HG2	1:D:160:THR:HG23	1.84	0.60
1:B:341:LEU:HD13	1:B:371:LEU:HD21	1.83	0.59
1:C:52:ALA:HB2	1:C:512:PHE:CD2	2.38	0.59
1:C:335:VAL:HG22	1:C:368:CYS:HB2	1.84	0.59
1:B:134:LEU:HD13	1:B:142:VAL:HG23	1.83	0.59
1:C:402:ARG:O	1:C:406:GLU:HG3	2.02	0.59
1:C:34:ASP:O	1:C:402:ARG:NH1	2.36	0.59
1:C:226:VAL:HG12	1:C:228:LEU:HG	1.86	0.58
1:B:193:LEU:HD23	1:B:207:VAL:HA	1.85	0.58
1:A:31:ALA:HB2	1:A:457:ARG:HH12	1.69	0.57
1:B:201:GLU:CD	1:B:201:GLU:H	2.07	0.57
1:B:54:SER:HB2	1:B:478:GLY:HA2	1.86	0.56
1:A:31:ALA:HB1	1:A:457:ARG:HH22	1.71	0.56
1:C:54:SER:HB2	1:C:477:ARG:HG2	1.88	0.55
1:C:70:ARG:HH11	1:C:70:ARG:HG2	1.71	0.55
1:B:26:GLN:HG2	5:B:836:HOH:O	2.06	0.55
1:A:25:GLN:HG2	1:A:48:GLU:H	1.72	0.54
1:B:409:ARG:NH2	5:B:707:HOH:O	2.41	0.54
1:D:146:LYS:NZ	1:D:208:GLU:O	2.36	0.54
1:A:521:VAL:HG21	1:A:538:LEU:HD12	1.90	0.54
1:A:25:GLN:CG	1:A:48:GLU:H	2.22	0.53
1:A:282:GLU:HG2	1:A:303:ALA:HB3	1.90	0.53
1:C:489:GLU:CD	1:C:498:ARG:HE	2.11	0.53
1:A:169:VAL:HG12	1:A:171:TYR:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:521:VAL:HG23	1:D:538:LEU:HD23	1.91	0.53
1:D:175:VAL:HG23	1:D:176:ARG:HG3	1.90	0.53
1:C:134:LEU:HD23	1:C:162:GLY:HA3	1.90	0.52
1:B:363:LEU:O	4:B:603:WV2:N1	2.42	0.52
1:A:127:PRO:HG2	1:A:254:PHE:CD2	2.45	0.52
1:C:517:ASP:O	1:C:540:ILE:HG12	2.10	0.52
1:C:400:TYR:OH	1:C:402:ARG:CZ	2.58	0.51
1:A:214:GLY:H	1:A:217:LYS:HZ2	1.58	0.51
1:C:288:LYS:HE2	1:D:46:ASP:OD2	2.10	0.51
1:D:52:ALA:CB	1:D:512:PHE:CE2	2.90	0.51
1:C:66:ARG:NH2	1:C:96:GLU:HG3	2.19	0.51
1:B:127:PRO:HG2	1:B:254:PHE:HD2	1.76	0.51
1:C:155:ASP:HB3	1:C:158:PHE:CD2	2.44	0.51
1:D:521:VAL:CG2	1:D:538:LEU:HD23	2.41	0.50
1:C:131:THR:CG2	1:C:217:LYS:H	2.22	0.50
1:A:54:SER:HB2	1:A:478:GLY:HA2	1.94	0.50
1:C:512:PHE:N	1:C:512:PHE:CD1	2.80	0.50
1:A:228:LEU:O	1:A:256:ARG:NH2	2.34	0.50
1:D:243:VAL:HG11	1:D:271:GLU:HG2	1.94	0.50
1:A:231:LEU:HD22	1:A:235:ASP:HB3	1.94	0.49
1:D:123:ASP:OD1	1:D:280:LYS:NZ	2.37	0.49
1:A:35:THR:HB	1:B:407:GLU:CD	2.33	0.49
1:A:256:ARG:HG2	1:A:260:ASP:OD2	2.12	0.49
1:B:183:ARG:HA	1:B:193:LEU:O	2.12	0.49
1:C:253:SER:HA	1:C:280:LYS:HD3	1.94	0.49
1:D:117:PRO:HG2	1:D:481:PRO:HG2	1.95	0.49
1:A:261:VAL:HG11	1:A:296:VAL:HG23	1.93	0.49
1:C:174:ILE:HG13	1:C:221:LEU:HD11	1.95	0.49
1:B:536:ARG:HG2	1:C:534:ILE:HG12	1.94	0.49
1:D:230:GLY:HA2	1:D:256:ARG:NH2	2.27	0.49
1:D:375:THR:HA	1:D:381:PRO:HB3	1.94	0.49
1:C:131:THR:HA	1:C:168:TRP:O	2.13	0.49
1:C:380:PHE:HB3	1:C:383:GLU:HB2	1.95	0.49
1:B:131:THR:O	1:B:216:ARG:HD2	2.13	0.49
1:C:333:PRO:HB3	1:C:475:LEU:O	2.13	0.49
1:B:256:ARG:HG2	1:B:285:GLU:HB3	1.95	0.48
1:D:68:VAL:HG12	1:D:72:LYS:HE3	1.95	0.48
1:A:33:ALA:HB1	1:A:38:GLU:HG2	1.94	0.48
1:C:69:GLU:HA	1:C:72:LYS:HD2	1.94	0.48
1:D:437:ALA:HB1	1:D:461:ILE:HD13	1.95	0.48
1:B:429:ALA:HB1	1:C:421:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ILE:HG12	1:B:119:ALA:HB3	1.94	0.48
1:A:534:ILE:HG12	1:D:536:ARG:HG2	1.95	0.48
1:C:231:LEU:HD22	1:C:235:ASP:HB3	1.94	0.48
1:B:131:THR:O	1:B:216:ARG:NH1	2.41	0.48
1:C:62:GLY:O	1:C:66:ARG:HG3	2.14	0.48
1:D:24:GLN:HG3	1:D:28:LEU:HB2	1.96	0.48
1:D:52:ALA:HB2	1:D:512:PHE:CD2	2.48	0.48
1:D:486:GLU:OE2	1:D:498:ARG:NH1	2.44	0.47
1:B:135:GLN:NE2	1:B:161:ARG:HG3	2.29	0.47
1:B:175:VAL:HG23	1:B:176:ARG:CD	2.29	0.47
1:B:127:PRO:HG2	1:B:254:PHE:CD2	2.49	0.47
1:D:251:PHE:HD1	1:D:278:ILE:HB	1.79	0.47
1:A:410:ARG:NH1	1:D:402:ARG:HE	2.13	0.47
1:C:53:ARG:NH1	1:C:57:ILE:HG13	2.30	0.47
1:D:271:GLU:OE2	1:D:271:GLU:N	2.24	0.47
1:C:54:SER:HB3	1:C:478:GLY:HA2	1.96	0.47
1:C:452:SER:HB2	1:C:477:ARG:O	2.15	0.47
1:B:226:VAL:HG12	1:B:228:LEU:HG	1.96	0.46
1:B:363:LEU:HB3	4:B:603:WV2:C10	2.45	0.46
1:A:271:GLU:H	1:A:271:GLU:CD	2.17	0.46
1:B:251:PHE:HD1	1:B:278:ILE:HB	1.80	0.46
1:A:233:GLU:HG3	1:A:237:ARG:NH1	2.31	0.46
1:A:251:PHE:HD1	1:A:278:ILE:HB	1.80	0.46
1:C:243:VAL:HG11	1:C:271:GLU:CD	2.36	0.46
1:A:469:ALA:O	1:A:473:VAL:HG13	2.15	0.46
1:C:178:VAL:HG12	1:C:195:VAL:HG21	1.97	0.46
1:A:65:SER:HA	1:A:70:ARG:HG2	1.97	0.46
1:B:331:GLY:CA	1:B:453:ARG:HG3	2.46	0.46
1:C:355:THR:HA	1:C:391:ILE:HD13	1.98	0.46
1:B:282:GLU:HG2	1:B:303:ALA:HB3	1.97	0.46
1:B:123:ASP:HA	1:B:251:PHE:HB2	1.97	0.46
1:B:331:GLY:HA2	1:B:453:ARG:HG3	1.97	0.46
1:A:160:THR:HG22	5:A:805:HOH:O	2.16	0.45
1:C:536:ARG:HB3	1:C:538:LEU:HD21	1.97	0.45
1:D:513:LEU:HD23	1:D:513:LEU:HA	1.77	0.45
1:A:25:GLN:HA	1:A:47:SER:HG	1.79	0.45
1:B:409:ARG:NH1	1:C:428:GLU:OE2	2.49	0.45
1:C:350:PRO:HG3	1:C:387:MET:HG2	1.97	0.45
1:D:455:ARG:NH1	1:D:477:ARG:HB3	2.31	0.45
1:A:127:PRO:HG2	1:A:254:PHE:HD2	1.80	0.45
1:D:228:LEU:HB3	1:D:229:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:HB3	1:B:209:ASN:HB2	1.99	0.45
1:A:123:ASP:OD1	1:A:280:LYS:NZ	2.46	0.45
1:A:201:GLU:CD	1:A:201:GLU:H	2.21	0.45
1:D:53:ARG:HD3	1:D:389:HIS:HA	1.99	0.45
1:C:302:VAL:HG12	1:C:304:ARG:HG2	1.99	0.45
1:C:70:ARG:HG2	1:C:70:ARG:NH1	2.32	0.44
1:A:410:ARG:NH1	1:D:402:ARG:NE	2.65	0.44
1:B:58:ILE:HB	1:B:370:MET:HG3	2.00	0.44
1:B:195:VAL:HA	1:B:205:THR:HG22	1.98	0.44
1:B:421:VAL:CG2	1:C:433:CYS:HB3	2.47	0.44
1:A:409:ARG:HD2	1:D:428:GLU:OE1	2.18	0.44
1:C:66:ARG:HH22	1:C:96:GLU:CG	2.22	0.44
1:D:98:ILE:HG23	1:D:120:ILE:HD13	2.00	0.44
1:A:329:LEU:CD1	1:A:411:ALA:HB1	2.48	0.44
1:C:231:LEU:CD2	1:C:264:VAL:HG22	2.47	0.44
1:D:185:TYR:CZ	1:D:222:PRO:HG3	2.53	0.43
1:A:331:GLY:HA3	1:A:453:ARG:HD2	2.00	0.43
1:B:453:ARG:O	1:B:453:ARG:HG2	2.17	0.43
1:D:183:ARG:HD2	1:D:194:VAL:HG22	1.99	0.43
1:A:253:SER:HA	1:A:280:LYS:HD3	1.99	0.43
1:B:282:GLU:O	1:B:310:GLU:HG3	2.18	0.43
1:B:421:VAL:HG21	1:C:433:CYS:HB3	2.00	0.43
1:B:489:GLU:CD	1:B:498:ARG:HE	2.22	0.43
1:C:158:PHE:HA	1:C:161:ARG:HG3	2.01	0.43
1:C:426:ALA:HB2	1:C:535:MET:HG3	2.00	0.43
1:D:174:ILE:HD11	1:D:184:ILE:HD11	2.00	0.43
1:C:182:GLY:O	1:C:195:VAL:HG23	2.18	0.43
1:B:70:ARG:HA	1:B:73:GLU:OE1	2.19	0.43
1:C:163:ASN:CG	1:C:164:ALA:N	2.72	0.43
1:C:473:VAL:HB	1:C:479:VAL:HG11	2.01	0.43
1:A:174:ILE:HG13	1:A:221:LEU:HD11	2.01	0.43
1:B:335:VAL:HG22	1:B:368:CYS:HB2	2.01	0.43
1:C:386:LYS:HD2	1:C:386:LYS:HA	1.66	0.43
1:C:154:VAL:HG11	1:C:172:PRO:HA	2.00	0.42
1:C:154:VAL:HG12	1:C:169:VAL:HG23	2.00	0.42
1:B:450:LEU:HD23	1:B:450:LEU:HA	1.84	0.42
1:B:433:CYS:HB2	1:B:518:LEU:HD12	2.00	0.42
1:A:183:ARG:HD3	1:A:185:TYR:CZ	2.54	0.42
1:B:333:PRO:HB3	1:B:475:LEU:O	2.19	0.42
1:D:169:VAL:HG11	1:D:174:ILE:HG21	2.01	0.42
1:D:459:ALA:HB1	1:D:480:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLN:CG	1:B:161:ARG:HA	2.45	0.42
1:B:171:TYR:CE2	1:B:227:ASP:OD2	2.73	0.42
1:B:185:TYR:CD1	1:B:189:GLY:HA2	2.54	0.42
1:B:362:VAL:O	1:B:477:ARG:NH1	2.51	0.42
1:C:438:ILE:HA	1:C:520:ILE:O	2.20	0.42
1:D:195:VAL:HG13	1:D:203:LEU:HB3	2.02	0.42
1:B:469:ALA:O	1:B:473:VAL:HG13	2.19	0.42
1:B:341:LEU:HD11	1:B:358:VAL:HG21	2.01	0.42
1:B:200:PRO:HD2	1:B:201:GLU:OE2	2.20	0.42
1:C:153:THR:HG22	1:C:155:ASP:H	1.84	0.41
1:D:171:TYR:O	1:D:174:ILE:HG22	2.20	0.41
1:D:488:PRO:HA	1:D:495:ASP:OD1	2.20	0.41
1:C:453:ARG:HD2	1:C:454:TYR:CZ	2.55	0.41
1:B:66:ARG:NH2	1:B:93:TYR:O	2.43	0.41
1:B:24:GLN:NE2	1:B:25:GLN:H	2.19	0.41
1:C:260:ASP:O	1:C:264:VAL:HG23	2.20	0.41
1:C:345:ILE:HG22	1:C:346:THR:HG23	2.02	0.41
1:D:355:THR:HG23	1:D:391:ILE:HG12	2.02	0.41
1:D:489:GLU:HG3	1:D:498:ARG:HD3	2.02	0.41
1:A:288:LYS:HD2	1:A:288:LYS:HA	1.80	0.41
1:D:192:SER:HB3	1:D:209:ASN:HB2	2.02	0.41
1:B:216:ARG:HD2	1:B:216:ARG:HA	1.83	0.41
1:B:230:GLY:HA2	1:B:256:ARG:NH1	2.35	0.41
1:B:65:SER:HB2	1:B:74:MET:SD	2.60	0.41
1:A:225:GLN:HA	5:A:891:HOH:O	2.19	0.40
1:B:101:VAL:O	1:B:105:VAL:HG23	2.21	0.40
1:B:307:LEU:O	1:B:311:ILE:HG12	2.22	0.40
1:B:25:GLN:HB3	1:B:48:GLU:O	2.22	0.40
1:B:127:PRO:HB2	1:B:228:LEU:HD13	2.03	0.40
1:B:344:MET:HA	1:B:347:LYS:O	2.22	0.40
1:C:144:LEU:HD23	1:C:150:VAL:HG21	2.03	0.40
1:B:240:ARG:HD2	1:B:244:GLU:OE2	2.21	0.40
1:B:514:ARG:HH21	1:B:514:ARG:HG3	1.85	0.40
1:C:400:TYR:OH	1:C:402:ARG:NE	2.55	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	510/543 (94%)	500 (98%)	9 (2%)	1 (0%)	47	49
1	B	515/543 (95%)	503 (98%)	11 (2%)	1 (0%)	47	49
1	C	505/543 (93%)	494 (98%)	10 (2%)	1 (0%)	47	49
1	D	515/543 (95%)	504 (98%)	10 (2%)	1 (0%)	47	49
All	All	2045/2172 (94%)	2001 (98%)	40 (2%)	4 (0%)	47	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	338	THR
1	A	338	THR
1	B	338	THR
1	C	338	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	413/433 (95%)	405 (98%)	8 (2%)	57	63
1	B	413/433 (95%)	400 (97%)	13 (3%)	40	43
1	C	410/433 (95%)	396 (97%)	14 (3%)	37	39
1	D	414/433 (96%)	406 (98%)	8 (2%)	57	63
All	All	1650/1732 (95%)	1607 (97%)	43 (3%)	46	50

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	231	LEU
1	A	256	ARG
1	A	257	LYS
1	A	259	SER
1	A	402	ARG
1	A	498	ARG
1	A	529	SER
1	B	70	ARG
1	B	116	ARG
1	B	197	LYS
1	B	206	GLN
1	B	225	GLN
1	B	237	ARG
1	B	240	ARG
1	B	256	ARG
1	B	259	SER
1	B	356	SER
1	B	377	LYS
1	B	498	ARG
1	B	535	MET
1	C	28	LEU
1	C	54	SER
1	C	67	SER
1	C	149	GLN
1	C	159	ARG
1	C	161	ARG
1	C	165	ASN
1	C	176	ARG
1	C	192	SER
1	C	329	LEU
1	C	420	GLU
1	C	434	CYS
1	C	453	ARG
1	C	498	ARG
1	D	36	PHE
1	D	149	GLN
1	D	158	PHE
1	D	183	ARG
1	D	197	LYS
1	D	231	LEU
1	D	302	VAL

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Mol	Chain	Res	Type
1	D	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	GLN
1	B	135	GLN
1	C	449	GLN
1	D	135	GLN
1	D	165	ASN
1	D	501	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FBP	C	602	-	18,20,20	0.48	0	23,32,32	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	WV2	D	603	-	36,36,36	0.49	0	52,52,52	0.75	3 (5%)
3	FBP	D	602	-	18,20,20	0.48	0	23,32,32	0.62	0
3	FBP	A	602	-	18,20,20	0.46	0	23,32,32	0.65	0
4	WV2	B	603	-	36,36,36	0.46	0	52,52,52	0.85	2 (3%)
3	FBP	B	602	-	18,20,20	0.52	0	23,32,32	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FBP	C	602	-	-	2/13/32/32	0/1/1/1
4	WV2	D	603	-	-	6/23/35/35	0/5/5/5
3	FBP	D	602	-	-	2/13/32/32	0/1/1/1
3	FBP	A	602	-	-	3/13/32/32	0/1/1/1
4	WV2	B	603	-	-	5/23/35/35	1/5/5/5
3	FBP	B	602	-	-	3/13/32/32	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	WV2	C-C5-N	-3.15	118.34	119.55
4	D	603	WV2	C9-N1-S	2.81	132.01	123.24
4	B	603	WV2	C-S-N1	-2.61	103.02	107.35
4	D	603	WV2	C-S-N1	-2.50	103.20	107.35
4	D	603	WV2	C-C5-N	2.20	120.39	119.55

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	FBP	C4-C5-C6-O6
4	D	603	WV2	C9-N1-S-O
3	A	602	FBP	C4-C5-C6-O6
3	B	602	FBP	C4-C5-C6-O6
3	D	602	FBP	C4-C5-C6-O6
4	D	603	WV2	C9-N1-S-O2

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Mol	Chain	Res	Type	Atoms
3	C	602	FBP	O5-C5-C6-O6
4	D	603	WV2	C9-N1-S-C
4	B	603	WV2	N3-C16-C17-C19
4	B	603	WV2	N3-C16-C17-C18
4	D	603	WV2	N3-C16-C17-C19
4	B	603	WV2	C17-C16-N3-C20
4	D	603	WV2	C17-C16-N3-C20
3	D	602	FBP	O5-C5-C6-O6
3	A	602	FBP	O5-C5-C6-O6
4	D	603	WV2	C17-C16-N3-C15
3	A	602	FBP	O1-C1-C2-O5
3	B	602	FBP	O1-C1-C2-O5
3	B	602	FBP	O5-C5-C6-O6
4	B	603	WV2	C17-C16-N3-C15
4	B	603	WV2	C9-N1-S-O

All (1) ring outliers are listed below:

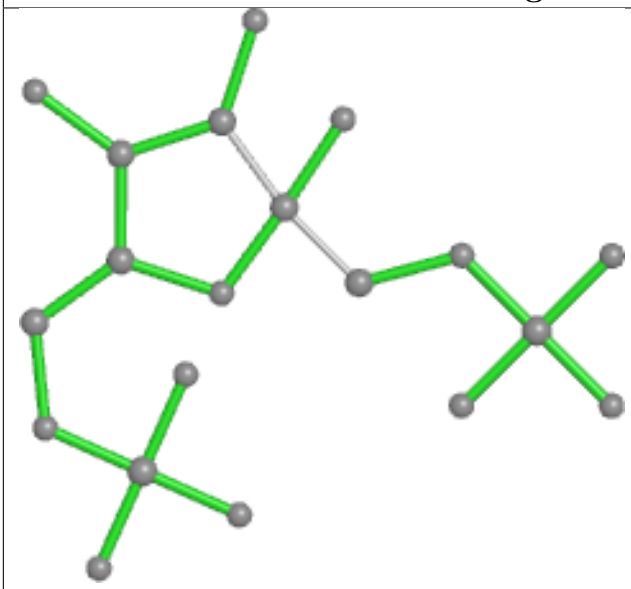
Mol	Chain	Res	Type	Atoms
4	B	603	WV2	C14-C15-C20-C21-N2-N3

1 monomer is involved in 2 short contacts:

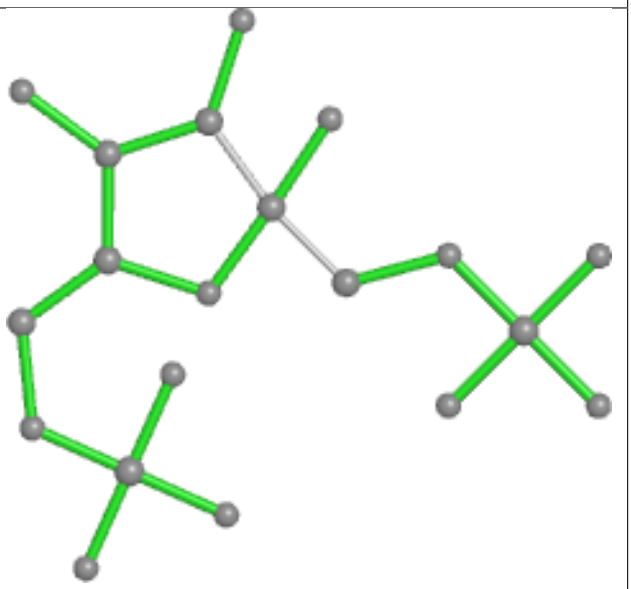
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	WV2	2	0

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.

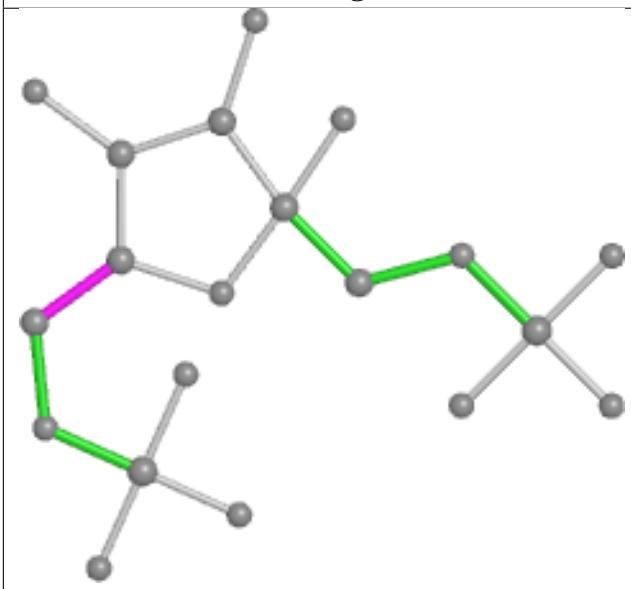
Ligand FBP C 602



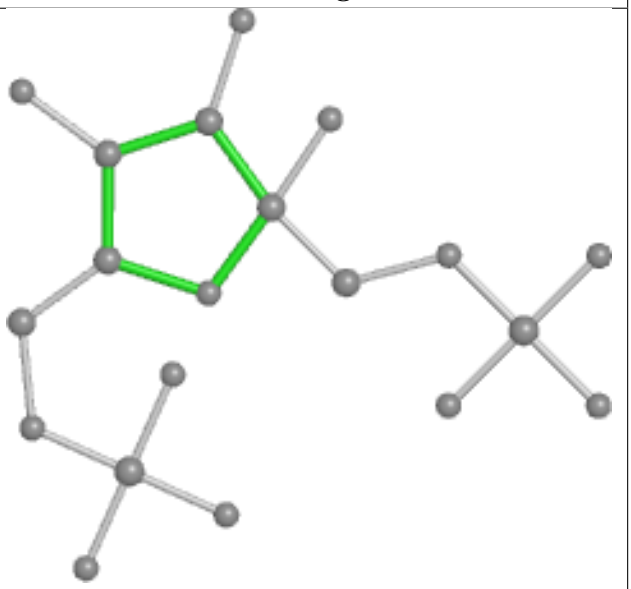
Bond lengths



Bond angles

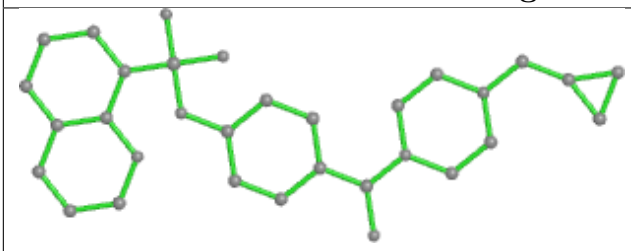


Torsions

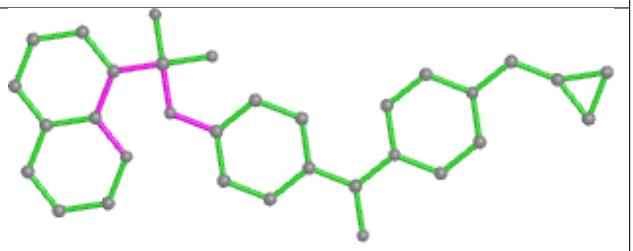


Rings

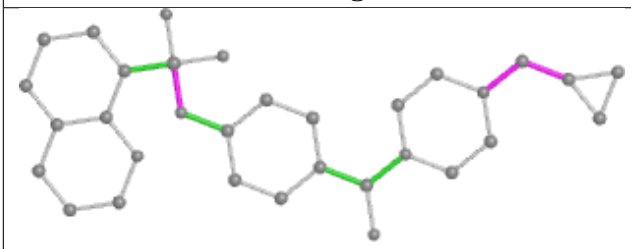
Ligand WV2 D 603



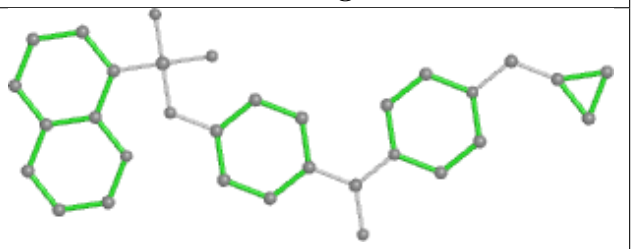
Bond lengths



Bond angles

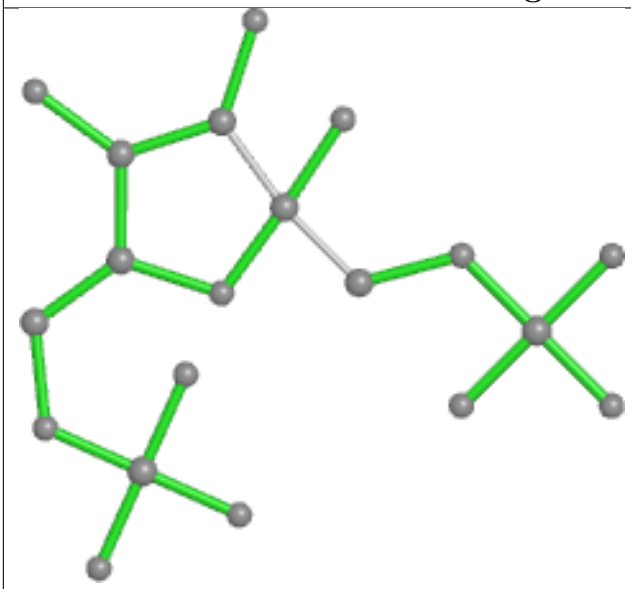


Torsions

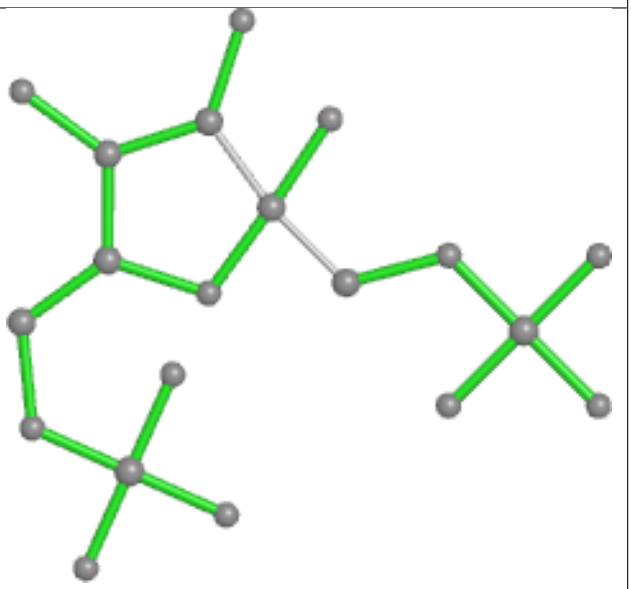


Rings

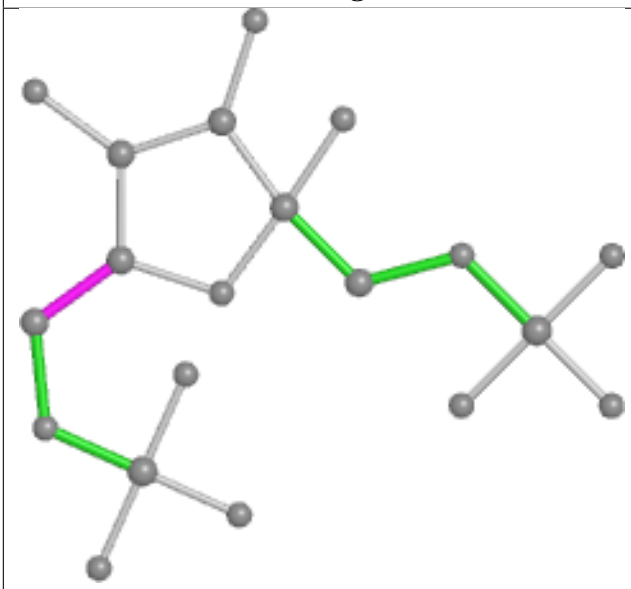
Ligand FBP D 602



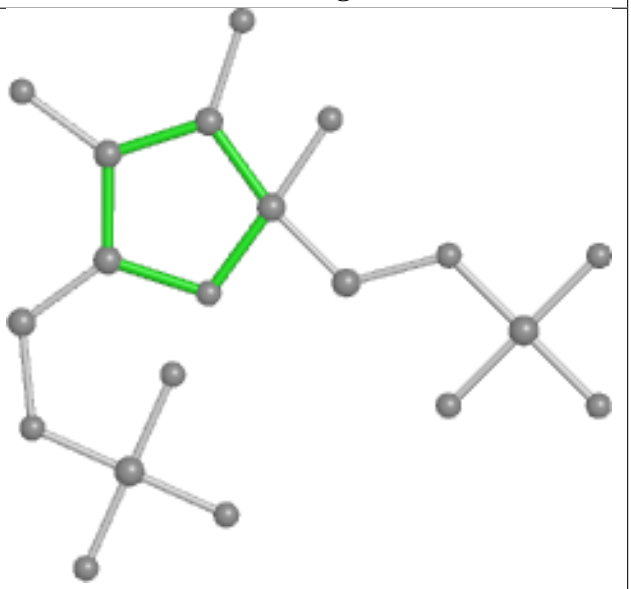
Bond lengths



Bond angles

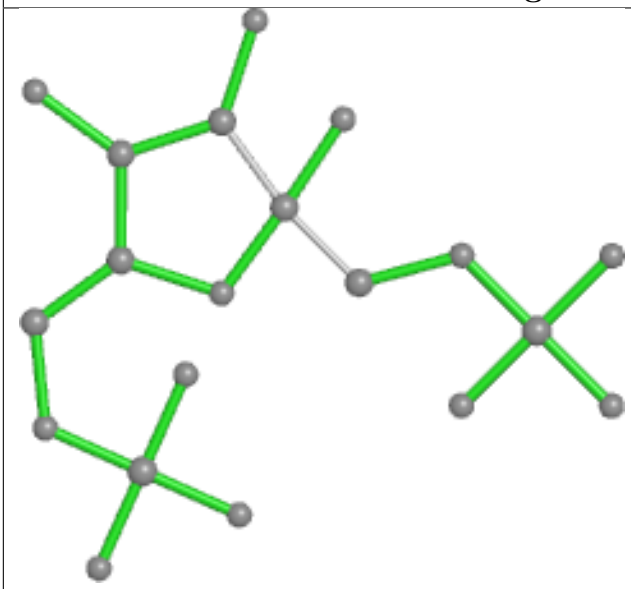


Torsions

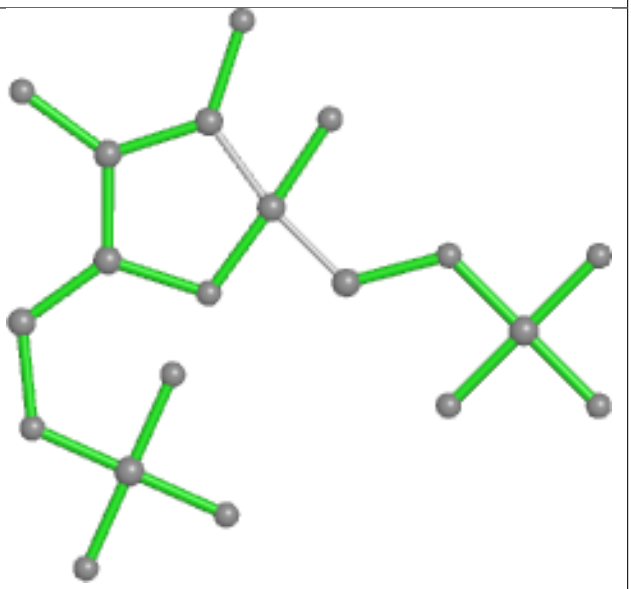


Rings

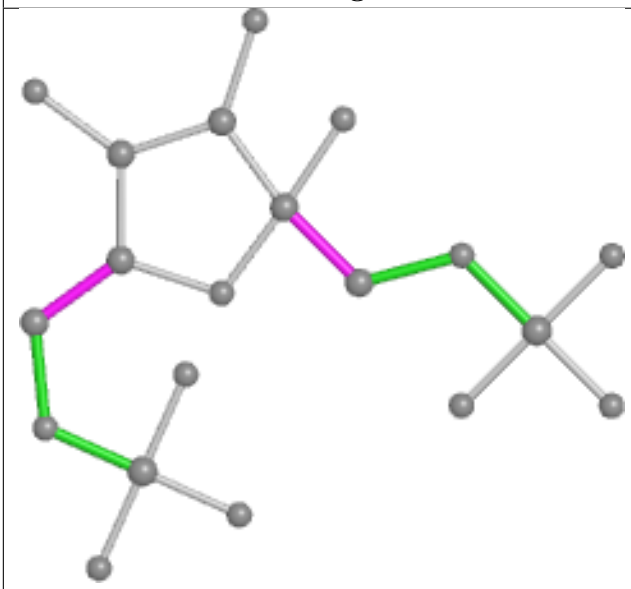
Ligand FBP A 602



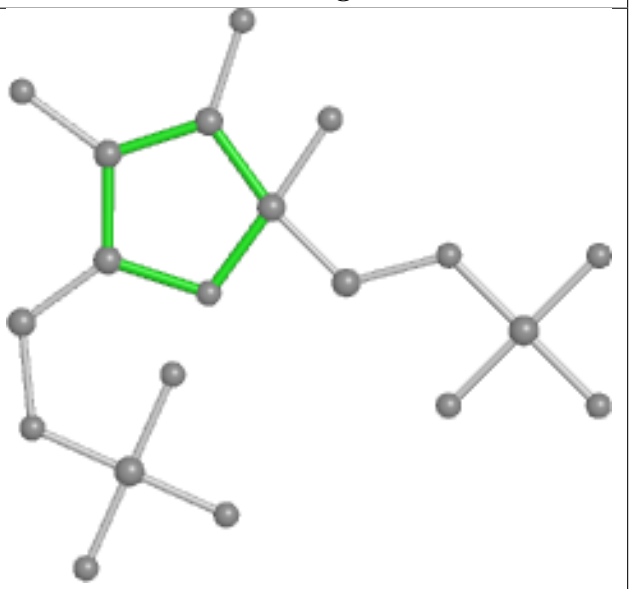
Bond lengths



Bond angles

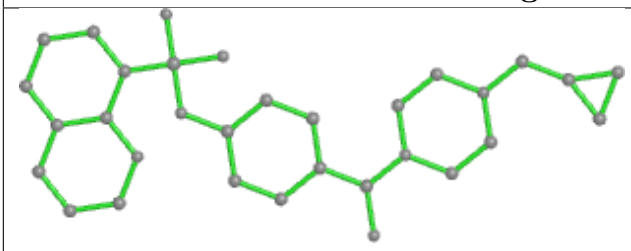


Torsions

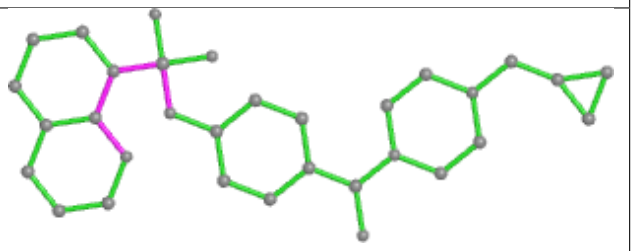


Rings

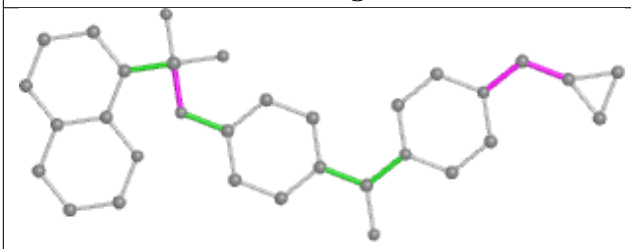
Ligand WV2 B 603



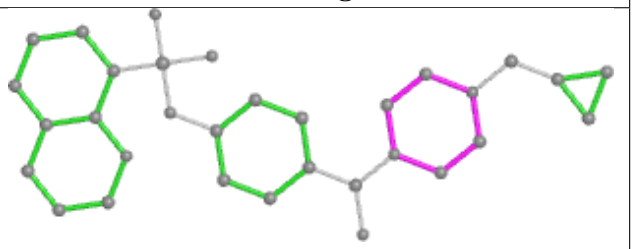
Bond lengths



Bond angles

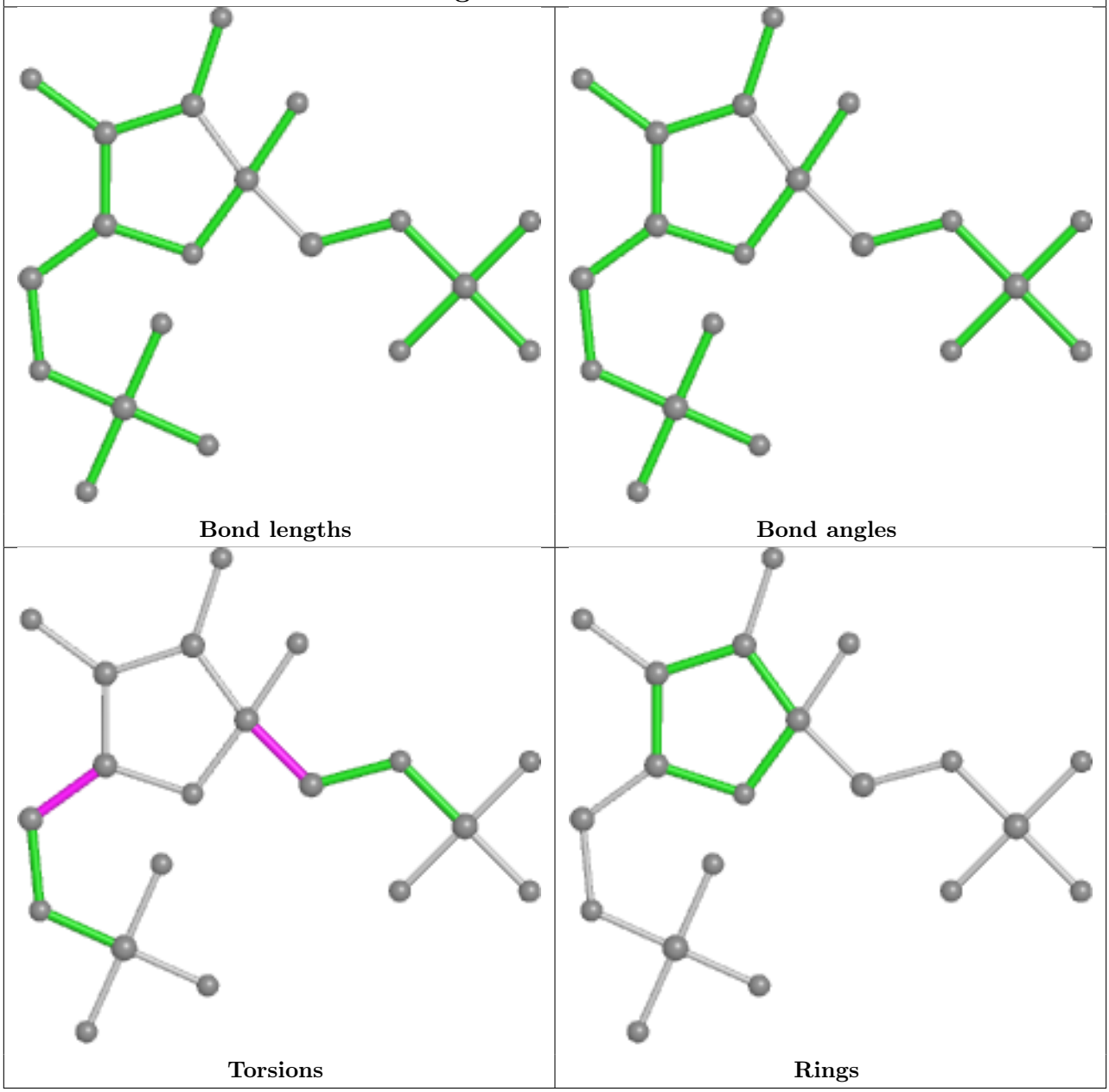


Torsions



Rings

Ligand FBP B 602



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, 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	514/543 (94%)	0.19	12 (2%)	60	65	12, 25, 42, 70	0
1	B	517/543 (95%)	0.39	19 (3%)	41	48	11, 27, 56, 65	0
1	C	511/543 (94%)	0.53	40 (7%)	13	17	20, 35, 62, 78	0
1	D	517/543 (95%)	0.33	20 (3%)	39	45	12, 24, 52, 66	0
All	All	2059/2172 (94%)	0.36	91 (4%)	34	40	11, 28, 56, 78	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	PRO	5.7
1	C	199	GLY	5.0
1	C	151	LEU	5.0
1	C	204	VAL	5.0
1	A	138	PRO	4.8
1	C	147	GLY	4.6
1	C	207	VAL	4.2
1	B	198	ILE	4.1
1	D	195	VAL	4.1
1	B	160	THR	4.0
1	D	181	GLY	4.0
1	D	145	VAL	3.9
1	D	139	GLU	3.8
1	C	144	LEU	3.8
1	C	160	THR	3.7
1	C	165	ASN	3.5
1	A	164	ALA	3.4
1	C	194	VAL	3.3
1	C	178	VAL	3.3
1	A	142	VAL	3.2
1	D	199	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	161	ARG	3.2
1	D	142	VAL	3.2
1	A	24	GLN	3.2
1	A	512	PHE	3.2
1	C	182	GLY	3.1
1	C	512	PHE	3.1
1	A	50	VAL	3.1
1	C	175	VAL	3.0
1	B	145	VAL	2.9
1	C	166	THR	2.9
1	B	143	GLU	2.9
1	C	32	MET	2.9
1	D	158	PHE	2.8
1	B	135	GLN	2.8
1	C	434	CYS	2.8
1	D	157	ALA	2.8
1	C	174	ILE	2.8
1	C	150	VAL	2.7
1	D	198	ILE	2.7
1	B	158	PHE	2.7
1	C	162	GLY	2.7
1	B	156	PRO	2.6
1	C	180	VAL	2.6
1	D	512	PHE	2.6
1	C	185	TYR	2.6
1	A	134	LEU	2.6
1	B	240	ARG	2.6
1	B	138	PRO	2.6
1	A	149	GLN	2.6
1	D	200	PRO	2.5
1	C	161	ARG	2.5
1	D	138	PRO	2.5
1	B	179	PRO	2.5
1	B	147	GLY	2.5
1	D	180	VAL	2.5
1	C	159	ARG	2.4
1	C	219	VAL	2.4
1	C	329	LEU	2.4
1	C	148	SER	2.4
1	D	133	ILE	2.4
1	C	203	LEU	2.3
1	A	167	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	226	VAL	2.3
1	A	52	ALA	2.3
1	C	205	THR	2.3
1	C	197	LYS	2.3
1	C	198	ILE	2.3
1	D	509	LEU	2.3
1	D	207	VAL	2.3
1	D	160	THR	2.3
1	C	158	PHE	2.3
1	B	176	ARG	2.3
1	B	196	GLN	2.2
1	D	182	GLY	2.2
1	C	142	VAL	2.2
1	C	157	ALA	2.2
1	C	179	PRO	2.2
1	A	515	VAL	2.2
1	C	227	ASP	2.2
1	D	137	GLY	2.2
1	B	159	ARG	2.2
1	C	152	VAL	2.1
1	D	203	LEU	2.1
1	B	178	VAL	2.1
1	B	214	GLY	2.1
1	C	181	GLY	2.1
1	B	363	LEU	2.0
1	C	134	LEU	2.0
1	C	480	PHE	2.0
1	B	166	THR	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,

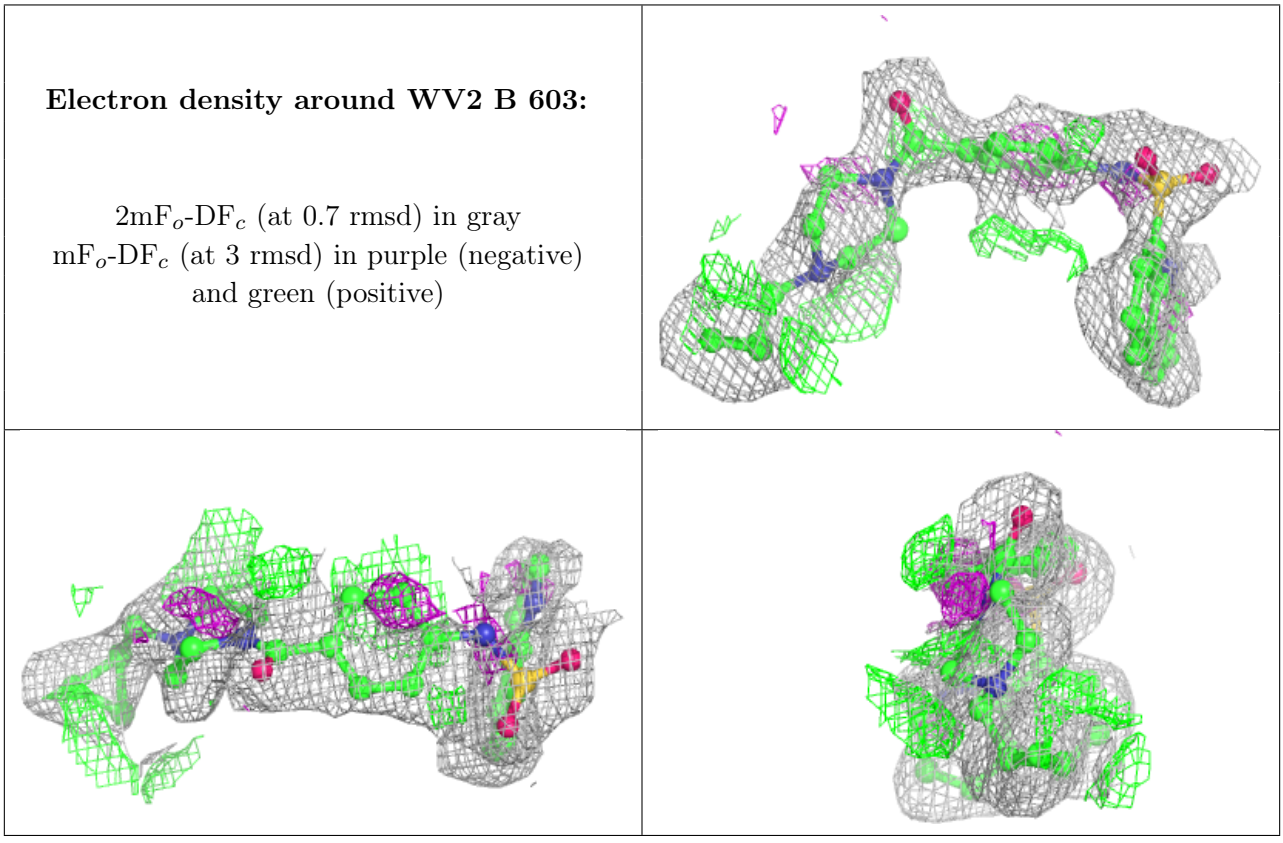
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	WV2	B	603	32/32	0.77	0.25	21,32,37,39	0
2	MG	A	601	1/1	0.80	0.13	36,36,36,36	0
2	MG	D	601	1/1	0.82	0.14	30,30,30,30	0
4	WV2	D	603	32/32	0.82	0.22	20,31,36,41	0
2	MG	C	601	1/1	0.88	0.13	41,41,41,41	0
2	MG	B	601	1/1	0.90	0.15	33,33,33,33	0
3	FBP	C	602	20/20	0.95	0.10	17,23,29,31	0
3	FBP	D	602	20/20	0.95	0.11	10,16,23,40	0
3	FBP	B	602	20/20	0.97	0.10	10,19,23,28	0
3	FBP	A	602	20/20	0.98	0.10	13,18,21,24	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.

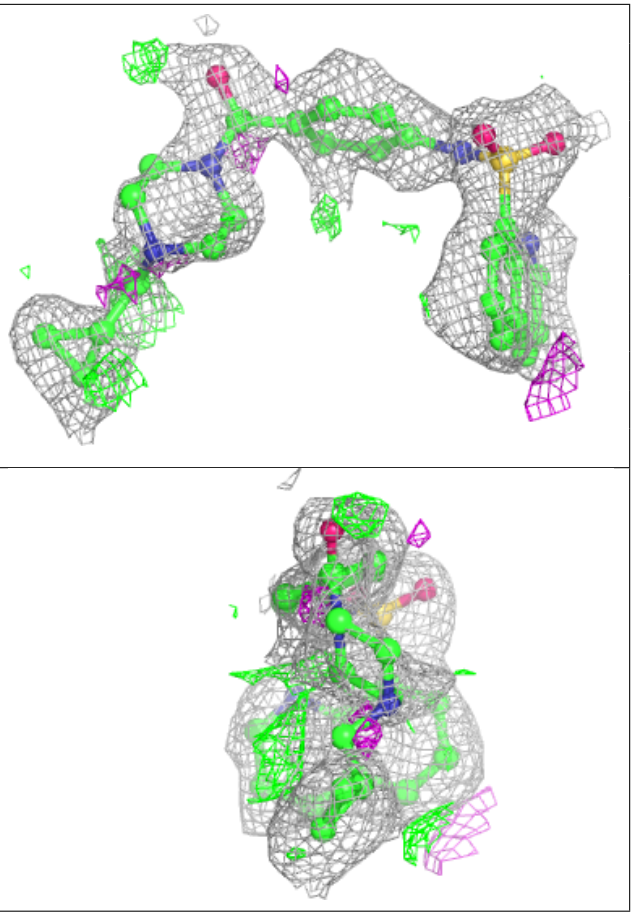
Electron density around WV2 B 603:

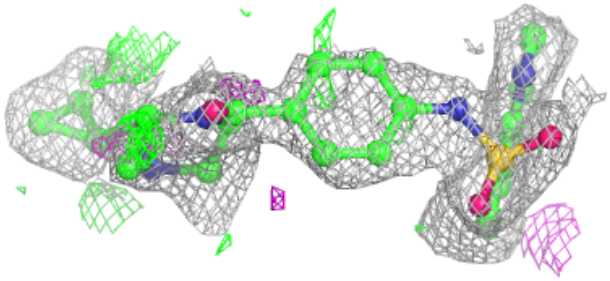
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around WV2 D 603:

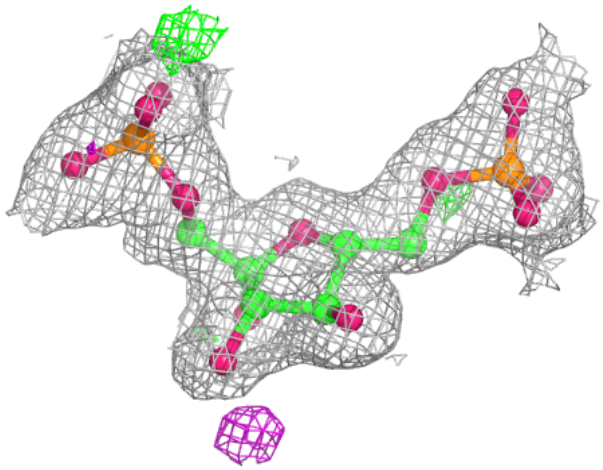
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

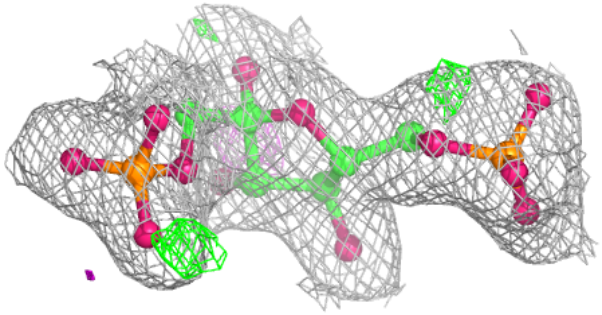


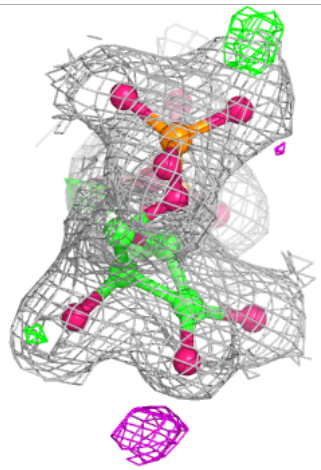


Electron density around FBP C 602:

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

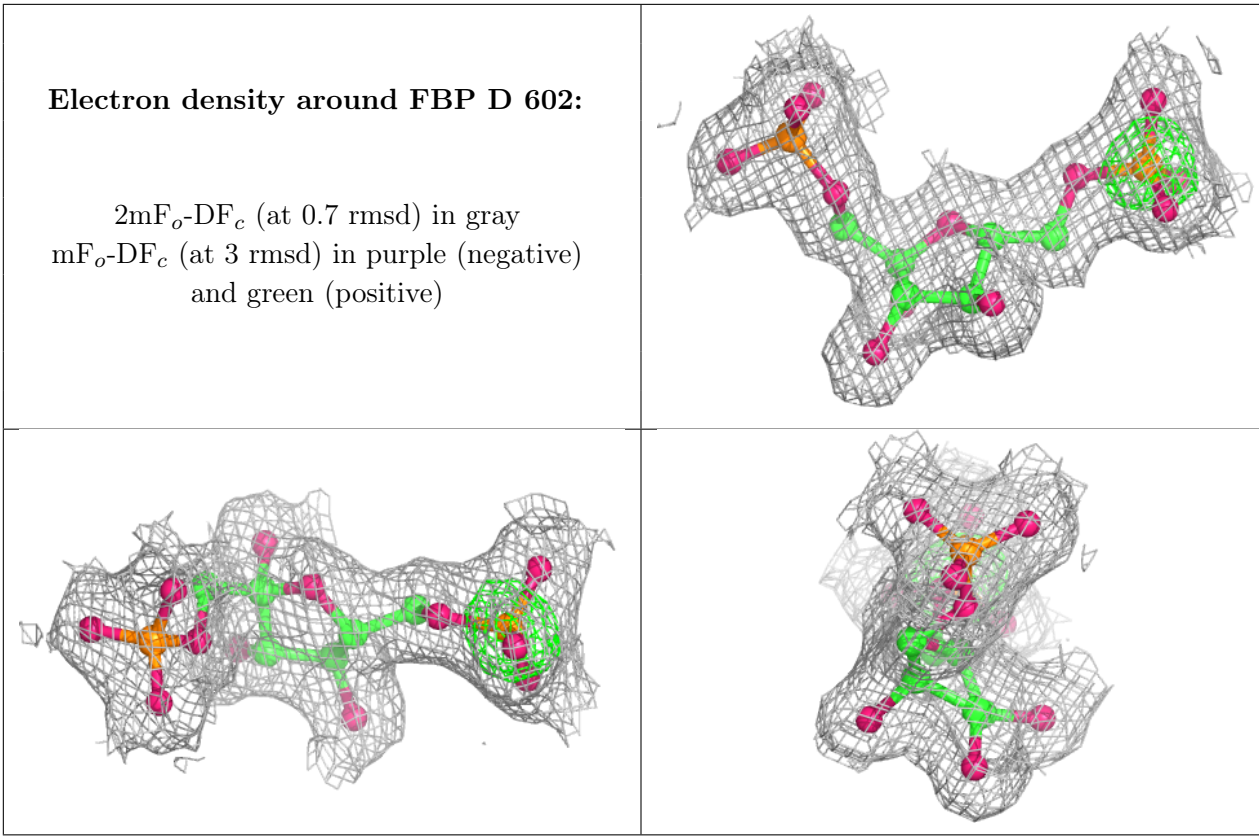






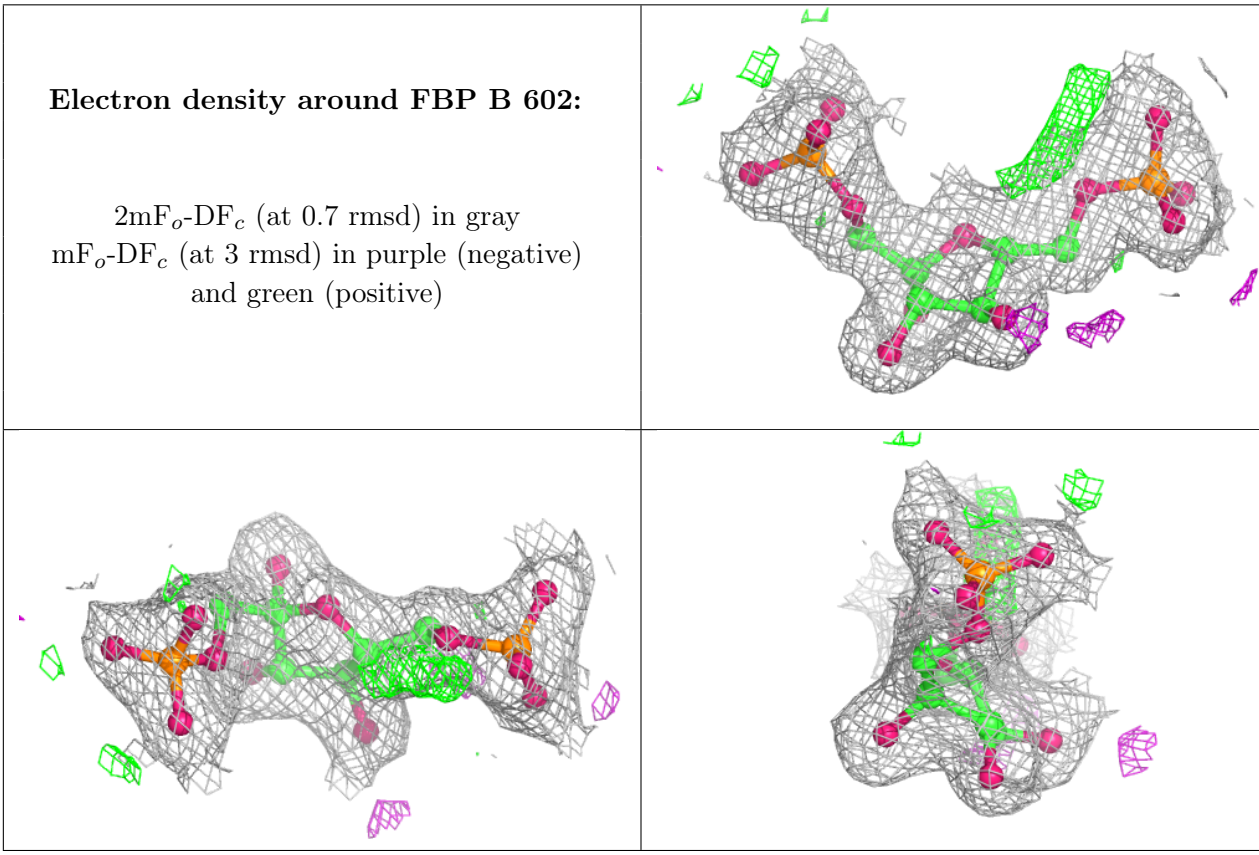
Electron density around FBP D 602:

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



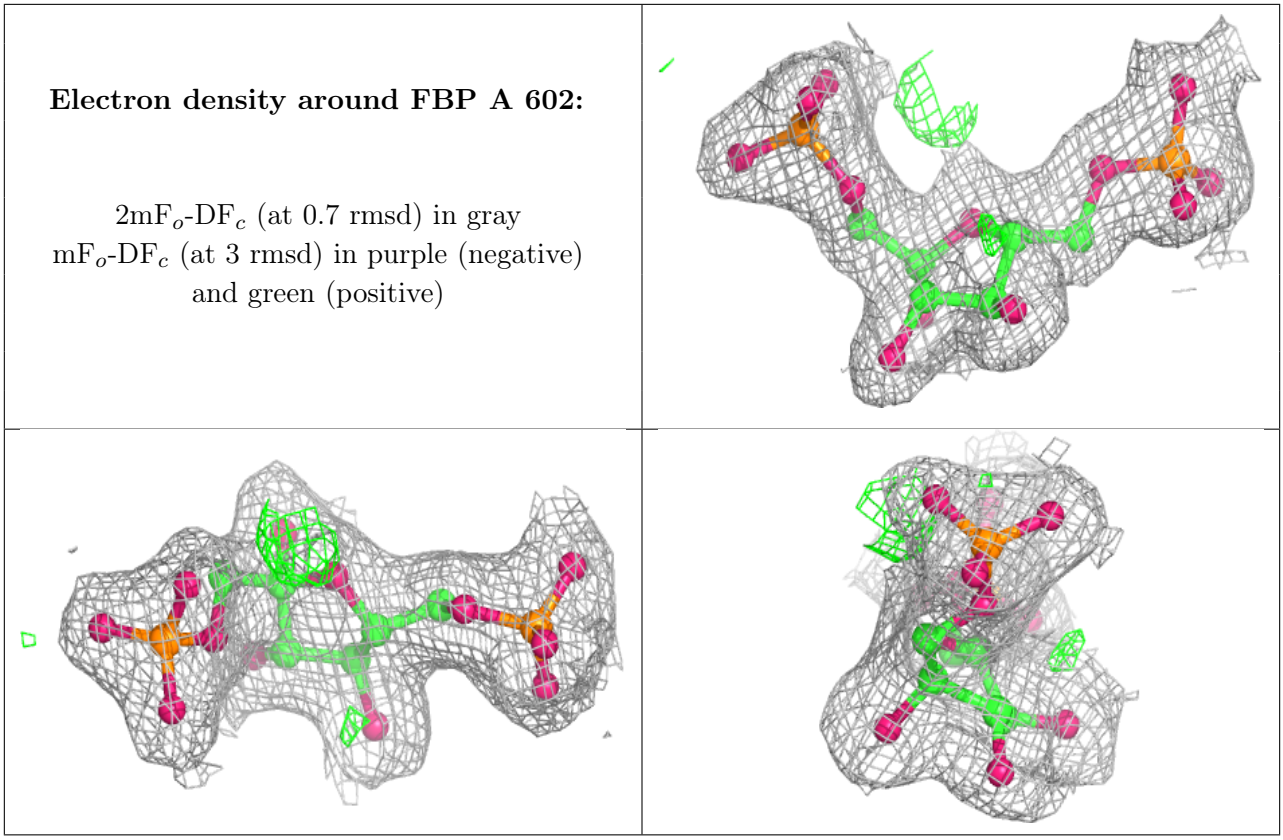
Electron density around FBP B 602:

$2mF_o$-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 602:

$2mF_o$-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.