Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:22 PM BST

PDB ID	:	6SU2
Title	:	Trypanosoma congolense pyruvate kinase in complex with citrate and glycerol
Authors	:	Sterckx, Y.G.-J.; Pinto Torres, J.E.
Deposited on	:	2019-09-12
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

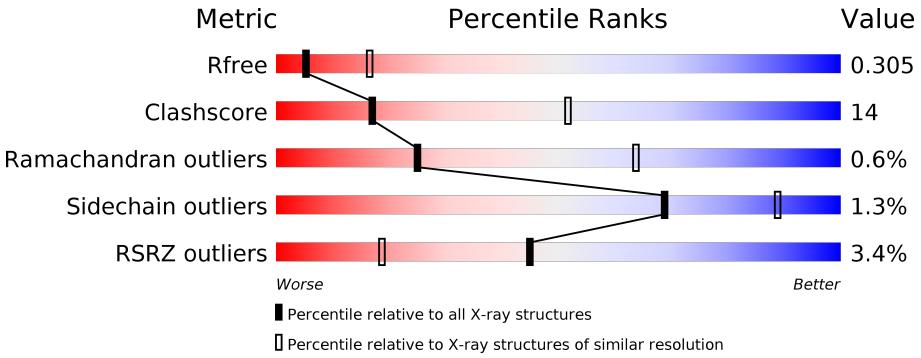
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	514	2% 80% 17%
1	B	514	3% 75% 18% 6%
1	C	514	5% 78% 18%
1	D	514	3% 79% 18%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FBP	A	601	-	-	X	-
2	FBP	B	601	-	-	X	-
2	FBP	C	601	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14203 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	498	Total	C	N	O	S	0	0	0
			3597	2233	642	696	26			
1	B	481	Total	C	N	O	S	0	0	0
			3381	2094	601	661	25			
1	C	497	Total	C	N	O	S	0	0	0
			3517	2178	626	688	25			
1	D	498	Total	C	N	O	S	0	0	0
			3575	2219	635	695	26			

There are 60 discrepancies between the modelled and reference sequences:

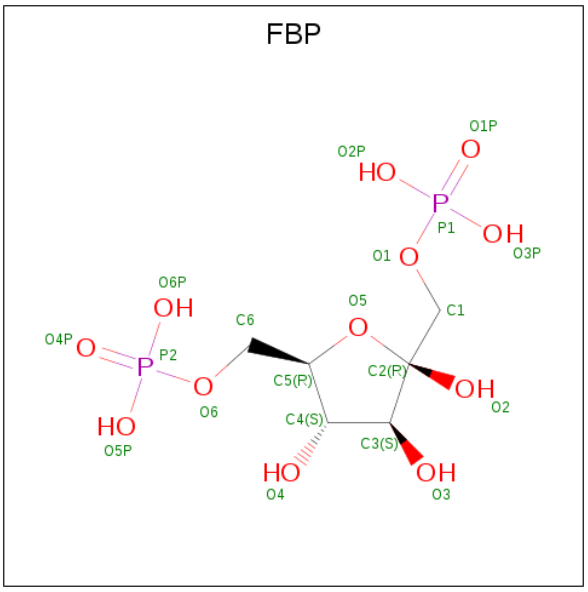
Chain	Residue	Modelled	Actual	Comment	Reference
A	500	GLU	-	expression tag	UNP G0UYF4
A	501	ASN	-	expression tag	UNP G0UYF4
A	502	LEU	-	expression tag	UNP G0UYF4
A	503	TYR	-	expression tag	UNP G0UYF4
A	504	PHE	-	expression tag	UNP G0UYF4
A	505	GLN	-	expression tag	UNP G0UYF4
A	506	SER	-	expression tag	UNP G0UYF4
A	507	GLY	-	expression tag	UNP G0UYF4
A	508	GLY	-	expression tag	UNP G0UYF4
A	509	HIS	-	expression tag	UNP G0UYF4
A	510	HIS	-	expression tag	UNP G0UYF4
A	511	HIS	-	expression tag	UNP G0UYF4
A	512	HIS	-	expression tag	UNP G0UYF4
A	513	HIS	-	expression tag	UNP G0UYF4
A	514	HIS	-	expression tag	UNP G0UYF4
B	500	GLU	-	expression tag	UNP G0UYF4
B	501	ASN	-	expression tag	UNP G0UYF4
B	502	LEU	-	expression tag	UNP G0UYF4
B	503	TYR	-	expression tag	UNP G0UYF4
B	504	PHE	-	expression tag	UNP G0UYF4
B	505	GLN	-	expression tag	UNP G0UYF4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	SER	-	expression tag	UNP G0UYF4
B	507	GLY	-	expression tag	UNP G0UYF4
B	508	GLY	-	expression tag	UNP G0UYF4
B	509	HIS	-	expression tag	UNP G0UYF4
B	510	HIS	-	expression tag	UNP G0UYF4
B	511	HIS	-	expression tag	UNP G0UYF4
B	512	HIS	-	expression tag	UNP G0UYF4
B	513	HIS	-	expression tag	UNP G0UYF4
B	514	HIS	-	expression tag	UNP G0UYF4
C	500	GLU	-	expression tag	UNP G0UYF4
C	501	ASN	-	expression tag	UNP G0UYF4
C	502	LEU	-	expression tag	UNP G0UYF4
C	503	TYR	-	expression tag	UNP G0UYF4
C	504	PHE	-	expression tag	UNP G0UYF4
C	505	GLN	-	expression tag	UNP G0UYF4
C	506	SER	-	expression tag	UNP G0UYF4
C	507	GLY	-	expression tag	UNP G0UYF4
C	508	GLY	-	expression tag	UNP G0UYF4
C	509	HIS	-	expression tag	UNP G0UYF4
C	510	HIS	-	expression tag	UNP G0UYF4
C	511	HIS	-	expression tag	UNP G0UYF4
C	512	HIS	-	expression tag	UNP G0UYF4
C	513	HIS	-	expression tag	UNP G0UYF4
C	514	HIS	-	expression tag	UNP G0UYF4
D	500	GLU	-	expression tag	UNP G0UYF4
D	501	ASN	-	expression tag	UNP G0UYF4
D	502	LEU	-	expression tag	UNP G0UYF4
D	503	TYR	-	expression tag	UNP G0UYF4
D	504	PHE	-	expression tag	UNP G0UYF4
D	505	GLN	-	expression tag	UNP G0UYF4
D	506	SER	-	expression tag	UNP G0UYF4
D	507	GLY	-	expression tag	UNP G0UYF4
D	508	GLY	-	expression tag	UNP G0UYF4
D	509	HIS	-	expression tag	UNP G0UYF4
D	510	HIS	-	expression tag	UNP G0UYF4
D	511	HIS	-	expression tag	UNP G0UYF4
D	512	HIS	-	expression tag	UNP G0UYF4
D	513	HIS	-	expression tag	UNP G0UYF4
D	514	HIS	-	expression tag	UNP G0UYF4

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$) (labeled as "Ligand of Interest" by author).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0

Continued on next page...

Continued from previous page...

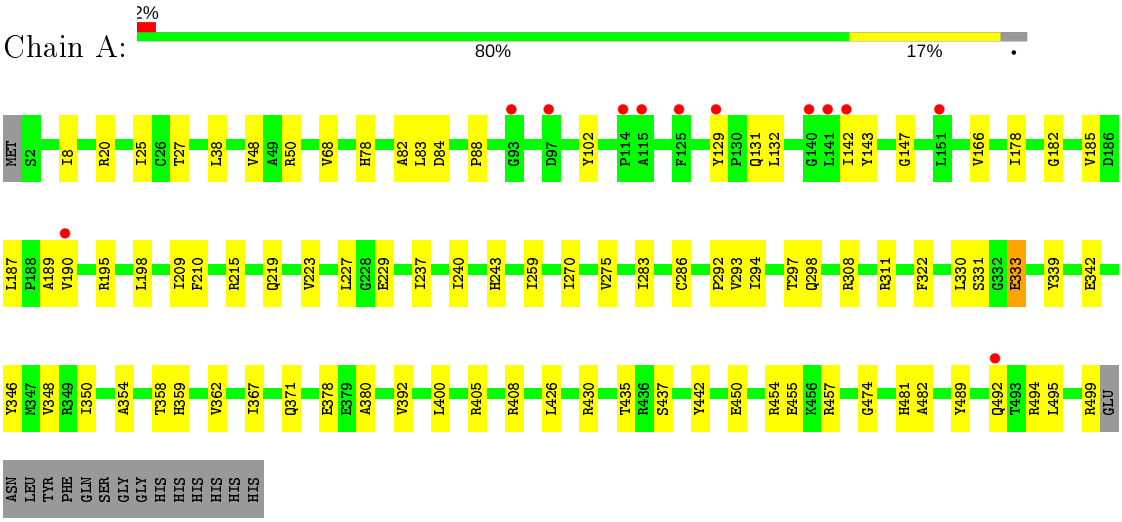
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	12	Total O 12 12	0	0
4	C	16	Total O 16 16	0	0
4	D	7	Total O 7 7	0	0

3 Residue-property plots (i)

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

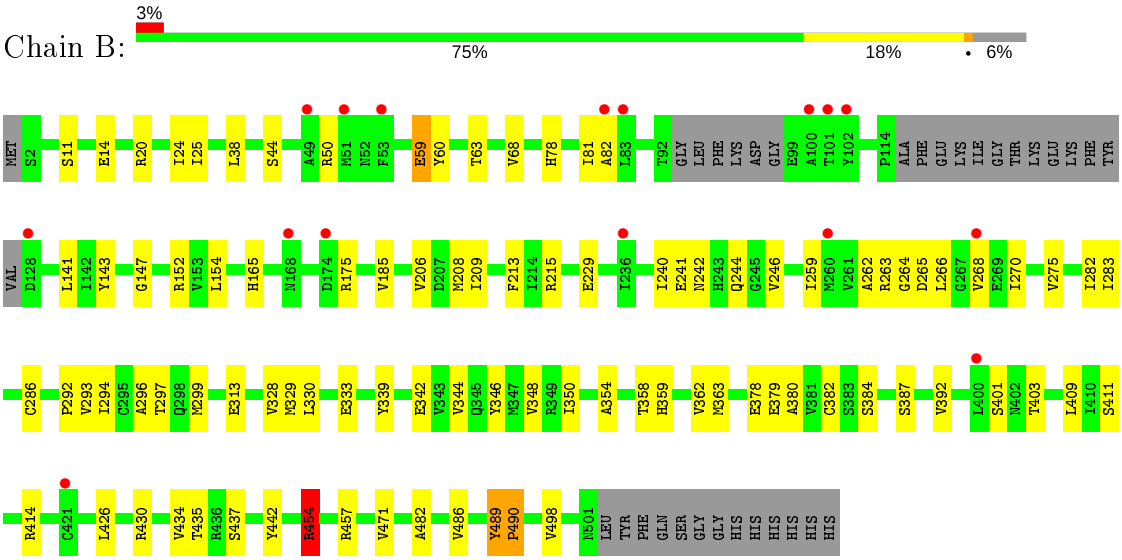
- Molecule 1: Pyruvate kinase

Chain A:



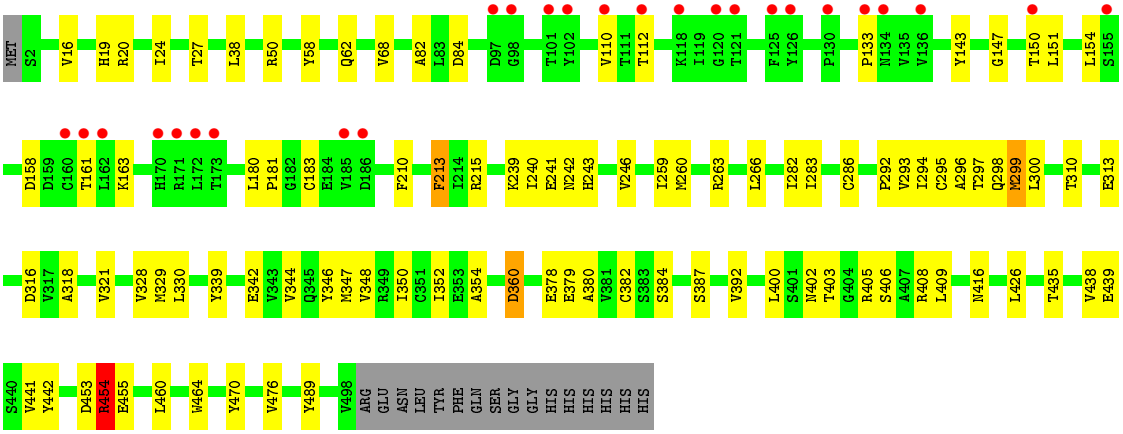
- Molecule 1: Pyruvate kinase

Chain B:

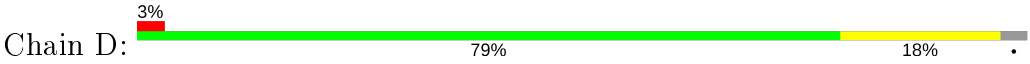


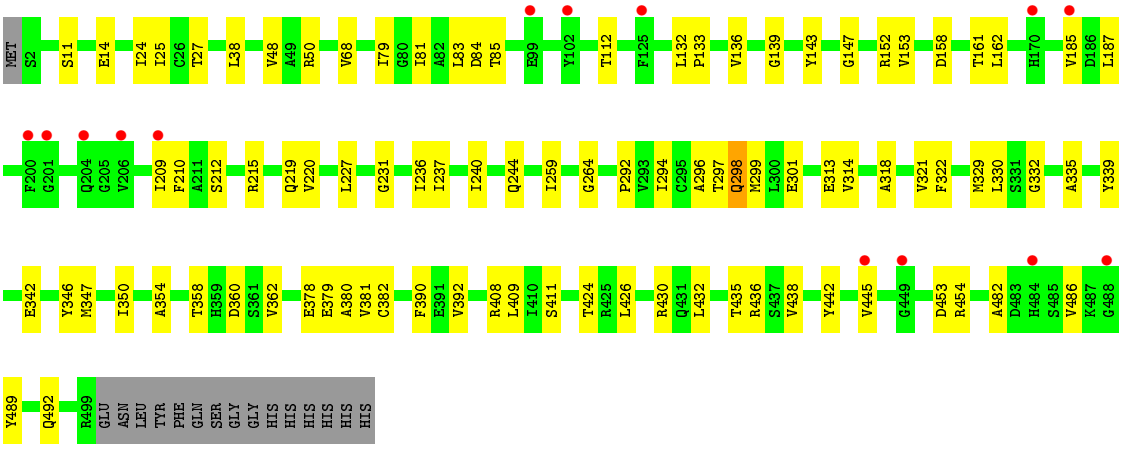
- Molecule 1: Pyruvate kinase

Chain C:



- Molecule 1: Pyruvate kinase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	112.77Å 182.46Å 244.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.74 – 3.00 49.05 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.74-3.00) 99.7 (49.05-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.250 , 0.284 0.273 , 0.305	Depositor DCC
R_{free} test set	2549 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	102.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 87.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14203	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: MG, 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	0.46	0/3653	0.73	0/4982
1	B	0.47	0/3429	0.72	0/4686
1	C	0.47	0/3570	0.71	0/4878
1	D	0.46	0/3630	0.72	0/4957
All	All	0.47	0/14282	0.72	0/19503

There are no bond length outliers.

There are no bond angle outliers.

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	3597	0	3390	88	0
1	B	3381	0	3124	96	0
1	C	3517	0	3261	118	0
1	D	3575	0	3372	87	0
2	A	20	0	10	12	0
2	B	20	0	10	8	0
2	C	20	0	10	7	0
2	D	20	0	10	1	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	0	0	0
4	B	12	0	0	0	0
4	C	16	0	0	0	0
4	D	7	0	0	0	0
All	All	14203	0	13187	383	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 14.

All (383) 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:D:50:ARG:HH21	1:D:84:ASP:CG	1.38	1.24
1:B:296:ALA:HB1	1:B:329:MET:CE	1.75	1.17
1:B:296:ALA:HB1	1:B:329:MET:HE3	1.18	1.15
1:A:454:ARG:HH11	2:A:601:FBP:C3	1.62	1.12
1:C:16:VAL:CG1	1:C:352:ILE:HG22	1.81	1.09
1:A:142:ILE:CG2	1:A:178:ILE:HD11	1.82	1.09
1:D:50:ARG:NH2	1:D:84:ASP:CG	2.07	1.08
1:B:242:ASN:OD1	1:B:244:GLN:HG2	1.54	1.06
1:D:11:SER:HB2	1:D:14:GLU:HG2	1.40	1.01
1:C:379:GLU:HG3	1:C:409:LEU:HD11	1.42	0.99
1:D:314:VAL:HG13	1:D:350:ILE:HD12	1.44	0.98
1:B:457:ARG:NH1	2:B:601:FBP:O1P	1.96	0.97
1:D:379:GLU:HG3	1:D:409:LEU:HD11	1.46	0.96
1:A:283:ILE:HG12	1:A:293:VAL:HG11	1.47	0.95
1:A:495:LEU:HD12	1:D:381:VAL:HG23	1.49	0.94
1:D:11:SER:CB	1:D:14:GLU:HG2	1.96	0.93
1:B:296:ALA:CB	1:B:329:MET:CE	2.46	0.93
1:C:263:ARG:HH12	1:C:299:MET:CE	1.82	0.92
1:A:142:ILE:HG21	1:A:178:ILE:HD11	1.50	0.92
1:C:283:ILE:HG12	1:C:293:VAL:HG11	1.50	0.90
1:B:283:ILE:HG12	1:B:293:VAL:HG11	1.50	0.90
1:A:454:ARG:NH1	2:A:601:FBP:C1	2.36	0.88
1:A:129:TYR:CE1	1:A:131:GLN:OE1	2.27	0.86
1:C:20:ARG:HB2	1:C:352:ILE:HD11	1.56	0.86
1:A:454:ARG:NH1	2:A:601:FBP:H11	1.89	0.86
1:B:379:GLU:HG3	1:B:409:LEU:HD11	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:VAL:HG21	1:D:354:ALA:HB3	1.57	0.85
1:A:454:ARG:HH11	2:A:601:FBP:H3	1.42	0.84
1:B:378:GLU:CG	1:B:489:TYR:CB	2.56	0.84
1:D:408:ARG:HG2	1:D:435:THR:HG21	1.58	0.84
1:C:321:VAL:HG21	1:C:354:ALA:HB3	1.56	0.84
1:C:392:VAL:HG12	1:C:476:VAL:HG11	1.57	0.84
1:C:408:ARG:HG2	1:C:435:THR:HG21	1.58	0.83
1:A:297:THR:HG22	1:A:298:GLN:HG3	1.58	0.83
1:B:401:SER:HB2	2:B:601:FBP:O4P	1.77	0.83
1:C:439:GLU:OE1	1:C:464:TRP:CH2	2.31	0.83
1:B:482:ALA:HB1	1:B:486:VAL:CG1	2.09	0.83
1:A:454:ARG:NH1	2:A:601:FBP:C3	2.42	0.82
1:A:408:ARG:HG2	1:A:435:THR:HG21	1.59	0.82
1:B:378:GLU:HG2	1:B:489:TYR:CB	2.09	0.82
1:C:379:GLU:HA	1:C:409:LEU:HD21	1.63	0.81
1:A:454:ARG:NH1	2:A:601:FBP:H3	1.96	0.80
1:B:296:ALA:HB2	1:B:329:MET:HG2	1.64	0.80
1:C:392:VAL:CG1	1:C:476:VAL:HG11	2.11	0.79
1:B:286:CYS:HB2	1:B:293:VAL:CG2	2.13	0.79
1:A:286:CYS:CB	1:A:293:VAL:CG2	2.60	0.79
1:A:190:VAL:HG12	1:A:195:ARG:HG3	1.65	0.78
1:C:180:LEU:HG	1:C:183:CYS:SG	2.23	0.78
1:C:16:VAL:CG1	1:C:352:ILE:CG2	2.60	0.78
1:C:263:ARG:HH12	1:C:299:MET:HE1	1.46	0.78
1:A:292:PRO:HG3	1:A:435:THR:HG22	1.66	0.77
1:B:262:ALA:O	1:B:266:LEU:HG	1.85	0.77
1:B:489:TYR:CB	1:B:490:PRO:CD	2.62	0.77
1:D:24:ILE:HG23	1:D:347:MET:CE	2.15	0.76
1:C:143:TYR:HB3	1:C:147:GLY:HA2	1.67	0.76
1:B:454:ARG:HH11	1:B:454:ARG:HG3	1.51	0.76
1:B:292:PRO:HG3	1:B:435:THR:HG22	1.68	0.76
1:B:296:ALA:CB	1:B:329:MET:HE2	2.15	0.75
1:C:297:THR:HG22	1:C:298:GLN:HG3	1.67	0.75
1:D:292:PRO:HG3	1:D:435:THR:HG22	1.68	0.75
1:B:379:GLU:HA	1:B:409:LEU:HD21	1.69	0.75
2:B:601:FBP:O2	2:B:601:FBP:O2P	2.05	0.75
1:D:379:GLU:HA	1:D:409:LEU:HD21	1.69	0.74
1:B:378:GLU:HG3	1:B:489:TYR:CB	2.17	0.74
1:C:400:LEU:O	2:C:601:FBP:H4	1.88	0.74
1:C:263:ARG:HH12	1:C:299:MET:HE3	1.53	0.73
1:B:296:ALA:CB	1:B:329:MET:CG	2.67	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ARG:NH1	1:C:299:MET:CE	2.52	0.73
1:D:11:SER:HB2	1:D:14:GLU:CG	2.15	0.73
1:C:292:PRO:HG3	1:C:435:THR:HG22	1.71	0.73
1:B:241:GLU:C	1:B:266:LEU:HD23	2.08	0.72
1:B:143:TYR:HB3	1:B:147:GLY:HA2	1.71	0.71
1:A:454:ARG:HH11	2:A:601:FBP:C1	2.02	0.71
1:B:380:ALA:CB	1:C:392:VAL:HG23	2.20	0.71
1:A:286:CYS:HB2	1:A:293:VAL:CG2	2.20	0.71
1:B:24:ILE:HG22	1:B:328:VAL:HG23	1.71	0.71
1:C:439:GLU:OE1	1:C:464:TRP:HH2	1.74	0.71
1:B:286:CYS:CB	1:B:293:VAL:CG2	2.68	0.71
1:B:380:ALA:CB	1:C:392:VAL:CG2	2.69	0.71
2:C:601:FBP:O2P	2:C:601:FBP:O2	2.05	0.71
1:D:143:TYR:HB3	1:D:147:GLY:HA2	1.72	0.71
1:C:16:VAL:HG11	1:C:352:ILE:HG22	1.71	0.70
1:D:158:ASP:HB2	1:D:161:THR:H	1.55	0.70
1:B:482:ALA:HB1	1:B:486:VAL:HG13	1.72	0.70
1:C:299:MET:SD	1:C:328:VAL:HG13	2.31	0.70
1:C:439:GLU:OE1	1:C:464:TRP:CZ3	2.43	0.70
1:C:286:CYS:SG	1:C:293:VAL:HG22	2.32	0.70
1:C:286:CYS:CB	1:C:293:VAL:CG2	2.69	0.70
1:A:454:ARG:CD	1:A:481:HIS:HB2	2.23	0.69
1:A:187:LEU:HB2	1:A:215:ARG:HH22	1.57	0.69
1:C:328:VAL:HG11	1:C:347:MET:HE2	1.73	0.69
1:C:405:ARG:HG2	2:C:601:FBP:O4P	1.93	0.69
1:A:454:ARG:NH1	1:A:482:ALA:HB3	2.07	0.68
1:C:150:THR:O	1:C:151:LEU:HD12	1.93	0.68
1:C:321:VAL:CG2	1:C:354:ALA:CB	2.71	0.68
1:D:264:GLY:HA2	1:D:297:THR:HG21	1.76	0.68
1:B:147:GLY:HA3	1:B:268:VAL:HG13	1.76	0.68
1:D:321:VAL:CG2	1:D:354:ALA:CB	2.70	0.68
1:C:16:VAL:HG12	1:C:352:ILE:CG2	2.24	0.68
1:C:318:ALA:O	1:C:321:VAL:HG22	1.94	0.67
1:A:25:ILE:HG12	1:A:48:VAL:HB	1.76	0.67
1:B:354:ALA:O	1:B:358:THR:HG23	1.94	0.67
1:C:242:ASN:OD1	1:C:243:HIS:N	2.28	0.66
1:B:296:ALA:CB	1:B:329:MET:HG2	2.25	0.66
1:C:16:VAL:HG12	1:C:352:ILE:HG22	1.76	0.66
1:C:310:THR:HG22	1:C:313:GLU:CD	2.15	0.66
1:C:263:ARG:NH1	1:C:299:MET:HE3	2.10	0.66
1:A:286:CYS:HB2	1:A:293:VAL:HG21	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ALA:O	1:D:321:VAL:HG22	1.94	0.66
1:A:454:ARG:HH11	2:A:601:FBP:C2	2.09	0.65
1:C:27:THR:HG22	1:C:50:ARG:HE	1.61	0.65
1:C:392:VAL:HG11	1:C:476:VAL:HG21	1.78	0.65
1:A:354:ALA:O	1:A:358:THR:HG23	1.97	0.65
1:A:454:ARG:HH12	2:A:601:FBP:H11	1.62	0.64
1:D:354:ALA:O	1:D:358:THR:HG23	1.98	0.64
1:C:263:ARG:NH1	1:C:299:MET:HE1	2.12	0.64
1:B:11:SER:OG	1:B:14:GLU:CB	2.45	0.63
1:A:190:VAL:HG12	1:A:195:ARG:CG	2.28	0.63
1:A:182:GLY:H	1:A:243:HIS:CE1	2.17	0.63
1:B:286:CYS:HB2	1:B:293:VAL:HG21	1.80	0.63
1:B:292:PRO:HG3	1:B:435:THR:CG2	2.27	0.63
1:B:296:ALA:HB2	1:B:329:MET:CG	2.29	0.63
1:A:495:LEU:HD12	1:D:381:VAL:CG2	2.27	0.63
1:D:330:LEU:HG	1:D:347:MET:HE1	1.81	0.63
1:D:215:ARG:HB2	1:D:219:GLN:OE1	1.99	0.62
1:B:241:GLU:HA	1:B:266:LEU:CD2	2.29	0.62
1:C:150:THR:C	1:C:151:LEU:HD12	2.20	0.62
1:D:321:VAL:CG2	1:D:354:ALA:HB3	2.29	0.62
1:C:328:VAL:HG12	1:C:347:MET:HE1	1.81	0.62
1:C:392:VAL:HG12	1:C:476:VAL:CG1	2.29	0.62
1:B:489:TYR:CB	1:B:490:PRO:HD3	2.29	0.62
1:A:292:PRO:HG3	1:A:435:THR:CG2	2.30	0.61
1:C:328:VAL:CG1	1:C:347:MET:CE	2.78	0.61
1:A:286:CYS:HB3	1:A:293:VAL:CG2	2.31	0.60
1:C:441:VAL:HG11	1:C:460:LEU:HG	1.83	0.60
1:C:328:VAL:HG12	1:C:347:MET:CE	2.31	0.60
1:C:403:THR:HB	2:C:601:FBP:O4P	2.01	0.60
1:B:242:ASN:OD1	1:B:244:GLN:CG	2.42	0.60
1:D:432:LEU:HD23	1:D:438:VAL:HG11	1.83	0.60
1:D:24:ILE:HG23	1:D:347:MET:HE3	1.84	0.59
1:C:402:ASN:N	2:C:601:FBP:O5P	2.35	0.59
1:A:454:ARG:NE	1:A:481:HIS:HB2	2.18	0.59
1:D:297:THR:HG22	1:D:298:GLN:HG2	1.85	0.58
1:A:359:HIS:HB3	1:A:362:VAL:HG22	1.85	0.58
1:B:264:GLY:N	1:B:297:THR:OG1	2.36	0.58
1:B:330:LEU:HB3	1:B:333:GLU:HB2	1.86	0.57
1:A:454:ARG:HD3	1:A:481:HIS:CB	2.35	0.57
1:C:154:LEU:N	1:C:163:LYS:O	2.30	0.57
1:C:292:PRO:HG3	1:C:435:THR:CG2	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ALA:CB	1:D:392:VAL:HG13	2.34	0.57
1:D:292:PRO:HG3	1:D:435:THR:CG2	2.34	0.57
1:B:382:CYS:SG	1:B:409:LEU:HD23	2.44	0.57
1:C:16:VAL:HG13	1:C:352:ILE:HG22	1.76	0.57
1:D:68:VAL:HG21	1:D:81:ILE:HD12	1.86	0.57
1:C:58:TYR:O	1:C:62:GLN:HB2	2.05	0.56
1:A:378:GLU:HG2	1:A:489:TYR:HB2	1.88	0.56
1:C:378:GLU:HG2	1:C:489:TYR:HB2	1.87	0.56
1:C:154:LEU:CB	1:C:163:LYS:O	2.54	0.56
1:D:321:VAL:HG23	1:D:354:ALA:HB1	1.87	0.56
1:D:50:ARG:NH2	1:D:84:ASP:OD2	2.25	0.56
1:A:308:ARG:HH21	1:A:311:ARG:HH12	1.53	0.56
1:B:384:SER:HA	1:B:387:SER:OG	2.05	0.56
1:A:286:CYS:HB3	1:A:293:VAL:HG23	1.87	0.56
1:A:454:ARG:HD3	1:A:481:HIS:HB2	1.88	0.56
1:B:241:GLU:OE2	1:B:265:ASP:OD2	2.24	0.56
1:B:380:ALA:HB3	1:C:392:VAL:CG2	2.36	0.56
1:C:426:LEU:HD21	1:C:442:TYR:CD2	2.41	0.56
1:C:310:THR:HG23	1:C:313:GLU:H	1.70	0.56
1:B:457:ARG:HH12	2:B:601:FBP:P1	2.29	0.56
1:C:27:THR:HG22	1:C:50:ARG:NE	2.20	0.55
1:D:378:GLU:HG2	1:D:489:TYR:HB2	1.87	0.55
1:B:241:GLU:CA	1:B:266:LEU:CD2	2.85	0.55
1:B:392:VAL:HG13	1:C:380:ALA:CB	2.37	0.55
1:D:314:VAL:CG1	1:D:350:ILE:HD12	2.28	0.55
1:D:321:VAL:CG2	1:D:354:ALA:HB1	2.37	0.54
1:B:454:ARG:NH1	1:B:454:ARG:HG3	2.20	0.54
1:A:286:CYS:SG	1:A:293:VAL:HG22	2.47	0.54
1:D:382:CYS:SG	1:D:409:LEU:HD23	2.48	0.54
1:C:321:VAL:HG23	1:C:354:ALA:HB1	1.90	0.54
1:C:286:CYS:HB2	1:C:293:VAL:CG2	2.38	0.53
1:B:283:ILE:CG1	1:B:293:VAL:HG11	2.30	0.53
1:C:246:VAL:HG12	1:C:282:ILE:HD11	1.89	0.53
1:D:426:LEU:HD23	1:D:442:TYR:CD1	2.43	0.53
1:A:426:LEU:HD21	1:A:442:TYR:CD2	2.43	0.53
1:B:411:SER:O	1:B:414:ARG:NH1	2.41	0.53
1:C:286:CYS:HB2	1:C:293:VAL:HG21	1.90	0.53
1:B:270:ILE:HD11	1:B:275:VAL:HG22	1.90	0.53
1:D:187:LEU:O	1:D:215:ARG:NH2	2.41	0.53
1:C:300:LEU:HD12	1:C:330:LEU:HD21	1.91	0.53
1:C:360:ASP:OD2	1:C:416:ASN:HB3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:PRO:HA	1:D:162:LEU:HD11	1.91	0.53
1:D:426:LEU:HD21	1:D:442:TYR:CD2	2.44	0.53
1:D:346:TYR:O	1:D:350:ILE:HG12	2.09	0.53
1:A:283:ILE:HG12	1:A:293:VAL:CG1	2.31	0.52
1:A:143:TYR:HB3	1:A:147:GLY:HA2	1.91	0.52
1:B:241:GLU:CA	1:B:266:LEU:HD23	2.38	0.52
1:A:286:CYS:CB	1:A:293:VAL:HG22	2.39	0.52
1:B:426:LEU:HD21	1:B:442:TYR:CD2	2.45	0.52
1:A:392:VAL:HG13	1:D:380:ALA:CB	2.39	0.52
1:B:426:LEU:HD23	1:B:442:TYR:CD1	2.45	0.52
1:B:296:ALA:HB1	1:B:329:MET:CG	2.37	0.52
1:D:185:VAL:O	1:D:215:ARG:NE	2.43	0.51
1:D:298:GLN:HB2	1:D:301:GLU:HB2	1.92	0.51
1:D:50:ARG:NH2	1:D:84:ASP:CB	2.74	0.51
1:B:154:LEU:HD21	1:B:165:HIS:HB2	1.92	0.51
1:D:220:VAL:HG13	1:D:236:ILE:HG21	1.93	0.51
1:A:8:ILE:HG13	1:A:8:ILE:O	2.10	0.51
1:A:283:ILE:CG1	1:A:293:VAL:HG11	2.29	0.51
1:C:321:VAL:CG2	1:C:354:ALA:HB1	2.39	0.51
1:D:38:LEU:HD22	1:D:68:VAL:HG12	1.92	0.51
1:A:88:PRO:HB2	1:A:187:LEU:HD13	1.92	0.51
1:C:299:MET:O	1:C:313:GLU:HG2	2.11	0.51
1:D:11:SER:CB	1:D:14:GLU:CG	2.82	0.51
1:A:129:TYR:CD1	1:A:131:GLN:OE1	2.63	0.50
1:B:20:ARG:HD3	1:B:348:VAL:HG13	1.93	0.50
1:A:454:ARG:NH1	2:A:601:FBP:O1	2.43	0.50
1:C:441:VAL:HG12	1:C:460:LEU:CD2	2.42	0.50
1:A:454:ARG:HH12	1:A:482:ALA:HB3	1.73	0.50
1:A:454:ARG:NH1	2:A:601:FBP:O3	2.44	0.50
1:C:328:VAL:CG1	1:C:347:MET:HE2	2.38	0.50
1:D:50:ARG:NH2	1:D:84:ASP:OD1	2.40	0.50
1:A:190:VAL:CG1	1:A:195:ARG:HG3	2.39	0.49
1:C:299:MET:HG3	1:C:329:MET:O	2.12	0.49
1:C:299:MET:CE	1:C:316:ASP:OD2	2.60	0.49
1:C:384:SER:HA	1:C:387:SER:OG	2.11	0.49
1:B:50:ARG:HA	1:B:82:ALA:HB3	1.94	0.49
1:C:339:TYR:HB3	1:C:342:GLU:HB2	1.94	0.49
1:D:339:TYR:HB3	1:D:342:GLU:HB2	1.94	0.49
1:D:321:VAL:HG21	1:D:354:ALA:CB	2.27	0.49
1:C:382:CYS:SG	1:C:409:LEU:HD23	2.53	0.49
1:D:68:VAL:HG21	1:D:81:ILE:CD1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:TYR:HB3	1:B:342:GLU:HB2	1.94	0.49
1:A:83:LEU:HB3	1:A:209:ILE:HD13	1.94	0.48
1:A:494:ARG:HB3	1:D:492:GLN:HG2	1.95	0.48
1:C:50:ARG:HA	1:C:82:ALA:HB3	1.95	0.48
1:C:321:VAL:CG2	1:C:354:ALA:HB3	2.27	0.48
1:A:339:TYR:HB3	1:A:342:GLU:HB2	1.95	0.48
1:B:44:SER:HB3	1:B:344:VAL:HG23	1.96	0.48
1:A:481:HIS:O	1:A:492:GLN:HB3	2.13	0.48
1:C:20:ARG:HD3	1:C:348:VAL:HG13	1.95	0.48
1:C:38:LEU:HD22	1:C:68:VAL:HG12	1.95	0.48
1:B:262:ALA:O	1:B:266:LEU:CG	2.60	0.48
1:D:24:ILE:CG2	1:D:347:MET:CE	2.89	0.48
1:C:360:ASP:OD2	1:C:416:ASN:CB	2.61	0.48
1:D:83:LEU:HB3	1:D:209:ILE:HD13	1.96	0.48
1:C:426:LEU:HD23	1:C:442:TYR:CD1	2.49	0.47
1:A:454:ARG:HD3	1:A:481:HIS:CG	2.48	0.47
1:B:185:VAL:HG13	1:B:215:ARG:HH21	1.77	0.47
1:A:190:VAL:CG1	1:A:195:ARG:CG	2.92	0.47
1:A:50:ARG:HA	1:A:82:ALA:HB3	1.96	0.47
1:B:346:TYR:O	1:B:350:ILE:HG13	2.14	0.47
1:D:296:ALA:HA	1:D:329:MET:HB3	1.96	0.47
1:C:283:ILE:CG1	1:C:293:VAL:HG11	2.32	0.47
1:A:198:LEU:HD22	1:A:227:LEU:HD11	1.97	0.47
1:B:241:GLU:HA	1:B:266:LEU:HD23	1.96	0.47
1:B:25:ILE:HB	1:B:329:MET:HB3	1.97	0.47
1:B:471:VAL:HG11	1:B:498:VAL:HG21	1.97	0.47
1:C:215:ARG:HG2	1:C:242:ASN:HD22	1.80	0.47
1:D:237:ILE:HG21	1:D:294:ILE:HD12	1.96	0.47
1:D:85:THR:CG2	1:D:212:SER:H	2.28	0.47
1:A:322:PHE:HD1	1:A:358:THR:HG22	1.80	0.46
1:C:286:CYS:HB3	1:C:293:VAL:HG23	1.97	0.46
1:A:38:LEU:HD22	1:A:68:VAL:HG12	1.97	0.46
1:A:426:LEU:HD23	1:A:442:TYR:CD1	2.51	0.46
1:C:19:HIS:HB3	1:C:470:TYR:CE1	2.51	0.46
1:B:296:ALA:CB	1:B:329:MET:HG3	2.46	0.46
1:D:424:THR:HG22	1:D:445:VAL:HG23	1.98	0.46
1:C:286:CYS:HB3	1:C:293:VAL:CG2	2.44	0.46
1:D:215:ARG:HD2	1:D:244:GLN:OE1	2.16	0.46
1:D:79:ILE:O	1:D:430:ARG:HD2	2.15	0.46
1:A:185:VAL:HG13	1:A:215:ARG:HH21	1.80	0.46
1:B:240:ILE:C	1:B:266:LEU:HD21	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:HG2	1:C:242:ASN:ND2	2.31	0.46
1:D:322:PHE:HD1	1:D:358:THR:HG22	1.80	0.46
1:C:20:ARG:HG3	1:C:352:ILE:HG13	1.97	0.46
1:B:240:ILE:HD13	1:B:259:ILE:HG23	1.98	0.46
1:D:264:GLY:CA	1:D:297:THR:HG21	2.46	0.46
1:C:346:TYR:O	1:C:350:ILE:HG13	2.16	0.45
1:B:241:GLU:O	1:B:266:LEU:HD23	2.15	0.45
1:C:213:PHE:CD2	1:C:241:GLU:HG3	2.52	0.45
1:D:25:ILE:HG12	1:D:48:VAL:HB	1.98	0.45
1:B:454:ARG:CG	1:B:454:ARG:NH1	2.80	0.45
1:B:283:ILE:HG12	1:B:293:VAL:CG1	2.34	0.45
1:C:24:ILE:CD1	1:C:344:VAL:HG13	2.46	0.45
1:C:24:ILE:HD11	1:C:344:VAL:HG13	1.97	0.45
1:A:400:LEU:HD22	1:A:454:ARG:HD3	1.98	0.45
1:B:263:ARG:HD2	1:B:275:VAL:HG12	1.98	0.45
1:C:110:VAL:O	1:C:161:THR:HA	2.17	0.45
1:C:143:TYR:CE2	1:C:181:PRO:HG3	2.52	0.45
1:D:332:GLY:HA2	1:D:335:ALA:HB3	1.99	0.45
1:D:426:LEU:CD2	1:D:442:TYR:CG	3.00	0.45
1:A:346:TYR:O	1:A:350:ILE:HG13	2.17	0.44
1:A:474:GLY:H	1:A:499:ARG:H	1.66	0.44
1:B:38:LEU:HD22	1:B:68:VAL:HG12	1.98	0.44
1:B:78:HIS:HB3	1:B:430:ARG:HG2	1.99	0.44
1:A:426:LEU:CD2	1:A:442:TYR:CG	3.00	0.44
1:D:318:ALA:O	1:D:321:VAL:CG2	2.65	0.44
1:C:441:VAL:CG1	1:C:460:LEU:HG	2.47	0.44
1:A:240:ILE:HD13	1:A:259:ILE:HG23	1.98	0.44
1:B:380:ALA:HB1	1:C:392:VAL:HG23	1.97	0.44
1:B:44:SER:CB	1:B:344:VAL:HG23	2.47	0.44
1:B:296:ALA:HB1	1:B:329:MET:HG3	1.99	0.44
1:A:102:TYR:HB3	1:A:166:VAL:HG11	1.99	0.44
1:B:286:CYS:CB	1:B:293:VAL:HG22	2.44	0.44
1:C:240:ILE:HD13	1:C:259:ILE:HG23	1.99	0.44
1:D:264:GLY:N	1:D:297:THR:OG1	2.50	0.44
1:A:142:ILE:CG2	1:A:178:ILE:CD1	2.75	0.44
1:C:241:GLU:HA	1:C:266:LEU:HB2	2.00	0.44
1:A:219:GLN:O	1:A:223:VAL:HG23	2.18	0.43
1:C:439:GLU:OE1	1:C:464:TRP:HZ3	2.00	0.43
1:D:227:LEU:HD12	1:D:231:GLY:HA3	2.00	0.43
1:B:60:TYR:O	1:B:63:THR:OG1	2.27	0.43
1:B:242:ASN:OD1	1:B:244:GLN:NE2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:HIS:CE1	1:A:492:GLN:HG2	2.53	0.43
1:A:454:ARG:NE	2:A:601:FBP:O3	2.50	0.43
1:B:141:LEU:HA	1:B:152:ARG:HA	2.00	0.43
1:B:246:VAL:HG22	1:B:282:ILE:HD11	2.00	0.43
1:C:84:ASP:HA	1:C:210:PHE:HB2	2.01	0.43
1:B:59:GLU:O	1:B:63:THR:OG1	2.37	0.43
1:C:321:VAL:HG21	1:C:354:ALA:CB	2.28	0.43
1:D:27:THR:HG22	1:D:50:ARG:HD3	2.00	0.43
1:D:84:ASP:HA	1:D:210:PHE:HB2	2.01	0.43
1:A:237:ILE:HG21	1:A:294:ILE:HD12	2.00	0.42
1:D:27:THR:HG22	1:D:50:ARG:HH11	1.84	0.42
1:C:283:ILE:HG12	1:C:293:VAL:CG1	2.35	0.42
1:A:189:ALA:HB2	1:A:219:GLN:HG2	2.01	0.42
1:A:270:ILE:HD11	1:A:275:VAL:HG12	2.01	0.42
1:C:441:VAL:CG1	1:C:460:LEU:CD2	2.97	0.42
1:D:240:ILE:HD13	1:D:259:ILE:HG23	2.00	0.42
1:B:426:LEU:CD2	1:B:442:TYR:CG	3.03	0.42
1:C:426:LEU:CD2	1:C:442:TYR:CG	3.03	0.42
1:D:136:VAL:HG12	1:D:153:VAL:HG21	2.01	0.42
1:D:360:ASP:HB3	1:D:390:PHE:HE1	1.85	0.42
1:B:392:VAL:HG13	1:C:380:ALA:HB3	2.01	0.42
1:C:406:SER:OG	2:C:601:FBP:O6P	2.24	0.42
1:B:25:ILE:HD11	1:B:294:ILE:HD12	2.02	0.42
1:D:486:VAL:HG11	1:D:489:TYR:CZ	2.54	0.42
1:A:454:ARG:CD	1:A:481:HIS:CG	3.03	0.42
1:B:286:CYS:SG	1:B:293:VAL:HG22	2.59	0.42
1:B:362:VAL:O	1:B:363:MET:C	2.58	0.42
1:C:286:CYS:SG	1:C:293:VAL:CG2	3.05	0.42
1:D:139:GLY:O	1:D:152:ARG:NH1	2.53	0.42
1:B:208:MET:SD	1:B:434:VAL:HG11	2.60	0.41
2:B:601:FBP:O2	2:B:601:FBP:P1	2.78	0.41
1:C:180:LEU:H	1:C:180:LEU:HD23	1.84	0.41
1:D:132:LEU:HD12	1:D:136:VAL:CG2	2.50	0.41
1:D:209:ILE:HB	1:D:236:ILE:HD13	2.02	0.41
2:B:601:FBP:HO2	2:B:601:FBP:P1	2.38	0.41
1:D:299:MET:O	1:D:313:GLU:HG2	2.19	0.41
1:A:84:ASP:HA	1:A:210:PHE:HB2	2.03	0.41
1:D:112:THR:HG21	1:D:133:PRO:HD3	2.02	0.41
1:D:426:LEU:HD21	1:D:442:TYR:CG	2.56	0.41
1:A:367:ILE:O	1:A:371:GLN:HG2	2.21	0.41
1:D:378:GLU:HG3	1:D:489:TYR:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:HD21	1:A:442:TYR:CG	2.55	0.41
1:B:403:THR:HB	2:B:601:FBP:O6P	2.21	0.41
1:C:360:ASP:OD2	1:C:416:ASN:HA	2.20	0.41
1:D:482:ALA:HB2	2:D:601:FBP:HO4	1.85	0.41
1:B:81:ILE:CG2	1:B:206:VAL:HG12	2.50	0.41
2:C:601:FBP:O2	2:C:601:FBP:P1	2.79	0.41
1:D:426:LEU:CD2	1:D:442:TYR:CD1	3.04	0.41
1:B:401:SER:CB	2:B:601:FBP:O4P	2.60	0.41
1:C:400:LEU:CD2	1:C:454:ARG:HB2	2.50	0.41
1:B:299:MET:HB2	1:B:299:MET:HE3	1.55	0.41
1:C:294:ILE:HG22	1:C:295:CYS:O	2.21	0.41
1:A:20:ARG:HD3	1:A:348:VAL:HG13	2.03	0.40
1:A:454:ARG:NH2	1:A:482:ALA:O	2.54	0.40
1:C:296:ALA:HA	1:C:329:MET:HB3	2.04	0.40
1:C:299:MET:HE2	1:C:316:ASP:OD2	2.21	0.40
1:A:330:LEU:HD23	1:A:333:GLU:OE1	2.21	0.40
1:B:213:PHE:HD1	1:B:241:GLU:HB2	1.86	0.40
1:C:453:ASP:O	1:C:453:ASP:OD1	2.39	0.40
1:A:27:THR:HB	1:A:331:SER:HA	2.04	0.40
1:A:78:HIS:HB3	1:A:430:ARG:HG2	2.03	0.40
1:B:299:MET:O	1:B:313:GLU:HG2	2.22	0.40
1:C:112:THR:HG21	1:C:133:PRO:HD3	2.03	0.40
1:C:392:VAL:HG12	1:C:392:VAL:O	2.21	0.40
1:C:454:ARG:HG2	1:C:454:ARG:H	1.67	0.40
1:D:411:SER:OG	1:D:436:ARG:O	2.27	0.40
1:A:378:GLU:HG3	1:A:489:TYR:CD2	2.56	0.40
1:D:453:ASP:O	1:D:453:ASP:OD1	2.39	0.40
1:C:239:LYS:HE3	1:C:260:MET:HE1	2.04	0.40
1:D:24:ILE:CG2	1:D:347:MET:HE2	2.51	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	496/514 (96%)	466 (94%)	28 (6%)	2 (0%)	34 72
1	B	475/514 (92%)	445 (94%)	26 (6%)	4 (1%)	19 57
1	C	495/514 (96%)	464 (94%)	28 (6%)	3 (1%)	25 64
1	D	496/514 (96%)	470 (95%)	24 (5%)	2 (0%)	34 72
All	All	1962/2056 (95%)	1845 (94%)	106 (5%)	11 (1%)	25 64

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	489	TYR
1	C	158	ASP
1	C	454	ARG
1	D	298	GLN
1	D	454	ARG
1	B	437	SER
1	B	454	ARG
1	C	360	ASP
1	A	132	LEU
1	A	455	GLU
1	B	490	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	361/435 (83%)	355 (98%)	6 (2%)	60 85
1	B	330/435 (76%)	324 (98%)	6 (2%)	59 85
1	C	345/435 (79%)	340 (99%)	5 (1%)	67 88
1	D	361/435 (83%)	360 (100%)	1 (0%)	92 97
All	All	1397/1740 (80%)	1379 (99%)	18 (1%)	69 89

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

Mol	Chain	Res	Type
1	A	229	GLU
1	A	333	GLU
1	A	405	ARG
1	A	437	SER
1	A	450	GLU
1	A	457	ARG
1	B	59	GLU
1	B	175	ARG
1	B	209	ILE
1	B	229	GLU
1	B	359	HIS
1	B	454	ARG
1	C	213	PHE
1	C	299	MET
1	C	438	VAL
1	C	454	ARG
1	C	455	GLU
1	D	362	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	433	ASN
1	D	298	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	FBP	D	601	-	18,20,20	0.78	0	23,32,32	1.14	1 (4%)
2	FBP	C	601	-	18,20,20	0.71	0	23,32,32	0.99	0
2	FBP	B	601	-	18,20,20	0.70	0	23,32,32	1.14	4 (17%)
2	FBP	A	601	-	18,20,20	0.62	0	23,32,32	0.80	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
2	FBP	D	601	-	-	12/13/32/32	0/1/1/1
2	FBP	C	601	-	-	11/13/32/32	0/1/1/1
2	FBP	B	601	-	-	7/13/32/32	0/1/1/1
2	FBP	A	601	-	-	2/13/32/32	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})
2	D	601	FBP	O6P-P2-O5P	2.54	117.34	107.64
2	B	601	FBP	O6P-P2-O5P	2.41	116.86	107.64
2	B	601	FBP	O3P-P1-O2P	2.14	115.81	107.64
2	B	601	FBP	O5-C5-C6	2.10	114.08	109.45
2	B	601	FBP	O2P-P1-O1	-2.06	101.24	106.73

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C1-O1-P1-O2P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	601	FBP	C1-O1-P1-O3P
2	D	601	FBP	O1-C1-C2-O2
2	D	601	FBP	O1-C1-C2-C3
2	D	601	FBP	O1-C1-C2-O5
2	D	601	FBP	C4-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	D	601	FBP	C6-O6-P2-O4P
2	D	601	FBP	C6-O6-P2-O5P
2	D	601	FBP	C6-O6-P2-O6P
2	C	601	FBP	C1-O1-P1-O2P
2	C	601	FBP	C1-O1-P1-O3P
2	C	601	FBP	C2-C1-O1-P1
2	C	601	FBP	O1-C1-C2-C3
2	C	601	FBP	C4-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	C	601	FBP	C6-O6-P2-O6P
2	B	601	FBP	C1-O1-P1-O1P
2	B	601	FBP	C1-O1-P1-O2P
2	B	601	FBP	C1-O1-P1-O3P
2	B	601	FBP	C2-C1-O1-P1
2	B	601	FBP	C6-O6-P2-O5P
2	B	601	FBP	C6-O6-P2-O6P
2	C	601	FBP	C1-O1-P1-O1P
2	B	601	FBP	C6-O6-P2-O4P
2	C	601	FBP	C6-O6-P2-O5P
2	C	601	FBP	O1-C1-C2-O5
2	D	601	FBP	C2-C1-O1-P1
2	C	601	FBP	C6-O6-P2-O4P
2	A	601	FBP	C6-O6-P2-O4P
2	A	601	FBP	O5-C5-C6-O6

There are no ring outliers.

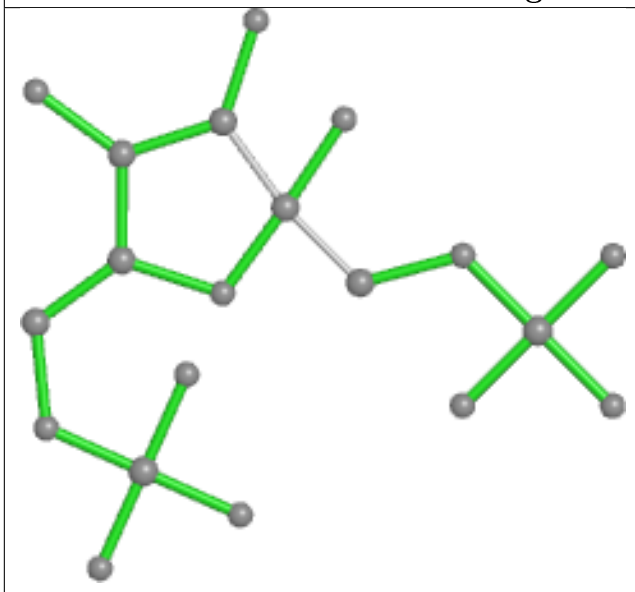
4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FBP	1	0
2	C	601	FBP	7	0
2	B	601	FBP	8	0
2	A	601	FBP	12	0

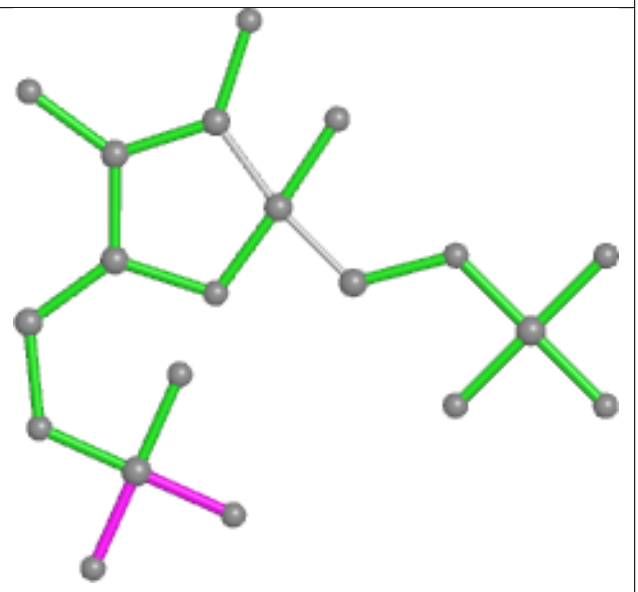
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

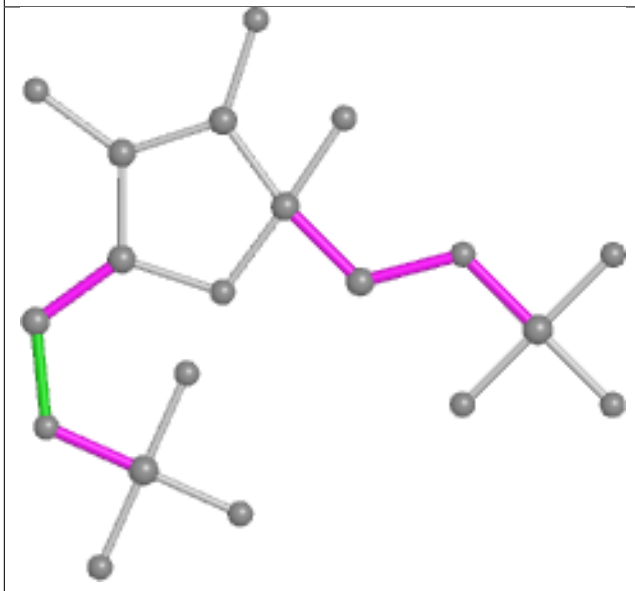
Ligand FBP D 601



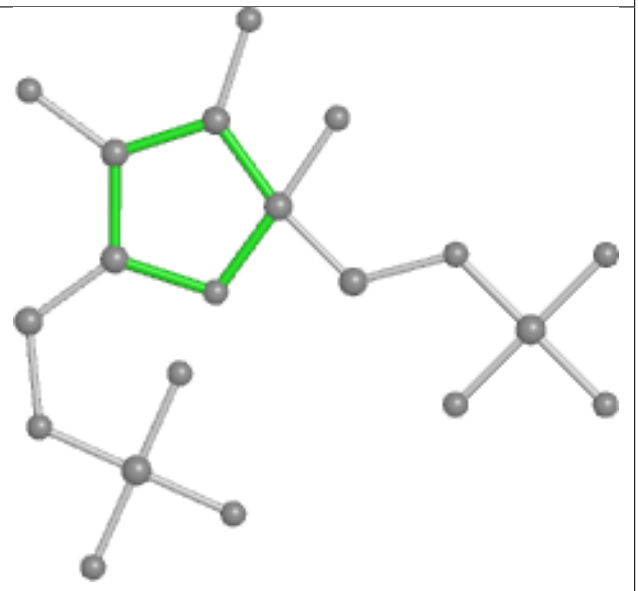
Bond lengths



Bond angles

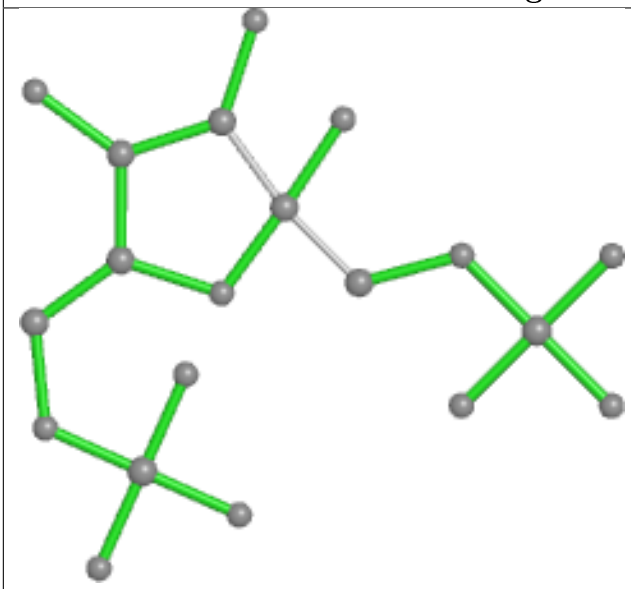


Torsions

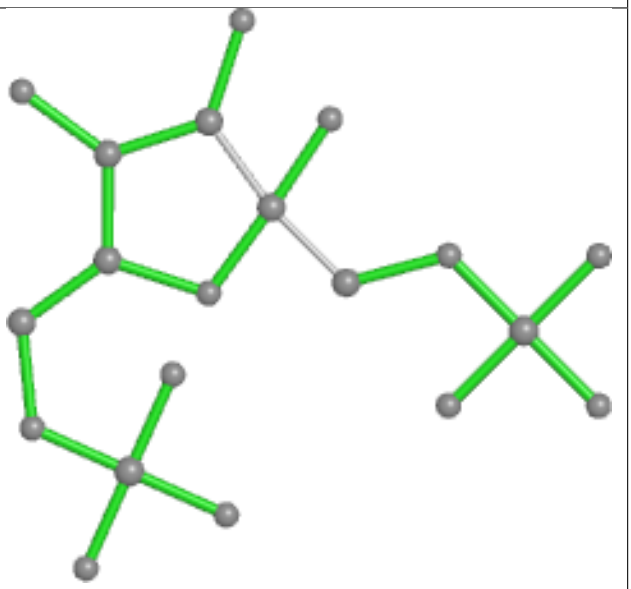


Rings

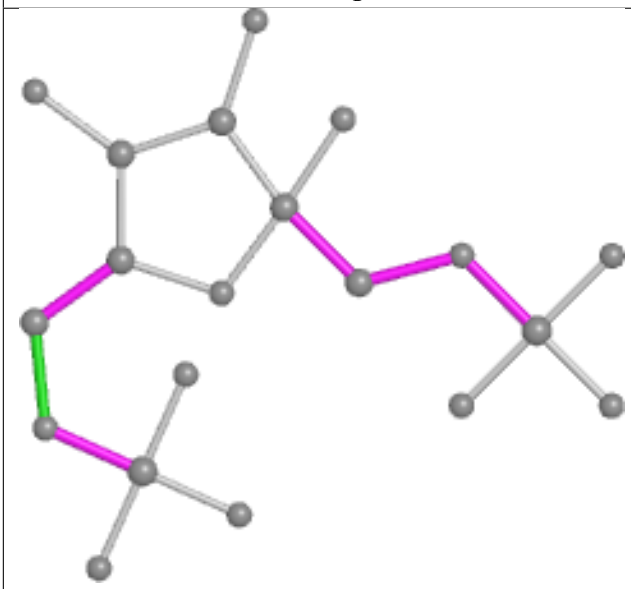
Ligand FBP C 601



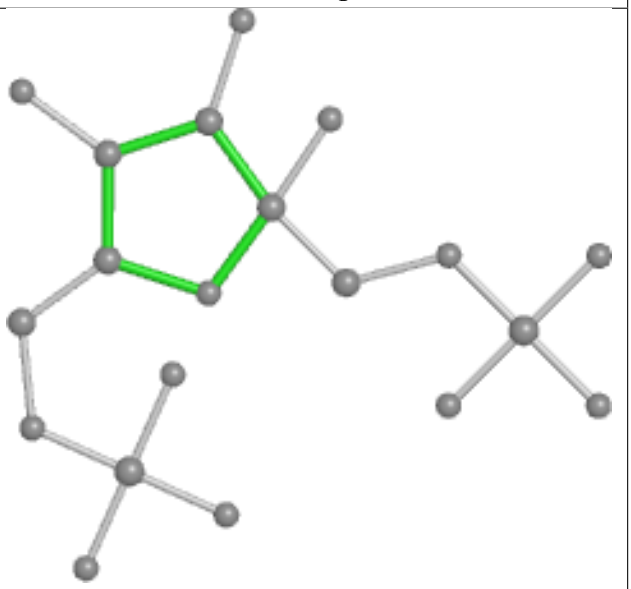
Bond lengths



Bond angles

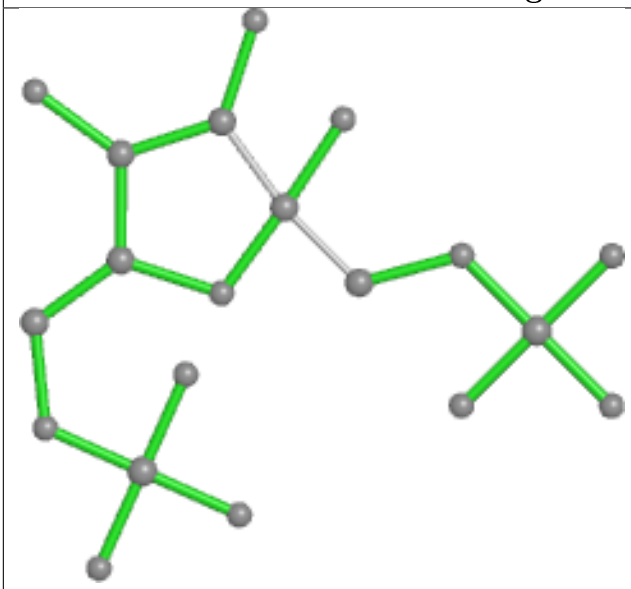


Torsions

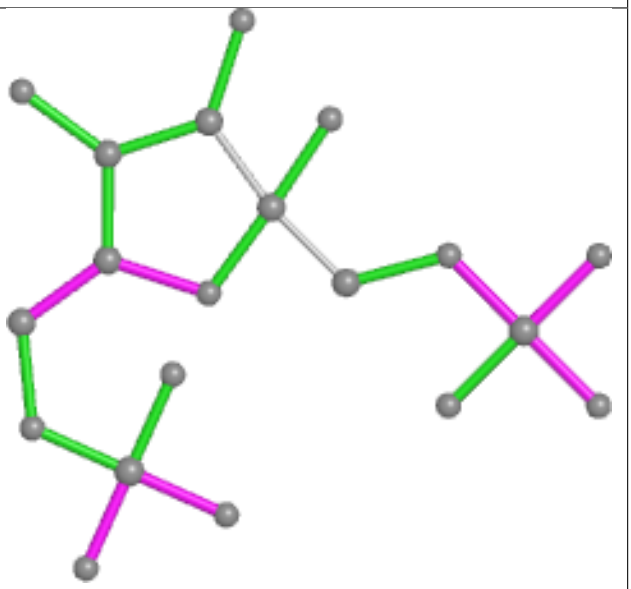


Rings

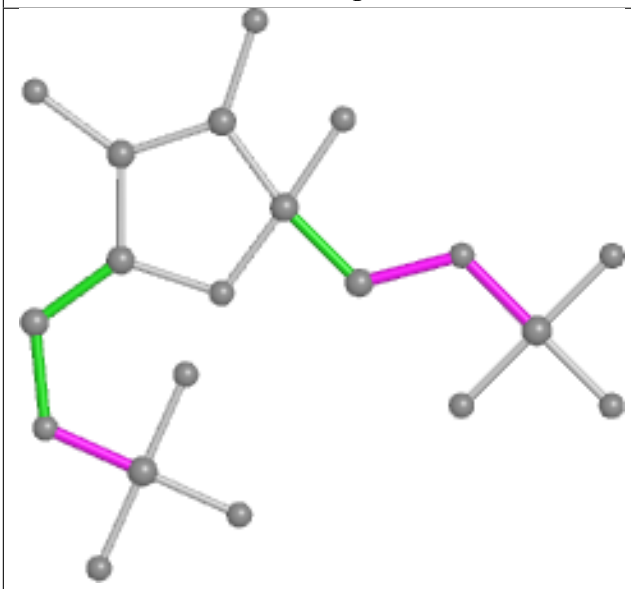
Ligand FBP B 601



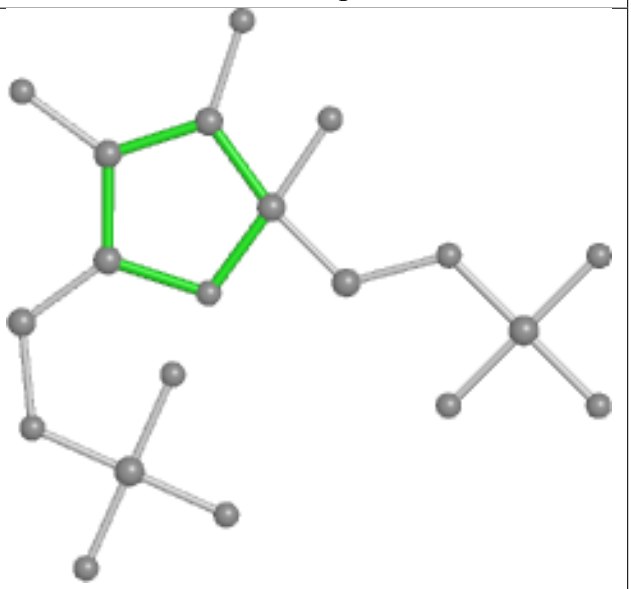
Bond lengths



Bond angles

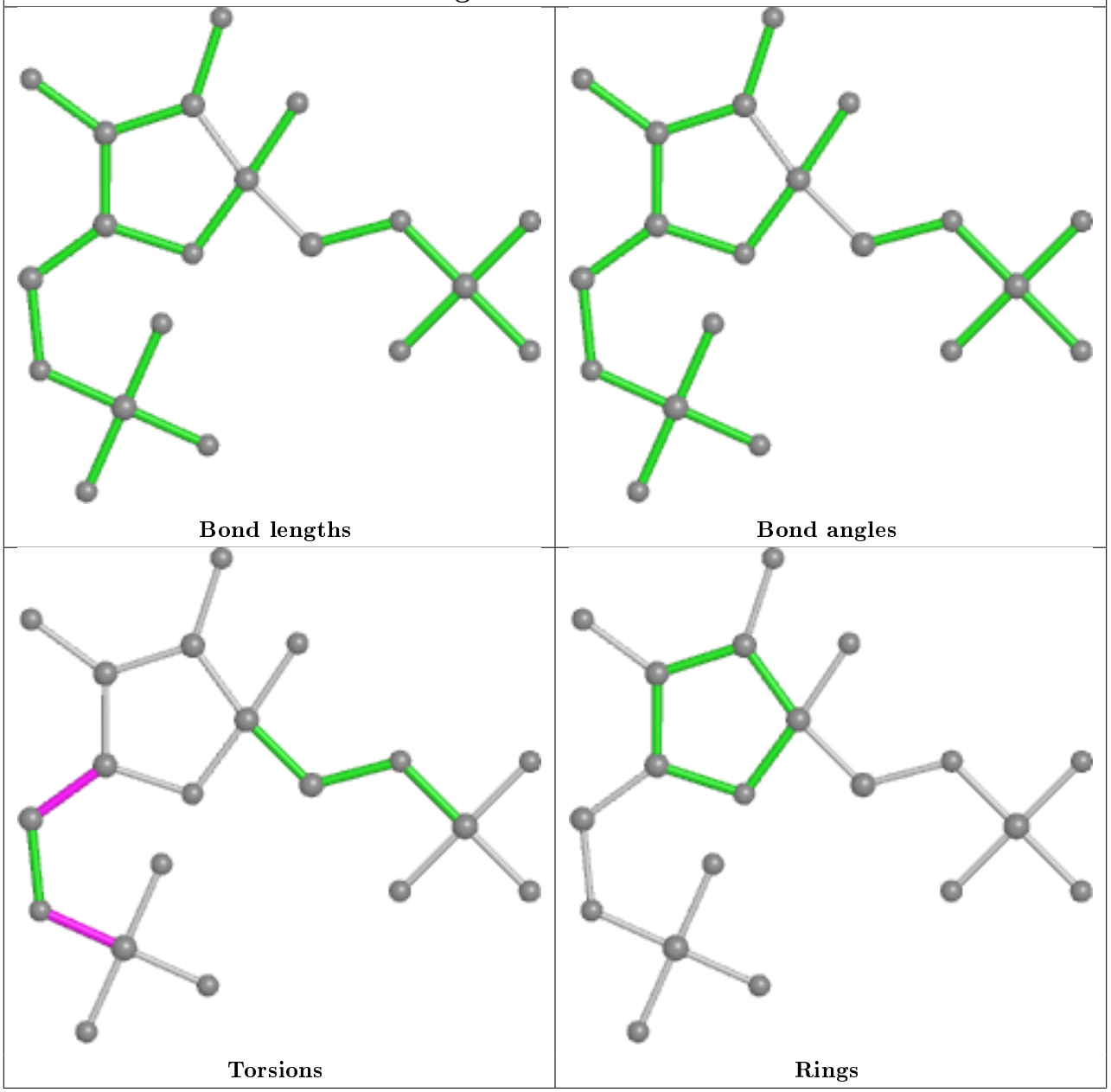


Torsions



Rings

Ligand FBP A 601



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	498/514 (96%)	0.05	12 (2%)	59	30	63, 92, 128, 142	0
1	B	481/514 (93%)	0.23	16 (3%)	46	20	74, 110, 140, 148	0
1	C	497/514 (96%)	0.34	26 (5%)	27	10	73, 97, 159, 169	0
1	D	498/514 (96%)	0.16	14 (2%)	53	25	68, 104, 139, 149	0
All	All	1974/2056 (96%)	0.19	68 (3%)	45	19	63, 102, 143, 169	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	THR	5.9
1	C	102	TYR	5.5
1	C	171	ARG	4.8
1	A	142	ILE	4.3
1	C	134	ASN	4.2
1	C	125	PHE	4.2
1	B	49	ALA	3.7
1	C	121	THR	3.7
1	C	172	LEU	3.7
1	A	114	PRO	3.4
1	A	151	LEU	3.3
1	B	128	ASP	3.3
1	D	484	HIS	3.2
1	A	97	ASP	3.2
1	C	130	PRO	3.1
1	D	206	VAL	3.1
1	C	150	THR	3.1
1	B	83	LEU	3.1
1	B	268	VAL	3.1
1	C	136	VAL	3.1
1	C	186	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	160	CYS	3.0
1	D	102	TYR	2.8
1	D	125	PHE	2.8
1	C	101	THR	2.7
1	D	201	GLY	2.7
1	B	236	ILE	2.7
1	B	260	MET	2.7
1	C	170	HIS	2.7
1	C	118	LYS	2.6
1	D	445	VAL	2.6
1	B	102	TYR	2.6
1	A	492	GLN	2.5
1	B	174	ASP	2.5
1	D	99	GLU	2.5
1	C	133	PRO	2.4
1	D	204	GLN	2.4
1	C	98	GLY	2.4
1	D	449	GLY	2.4
1	D	200	PHE	2.4
1	C	97	ASP	2.3
1	A	190	VAL	2.3
1	C	120	GLY	2.2
1	B	101	THR	2.2
1	C	185	VAL	2.2
1	D	209	ILE	2.2
1	A	141	LEU	2.2
1	A	115	ALA	2.2
1	A	125	PHE	2.2
1	C	162	LEU	2.1
1	C	155	SER	2.1
1	A	129	TYR	2.1
1	A	93	GLY	2.1
1	D	488	GLY	2.1
1	B	53	PHE	2.1
1	A	140	GLY	2.1
1	C	112	THR	2.1
1	C	173	THR	2.1
1	B	82	ALA	2.1
1	C	110	VAL	2.1
1	D	185	VAL	2.1
1	D	170	HIS	2.1
1	B	400	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	51	MET	2.0
1	B	168	ASN	2.0
1	B	421	CYS	2.0
1	B	100	ALA	2.0
1	C	126	TYR	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)

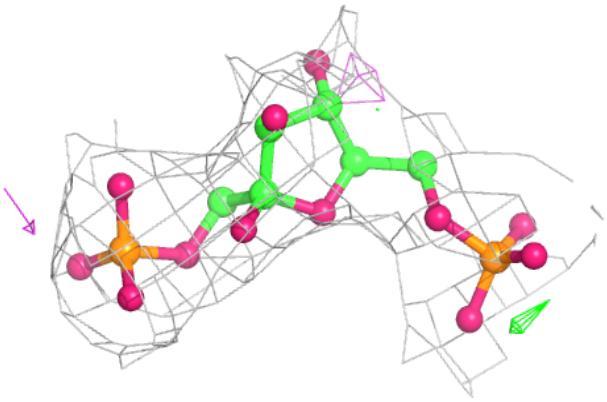
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

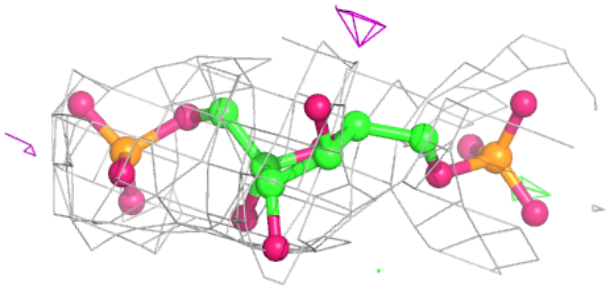
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FBP	D	601	20/20	0.74	0.23	136,146,147,148	0
2	FBP	C	601	20/20	0.81	0.24	153,164,176,176	0
3	MG	B	602	1/1	0.81	0.14	66,66,66,66	0
2	FBP	A	601	20/20	0.81	0.18	136,154,166,167	0
2	FBP	B	601	20/20	0.87	0.17	146,151,154,154	0
3	MG	A	602	1/1	0.91	0.21	80,80,80,80	0
3	MG	C	602	1/1	0.95	0.42	107,107,107,107	0
3	MG	D	602	1/1	0.95	0.31	89,89,89,89	0

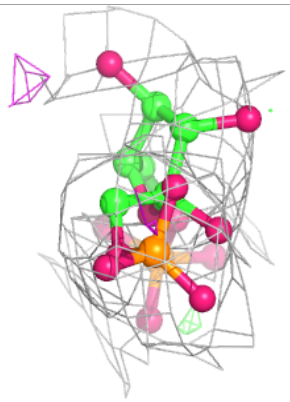
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP D 601:

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

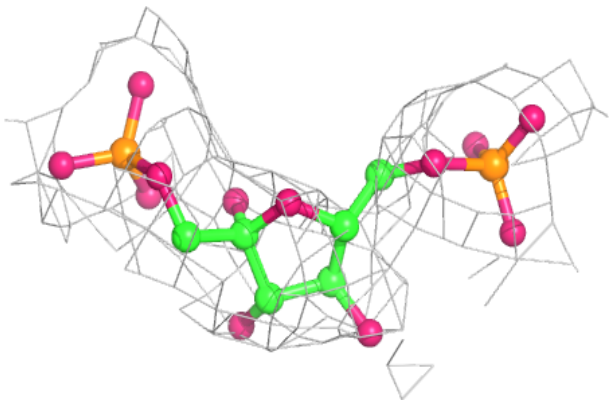


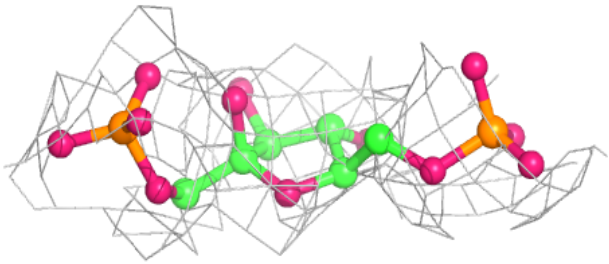




Electron density around FBP C 601:

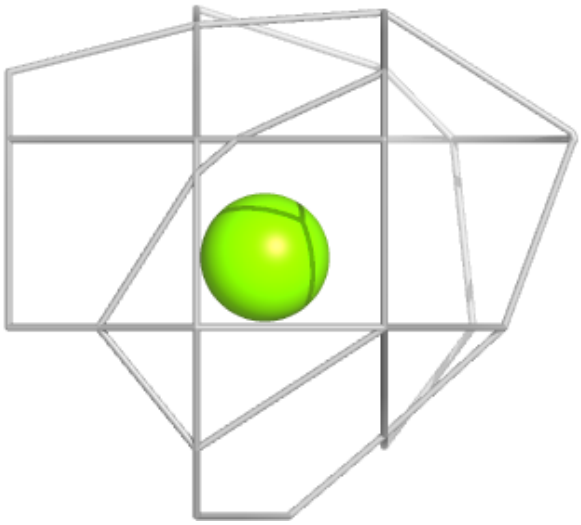
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

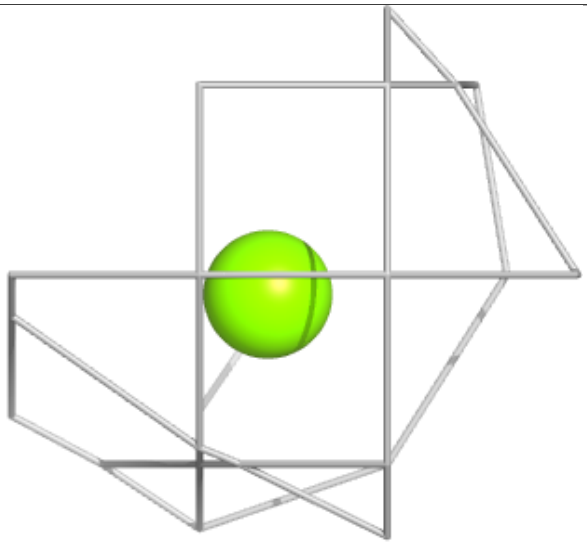


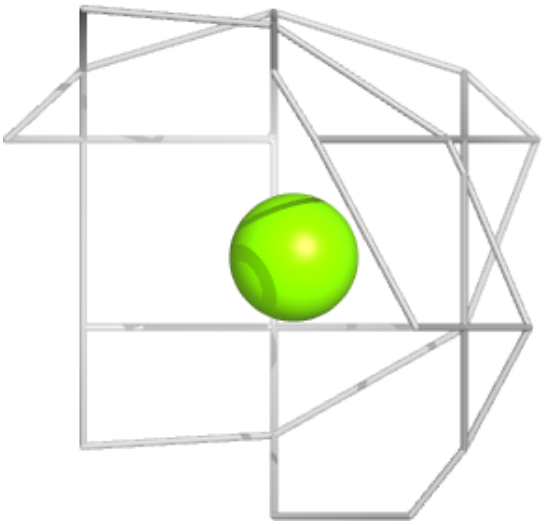


Electron density around MG B 602:

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

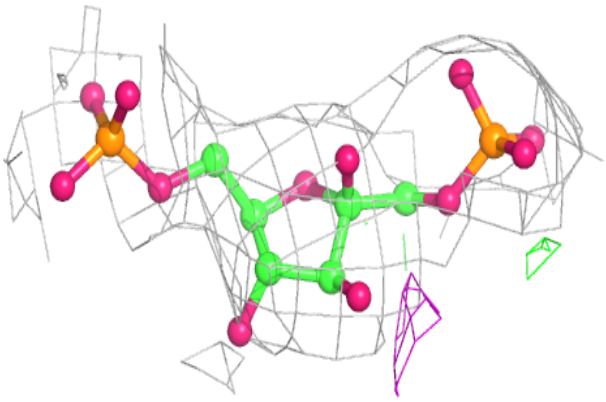


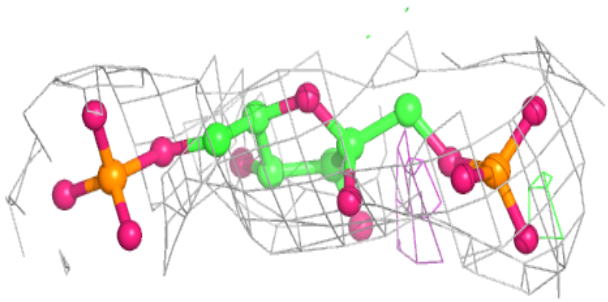


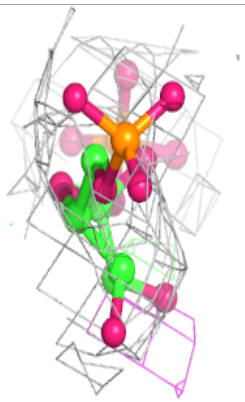


Electron density around FBP A 601:

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

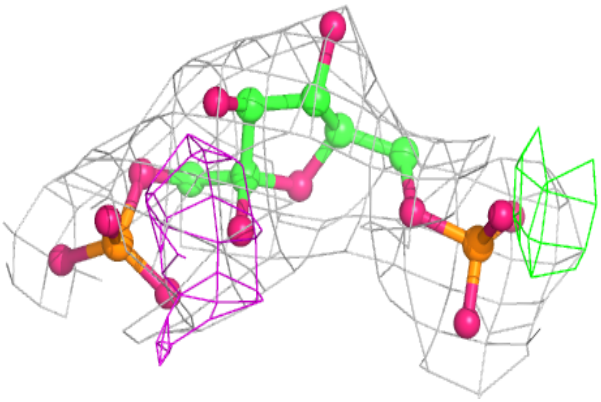


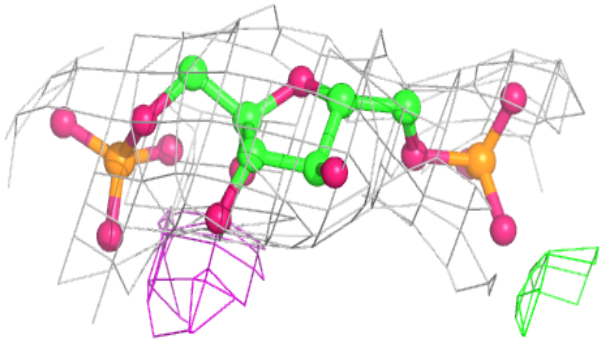


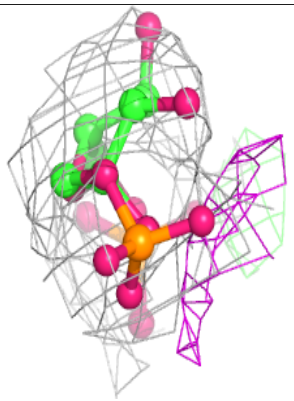


Electron density around FBP B 601:

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

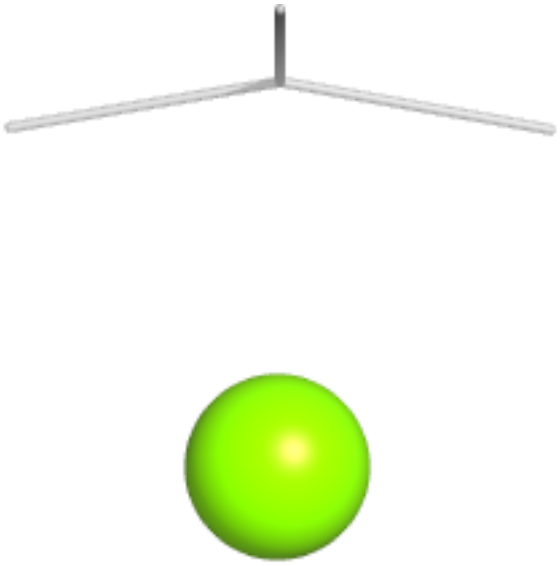


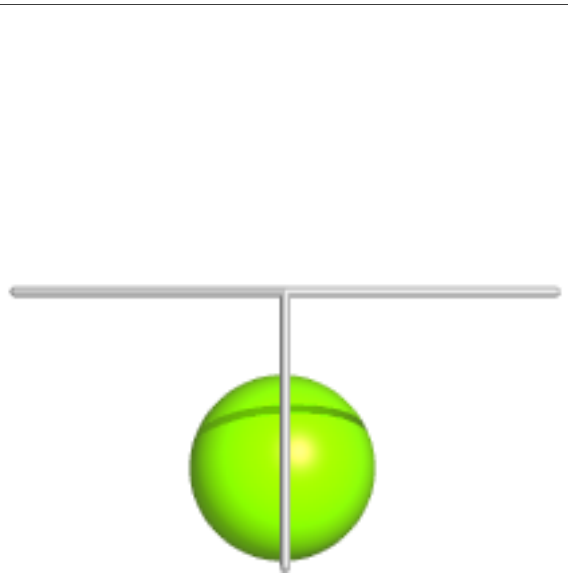


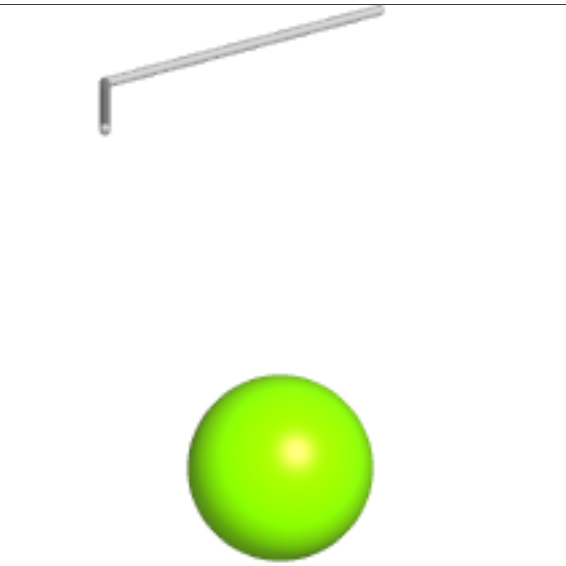


Electron density around MG A 602:

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

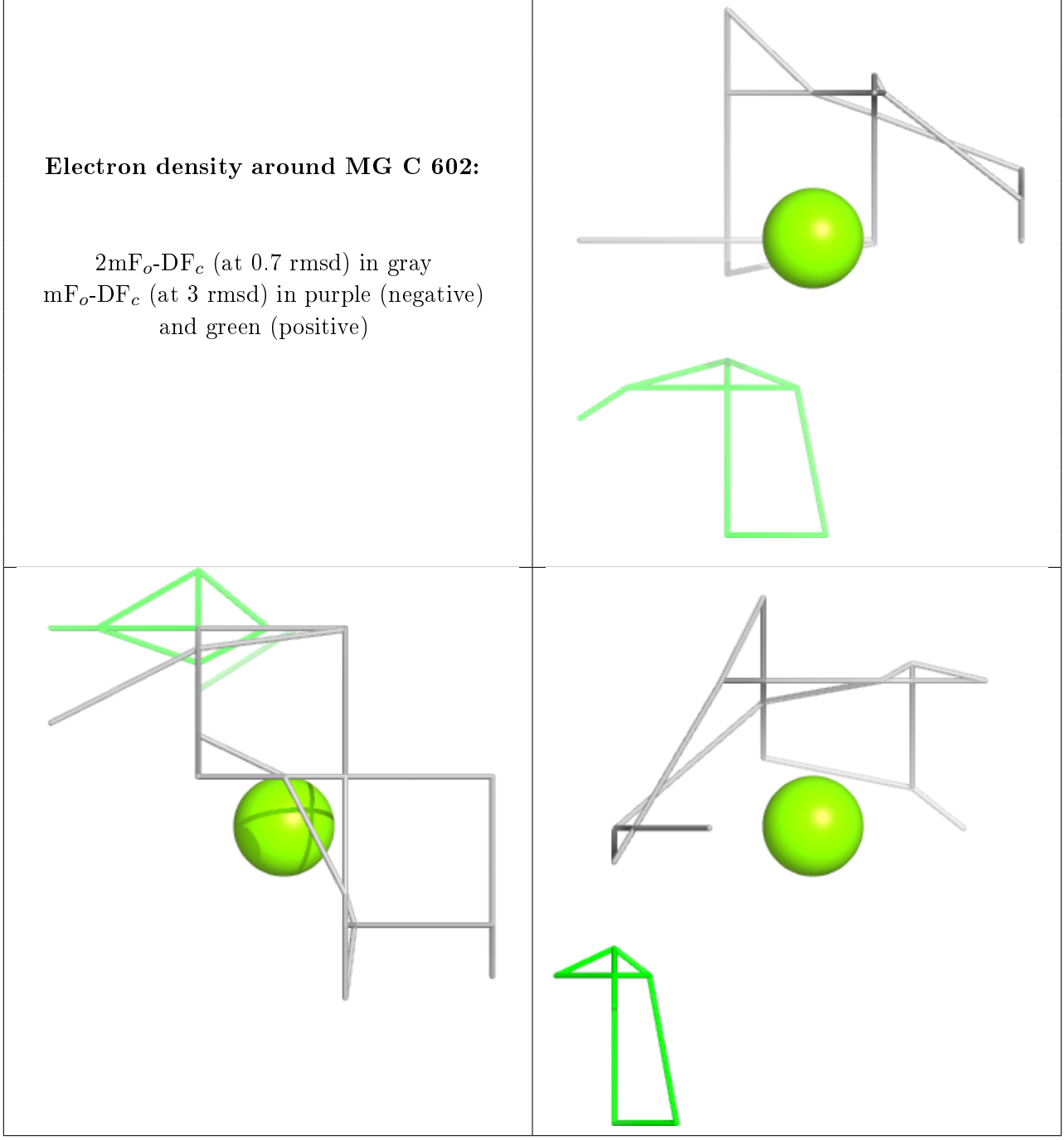






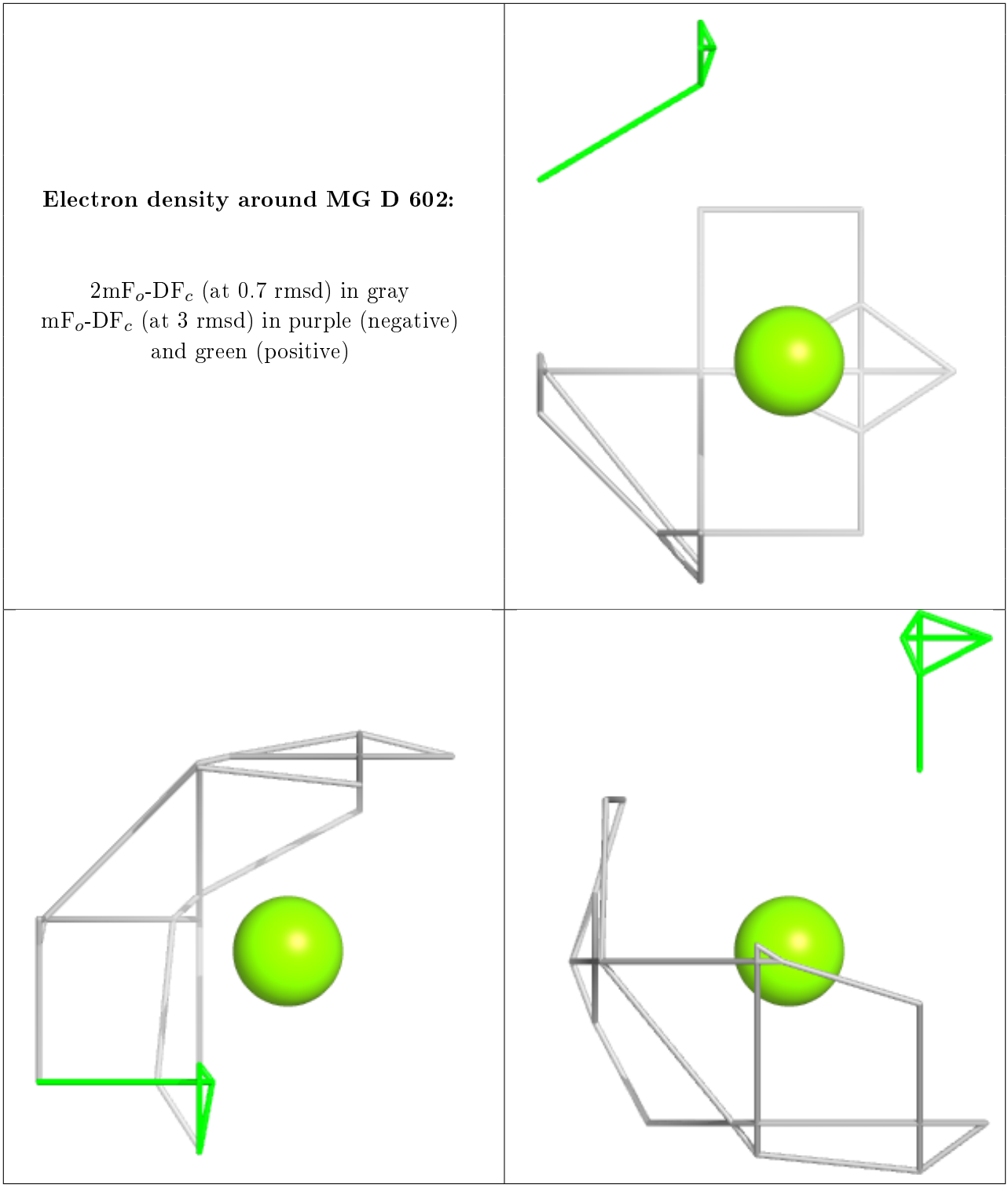
Electron density around MG C 602:

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



Electron density around MG 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)



6.5 Other polymers

There are no such residues in this entry.