Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:58 PM JST

PDB ID	:	6J9T
Title	:	Complex structure of Lactobacillus casei lactate dehydrogenase with fructose -1,6-bisphosphate
Authors	:	Arai, K.; Miyanaga, A.; Uchikoba, H.; Fushinobu, S.; Taguchi, H.
Deposited on	:	2019-01-24
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

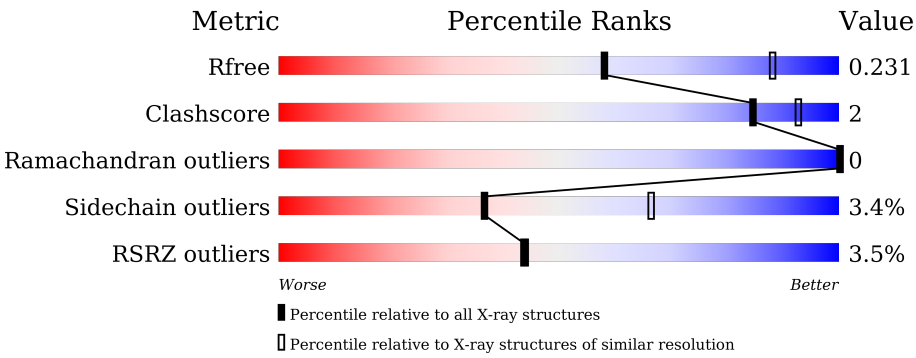
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	326	5% 88% 6% • 5%
1	B	326	2% 88% 8% • •
1	C	326	4% 87% 9% 5%
1	D	326	3% 87% 9% • •
1	E	326	3% 87% 7% • 6%
1	F	326	4% 90% 6% • •

2 Entry composition (i)

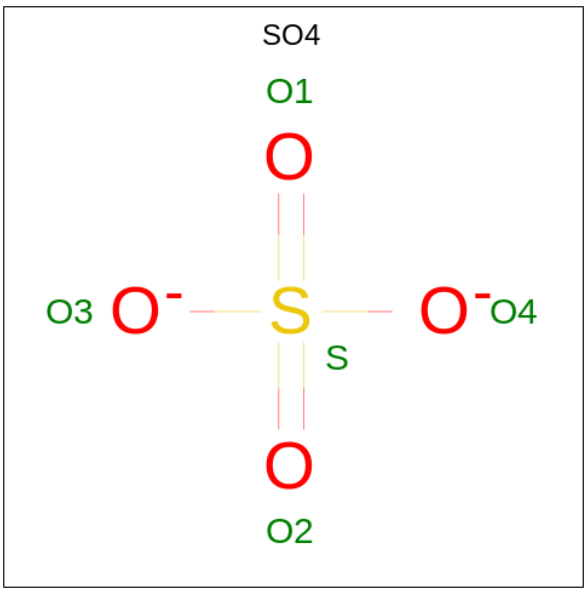
There are 4 unique types of molecules in this entry. The entry contains 14571 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase.

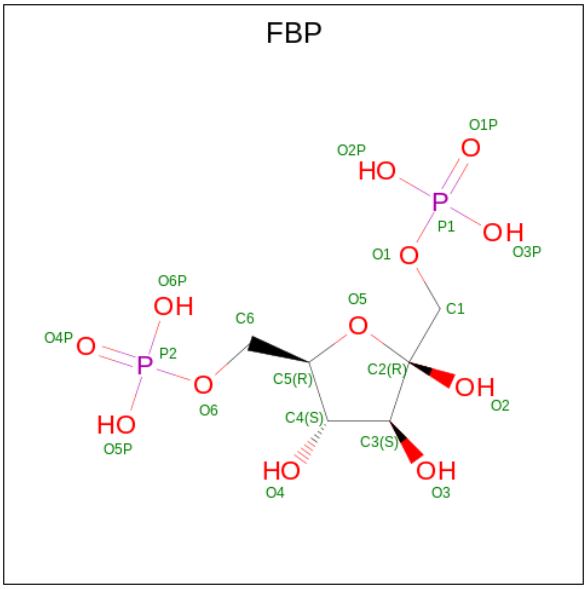
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2375	1514	395	460	6	0	0	0
1	B	316	2420	1544	402	468	6	0	0	0
1	C	311	2386	1523	396	461	6	0	0	0
1	D	314	2409	1538	400	465	6	0	0	0
1	E	308	2361	1507	391	457	6	0	0	0
1	F	316	2420	1544	402	468	6	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	C	1	5	4	1		0	0
2	D	1	5	4	1		0	0
2	E	1	5	4	1		0	0
2	F	1	5	4	1		0	0

- 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
			Total	C	O	P		
3	B	1	20	6	12	2	0	0
3	E	1	20	6	12	2	0	0
3	F	1	20	6	12	2	0	0

- Molecule 4 is water.

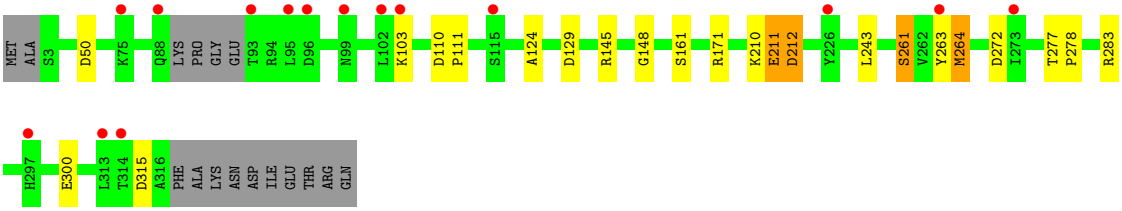
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	4	4	4	0	0
			Total	O		
4	B	10	10	10	0	0
			Total	O		
4	C	21	21	21	0	0
			Total	O		
4	D	27	27	27	0	0
			Total	O		
4	E	33	33	33	0	0
			Total	O		
4	F	15	15	15	0	0

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.

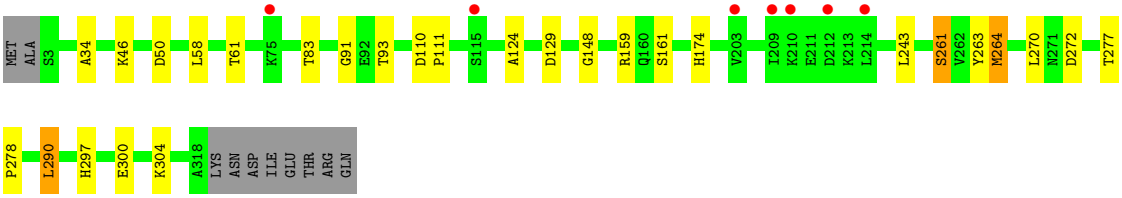
• Molecule 1: L-lactate dehydrogenase

Chain A:



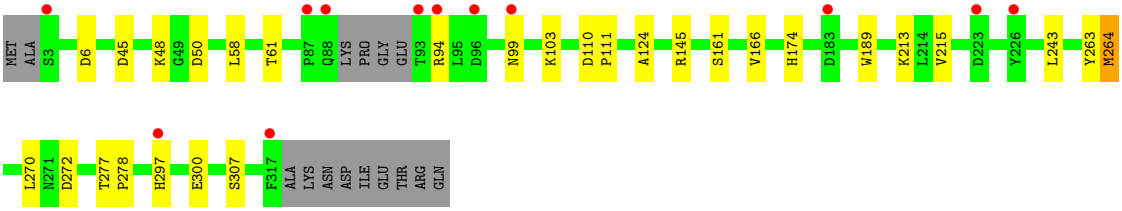
• Molecule 1: L-lactate dehydrogenase

Chain B:



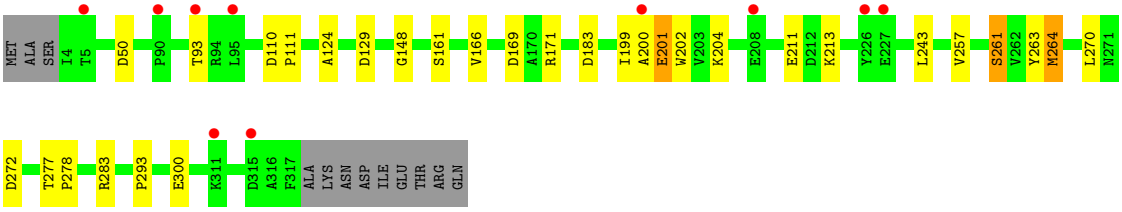
• Molecule 1: L-lactate dehydrogenase

Chain C:



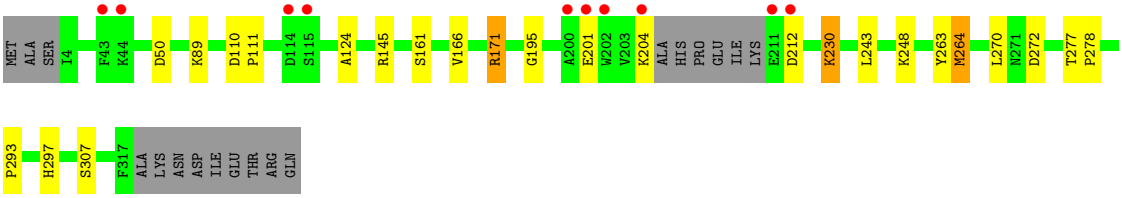
• Molecule 1: L-lactate dehydrogenase

Chain D:



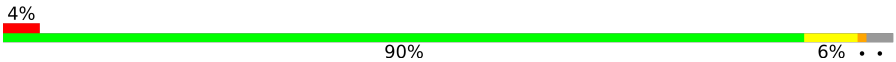
• Molecule 1: L-lactate dehydrogenase

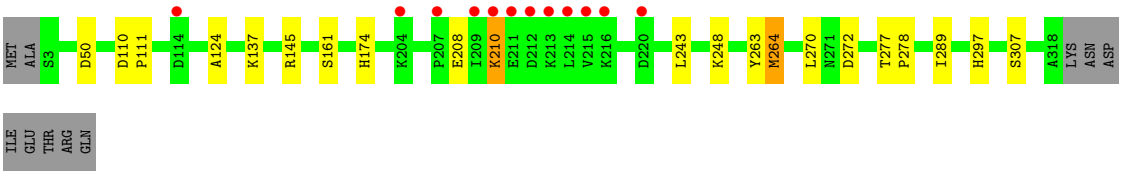
Chain E:



• Molecule 1: L-lactate dehydrogenase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.25Å 83.58Å 180.09Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	41.18 – 2.70 41.05 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.18-2.70) 99.9 (41.05-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.79 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.226 0.201 , 0.231	Depositor DCC
R_{free} test set	3405 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14571	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.64	0/2416	0.74	5/3277 (0.2%)
1	B	0.67	0/2464	0.80	5/3343 (0.1%)
1	C	0.65	0/2428	0.75	3/3293 (0.1%)
1	D	0.68	0/2453	0.79	3/3328 (0.1%)
1	E	0.67	0/2402	0.76	5/3257 (0.2%)
1	F	0.64	0/2464	0.73	2/3343 (0.1%)
All	All	0.66	0/14627	0.76	23/19841 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	304	LYS	CD-CE-NZ	9.32	133.15	111.70
1	A	264	MET	CA-CB-CG	8.43	127.62	113.30
1	E	171	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	B	290	LEU	CA-CB-CG	6.75	130.83	115.30
1	B	290	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	F	289	ILE	CG1-CB-CG2	-6.45	97.20	111.40
1	E	307	SER	N-CA-CB	6.42	120.14	110.50
1	D	171	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	212	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	C	45	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	83	THR	C-N-CA	-5.66	107.56	121.70
1	E	145	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	315	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	34	ALA	N-CA-CB	-5.49	102.41	110.10
1	F	145	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	C	94	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	C	145	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	D	183	ASP	CB-CG-OD2	-5.20	113.62	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	171	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	A	145	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	171	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	E	145	ARG	NE-CZ-NH2	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2375	0	2396	8	0
1	B	2420	0	2440	14	0
1	C	2386	0	2405	14	0
1	D	2409	0	2430	17	0
1	E	2361	0	2380	14	0
1	F	2420	0	2440	11	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	B	20	0	10	2	0
3	E	20	0	10	0	0
3	F	20	0	10	2	0
4	A	4	0	0	0	0
4	B	10	0	0	0	0
4	C	21	0	0	0	0
4	D	27	0	0	0	0
4	E	33	0	0	1	0
4	F	15	0	0	1	0
All	All	14571	0	14521	67	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 2.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:LEU:HA	1:C:61:THR:HG22	1.71	0.72
1:B:58:LEU:HA	1:B:61:THR:HG22	1.72	0.71
1:D:293:PRO:HG3	1:E:201:GLU:CD	2.11	0.70
1:D:199:ILE:O	1:D:200:ALA:C	2.28	0.69
1:D:202:TRP:C	1:D:202:TRP:CD1	2.70	0.65
1:D:202:TRP:CD1	1:D:202:TRP:O	2.50	0.65
1:F:174:HIS:ND1	3:F:402:FBP:O5P	2.18	0.63
1:F:210:LYS:HA	1:F:210:LYS:CE	2.28	0.63
1:A:129:ASP:OD1	1:A:261:SER:HB3	2.02	0.59
1:B:129:ASP:OD1	1:B:261:SER:HB3	2.03	0.59
1:D:293:PRO:CG	1:E:201:GLU:CD	2.71	0.58
1:F:210:LYS:HA	1:F:210:LYS:HE3	1.85	0.57
1:D:129:ASP:OD1	1:D:261:SER:HB3	2.04	0.57
1:E:248:LYS:NZ	4:E:501:HOH:O	2.34	0.56
1:D:201:GLU:O	1:D:204:LYS:HB2	2.07	0.54
1:E:264:MET:HG2	1:E:270:LEU:HB2	1.92	0.52
1:A:211:GLU:OE2	1:A:211:GLU:HA	2.11	0.51
1:A:283:ARG:HH21	1:A:283:ARG:HG2	1.76	0.51
1:F:264:MET:HG2	1:F:270:LEU:HB2	1.94	0.50
1:B:264:MET:HG2	1:B:270:LEU:HB2	1.95	0.49
1:E:263:TYR:CZ	1:E:272:ASP:HA	2.49	0.48
1:C:264:MET:HG2	1:C:270:LEU:HB2	1.93	0.48
1:B:159:ARG:NH2	3:B:402:FBP:O3P	2.47	0.48
1:C:110:ASP:HB2	1:C:111:PRO:HD3	1.95	0.48
1:F:110:ASP:HB2	1:F:111:PRO:HD3	1.95	0.48
1:D:264:MET:HG2	1:D:270:LEU:HB2	1.95	0.48
1:B:91:GLY:CA	1:C:189:TRP:CD1	2.97	0.47
1:C:124:ALA:HB2	1:C:243:LEU:HD21	1.96	0.47
1:B:277:THR:OG1	1:B:278:PRO:HD2	2.14	0.47
1:B:124:ALA:HB2	1:B:243:LEU:HD21	1.96	0.47
1:F:263:TYR:CZ	1:F:272:ASP:HA	2.50	0.47
1:D:110:ASP:HB2	1:D:111:PRO:HD3	1.97	0.46
1:B:93:THR:HG22	1:C:215:VAL:HG11	1.98	0.46
1:F:174:HIS:HE1	3:F:402:FBP:O5	1.98	0.46
1:A:263:TYR:CZ	1:A:272:ASP:HA	2.50	0.46
1:C:6:ASP:OD1	1:D:283:ARG:NH1	2.49	0.46
1:B:263:TYR:CZ	1:B:272:ASP:HA	2.51	0.46
1:D:124:ALA:HB2	1:D:243:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:HB2	1:A:111:PRO:HD3	1.97	0.45
1:E:110:ASP:HB2	1:E:111:PRO:HD3	1.97	0.45
1:E:124:ALA:HB2	1:E:243:LEU:HD21	1.99	0.45
1:F:277:THR:OG1	1:F:278:PRO:HD2	2.17	0.45
1:E:230:LYS:HE3	1:E:230:LYS:HB3	1.58	0.45
1:C:263:TYR:CZ	1:C:272:ASP:HA	2.53	0.44
1:F:124:ALA:HB2	1:F:243:LEU:HD21	1.99	0.44
1:B:110:ASP:HB2	1:B:111:PRO:HD3	1.99	0.43
1:A:277:THR:OG1	1:A:278:PRO:HD2	2.19	0.43
1:C:174:HIS:CE1	1:F:174:HIS:CE1	3.07	0.43
1:D:263:TYR:CZ	1:D:272:ASP:HA	2.53	0.43
1:A:124:ALA:HB2	1:A:243:LEU:HD21	1.99	0.43
1:B:174:HIS:HE1	3:B:402:FBP:O5	2.02	0.43
1:C:61:THR:O	1:E:171:ARG:HD2	2.19	0.42
1:C:277:THR:OG1	1:C:278:PRO:HD2	2.19	0.42
1:F:248:LYS:NZ	4:F:501:HOH:O	2.46	0.42
1:B:91:GLY:HA2	1:C:189:TRP:CD1	2.55	0.42
1:C:99:ASN:O	1:C:103:LYS:HG2	2.20	0.42
1:E:201:GLU:O	1:E:204:LYS:HB2	2.19	0.42
1:A:148:GLY:HA3	1:A:261:SER:OG	2.19	0.41
1:B:58:LEU:HA	1:B:61:THR:CG2	2.47	0.41
1:D:277:THR:OG1	1:D:278:PRO:HD2	2.21	0.41
1:D:293:PRO:HG2	1:E:201:GLU:OE2	2.19	0.41
1:D:148:GLY:HA3	1:D:261:SER:OG	2.20	0.41
1:D:201:GLU:OE1	1:E:293:PRO:HG3	2.21	0.41
1:E:277:THR:OG1	1:E:278:PRO:HD2	2.21	0.41
1:B:148:GLY:HA3	1:B:261:SER:OG	2.22	0.40
1:D:257:VAL:HG11	1:E:195:GLY:HA3	2.03	0.40
1:C:58:LEU:HA	1:C:61:THR:CG2	2.45	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	306/326 (94%)	300 (98%)	6 (2%)	0	100	100
1	B	314/326 (96%)	305 (97%)	9 (3%)	0	100	100
1	C	307/326 (94%)	300 (98%)	7 (2%)	0	100	100
1	D	312/326 (96%)	304 (97%)	8 (3%)	0	100	100
1	E	304/326 (93%)	297 (98%)	7 (2%)	0	100	100
1	F	314/326 (96%)	307 (98%)	7 (2%)	0	100	100
All	All	1857/1956 (95%)	1813 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	256/269 (95%)	247 (96%)	9 (4%)	36	65
1	B	260/269 (97%)	252 (97%)	8 (3%)	40	69
1	C	257/269 (96%)	248 (96%)	9 (4%)	36	65
1	D	259/269 (96%)	249 (96%)	10 (4%)	32	61
1	E	254/269 (94%)	246 (97%)	8 (3%)	40	69
1	F	260/269 (97%)	252 (97%)	8 (3%)	40	69
All	All	1546/1614 (96%)	1494 (97%)	52 (3%)	37	66

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	103	LYS
1	A	161	SER
1	A	210	LYS
1	A	211	GLU
1	A	212	ASP
1	A	261	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	264	MET
1	A	300	GLU
1	B	46	LYS
1	B	50	ASP
1	B	161	SER
1	B	261	SER
1	B	264	MET
1	B	290	LEU
1	B	297	HIS
1	B	300	GLU
1	C	48	LYS
1	C	50	ASP
1	C	161	SER
1	C	166	VAL
1	C	213	LYS
1	C	264	MET
1	C	297	HIS
1	C	300	GLU
1	C	307	SER
1	D	50	ASP
1	D	93	THR
1	D	161	SER
1	D	166	VAL
1	D	201	GLU
1	D	211	GLU
1	D	213	LYS
1	D	261	SER
1	D	264	MET
1	D	300	GLU
1	E	50	ASP
1	E	89	LYS
1	E	161	SER
1	E	166	VAL
1	E	212	ASP
1	E	230	LYS
1	E	264	MET
1	E	297	HIS
1	F	50	ASP
1	F	137	LYS
1	F	161	SER
1	F	208	GLU
1	F	210	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	264	MET
1	F	297	HIS
1	F	307	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	HIS

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)

9 ligands are modelled in this entry.

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	E	402	-	18,20,20	0.96	0	23,32,32	1.47	4 (17%)
2	SO4	E	401	-	4,4,4	0.61	0	6,6,6	0.65	0
2	SO4	D	401	-	4,4,4	0.54	0	6,6,6	1.05	0
2	SO4	F	401	-	4,4,4	0.43	0	6,6,6	1.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FBP	B	402	-	18,20,20	1.04	1 (5%)	23,32,32	2.57	8 (34%)
3	FBP	F	402	-	18,20,20	0.67	0	23,32,32	1.85	6 (26%)
2	SO4	A	401	-	4,4,4	0.52	0	6,6,6	0.65	0
2	SO4	B	401	-	4,4,4	0.69	0	6,6,6	0.89	0
2	SO4	C	401	-	4,4,4	0.49	0	6,6,6	0.42	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	F	402	-	-	7/13/32/32	0/1/1/1
3	FBP	E	402	-	-	6/13/32/32	0/1/1/1
3	FBP	B	402	-	-	7/13/32/32	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	FBP	P1-O3P	-2.01	1.47	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	FBP	O6-P2-O4P	5.95	123.18	106.47
3	B	402	FBP	O1-P1-O1P	5.15	120.92	106.47
3	B	402	FBP	O5P-P2-O6	-4.94	93.59	106.73
3	F	402	FBP	O1-P1-O1P	-4.33	94.34	106.47
3	B	402	FBP	O2P-P1-O1	-3.87	96.43	106.73
3	F	402	FBP	O2P-P1-O1	3.81	116.87	106.73
3	E	402	FBP	O1-P1-O1P	3.73	116.93	106.47
3	B	402	FBP	O6P-P2-O6	-3.67	96.98	106.73
3	B	402	FBP	O6P-P2-O5P	3.15	119.69	107.64
3	F	402	FBP	O6P-P2-O4P	2.78	121.57	110.68
3	E	402	FBP	P2-O6-C6	2.75	125.88	118.30
3	E	402	FBP	O6P-P2-O6	2.73	113.99	106.73
3	F	402	FBP	O6-P2-O4P	-2.66	99.00	106.47
3	B	402	FBP	O2P-P1-O1P	2.64	121.03	110.68
3	F	402	FBP	O6P-P2-O6	2.63	113.73	106.73
3	F	402	FBP	O2P-P1-O1P	2.56	120.71	110.68
3	E	402	FBP	O6-P2-O4P	-2.24	100.20	106.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	FBP	P1-O1-C1	2.04	123.91	118.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	FBP	C1-O1-P1-O2P
3	B	402	FBP	C1-O1-P1-O3P
3	B	402	FBP	O1-C1-C2-O2
3	B	402	FBP	O1-C1-C2-C3
3	B	402	FBP	O1-C1-C2-O5
3	E	402	FBP	O1-C1-C2-C3
3	E	402	FBP	C4-C5-C6-O6
3	E	402	FBP	C6-O6-P2-O5P
3	E	402	FBP	C6-O6-P2-O6P
3	F	402	FBP	C4-C5-C6-O6
3	F	402	FBP	C6-O6-P2-O4P
3	F	402	FBP	C6-O6-P2-O5P
3	F	402	FBP	C6-O6-P2-O6P
3	E	402	FBP	O5-C5-C6-O6
3	F	402	FBP	O5-C5-C6-O6
3	E	402	FBP	C6-O6-P2-O4P
3	B	402	FBP	C1-O1-P1-O1P
3	F	402	FBP	C5-C6-O6-P2
3	F	402	FBP	O1-C1-C2-C3
3	B	402	FBP	C4-C5-C6-O6

There are no ring outliers.

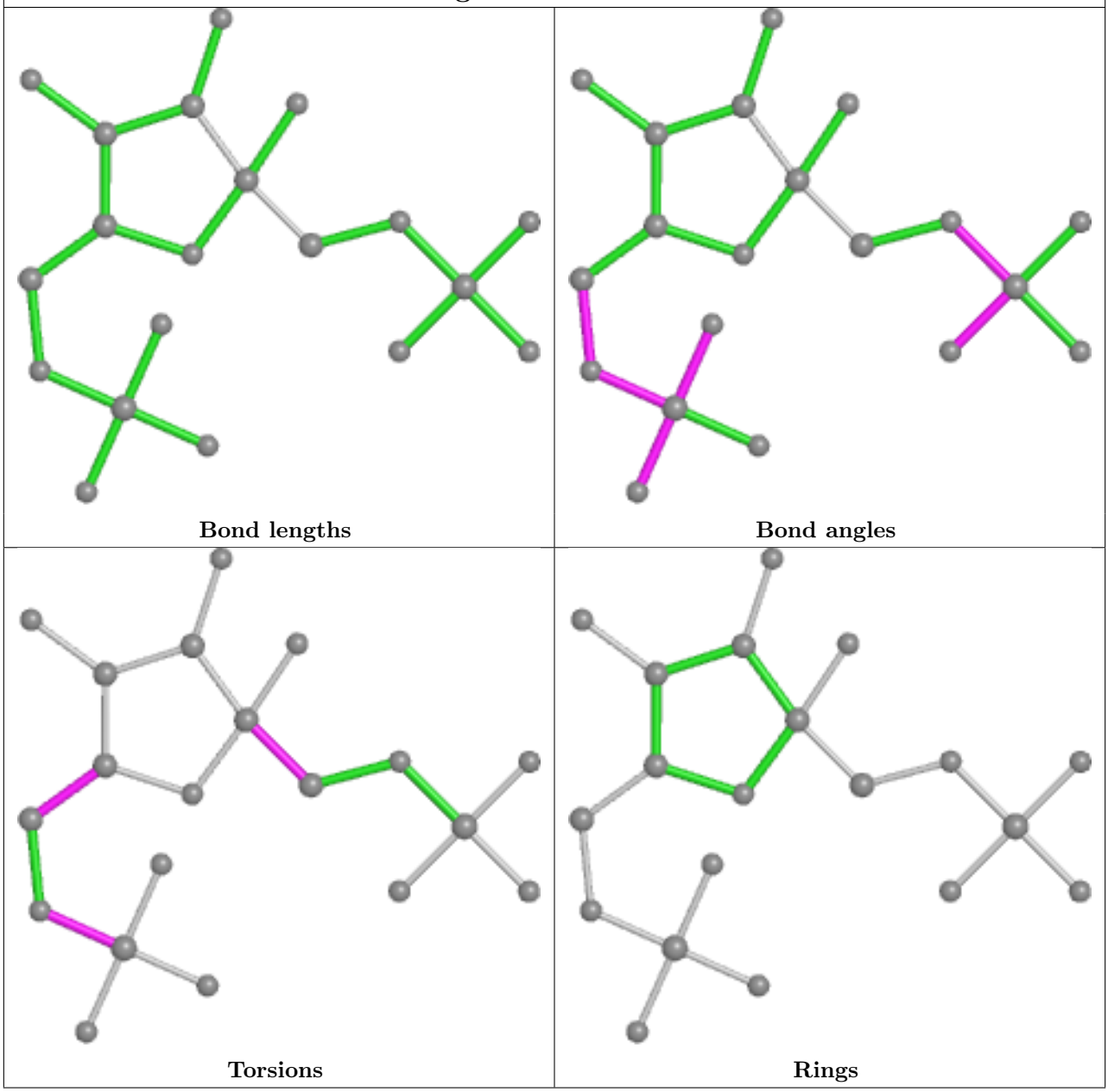
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	FBP	2	0
3	F	402	FBP	2	0

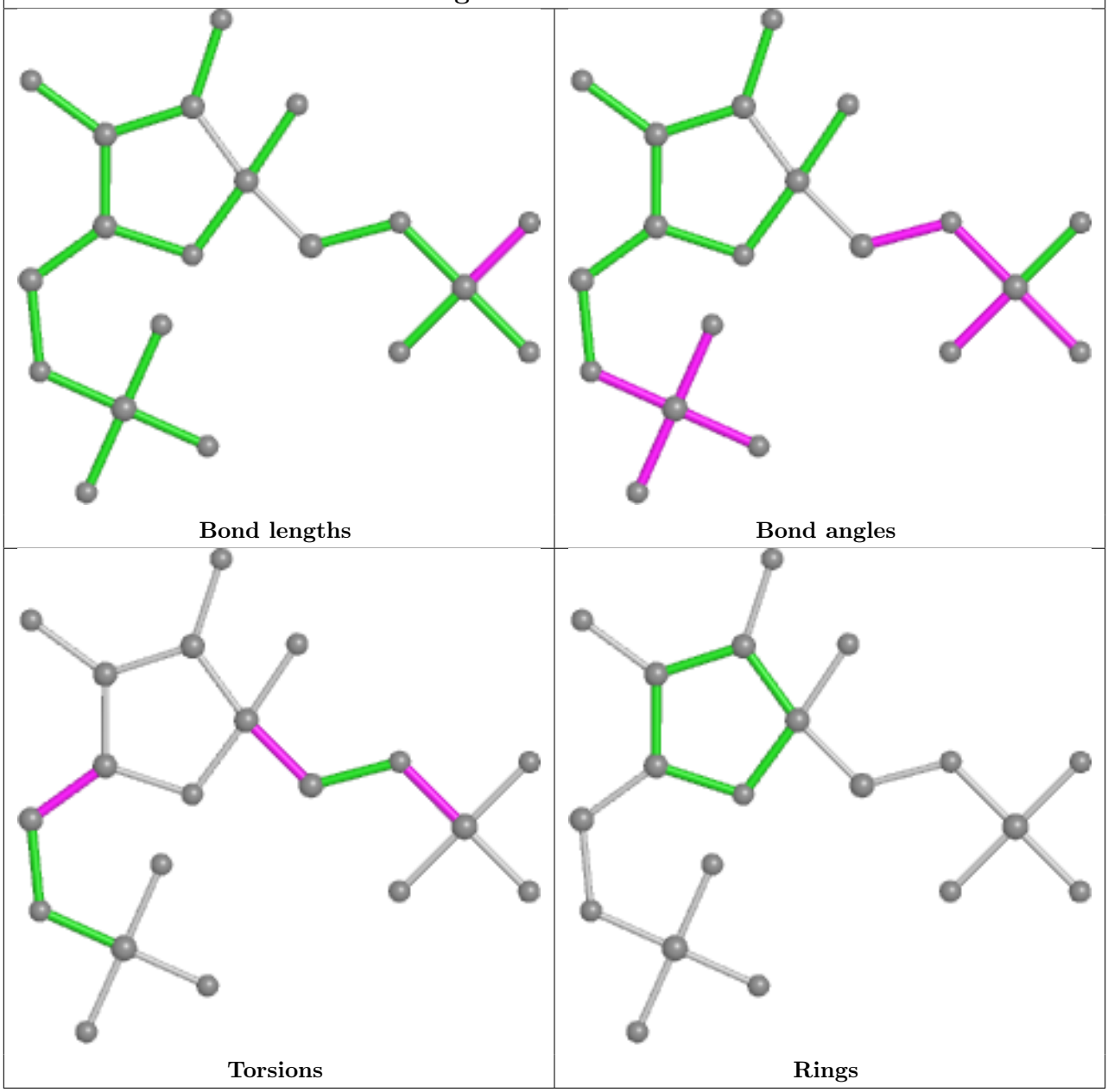
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

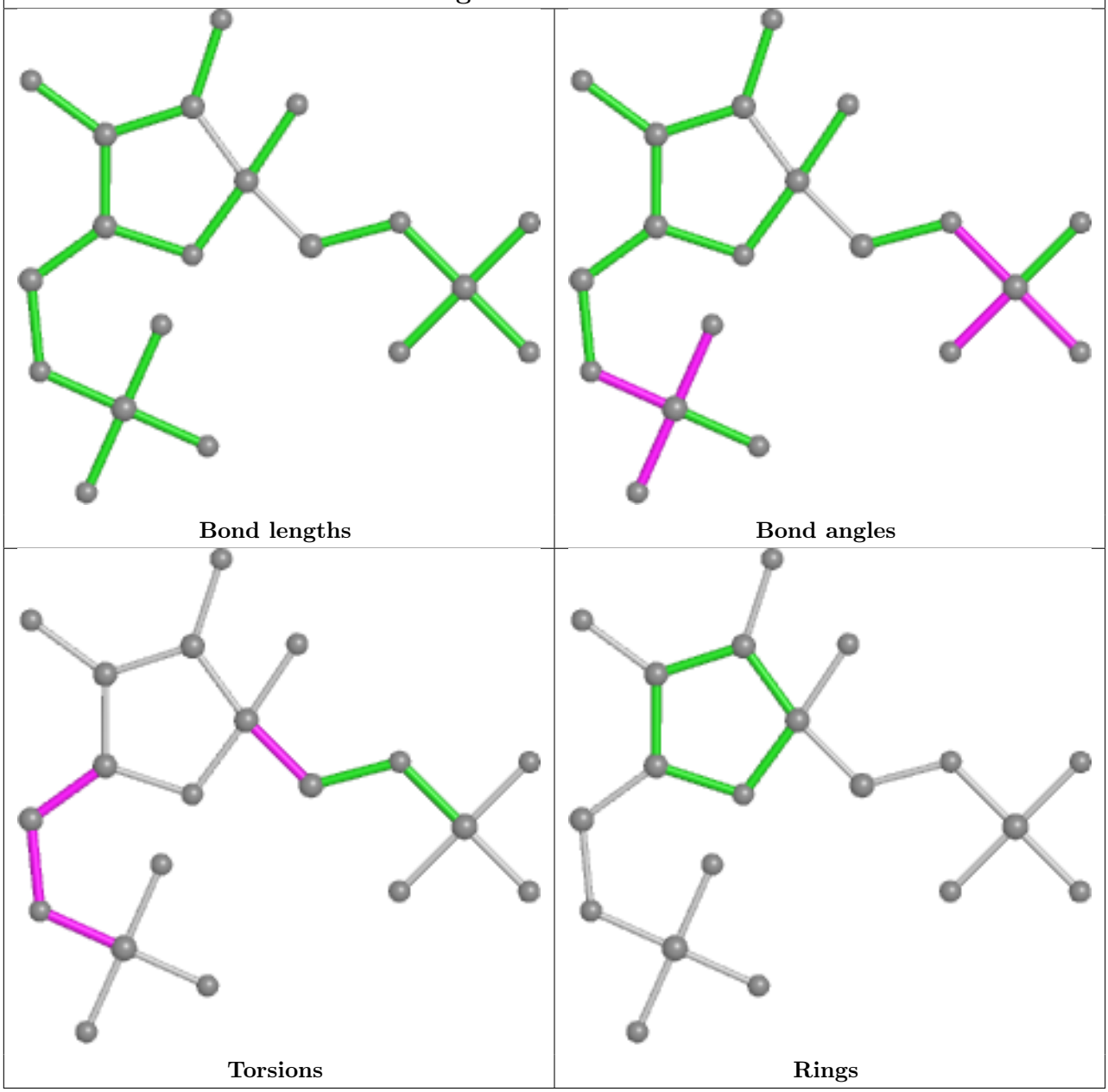
Ligand FBP E 402



Ligand FBP B 402



Ligand FBP F 402



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	310/326 (95%)	0.12	15 (4%)	30	28	28, 49, 77, 90	0
1	B	316/326 (96%)	-0.01	7 (2%)	62	63	25, 41, 67, 89	0
1	C	311/326 (95%)	0.05	12 (3%)	39	38	28, 48, 78, 88	0
1	D	314/326 (96%)	0.08	10 (3%)	47	48	24, 41, 77, 100	0
1	E	308/326 (94%)	0.01	10 (3%)	47	48	27, 40, 66, 107	0
1	F	316/326 (96%)	0.08	12 (3%)	40	39	29, 47, 74, 93	0
All	All	1875/1956 (95%)	0.06	66 (3%)	44	44	24, 44, 75, 107	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	211	GLU	5.5
1	D	90	PRO	5.0
1	F	204	LYS	4.7
1	B	212	ASP	4.5
1	D	226	TYR	4.1
1	F	212	ASP	4.1
1	C	96	ASP	4.0
1	A	93	THR	3.9
1	A	226	TYR	3.9
1	E	212	ASP	3.8
1	B	209	ILE	3.7
1	A	99	ASN	3.6
1	A	75	LYS	3.6
1	C	87	PRO	3.5
1	A	313	LEU	3.4
1	E	201	GLU	3.4
1	C	226	TYR	3.3
1	B	210	LYS	3.3
1	C	93	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	88	GLN	3.2
1	D	208	GLU	3.1
1	D	311	LYS	3.1
1	F	114	ASP	3.0
1	E	204	LYS	2.9
1	C	99	ASN	2.9
1	E	200	ALA	2.8
1	F	210	LYS	2.8
1	F	209	ILE	2.8
1	C	183	ASP	2.8
1	E	114	ASP	2.7
1	D	93	THR	2.7
1	C	3	SER	2.7
1	E	44	LYS	2.7
1	D	5	THR	2.7
1	D	200	ALA	2.6
1	A	314	THR	2.6
1	C	297	HIS	2.5
1	A	95	LEU	2.5
1	A	102	LEU	2.5
1	F	214	LEU	2.5
1	A	263	TYR	2.4
1	A	103	LYS	2.4
1	A	96	ASP	2.4
1	A	273	ILE	2.4
1	C	317	PHE	2.4
1	F	215	VAL	2.4
1	E	115	SER	2.3
1	E	43	PHE	2.3
1	A	297	HIS	2.3
1	E	202	TRP	2.3
1	B	115	SER	2.3
1	D	95	LEU	2.3
1	F	211	GLU	2.2
1	C	223	ASP	2.2
1	B	203	VAL	2.2
1	C	88	GLN	2.2
1	D	227	GLU	2.2
1	F	207	PRO	2.1
1	A	115	SER	2.1
1	C	94	ARG	2.1
1	F	220	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	216	LYS	2.1
1	D	315	ASP	2.1
1	F	213	LYS	2.0
1	B	75	LYS	2.0
1	B	214	LEU	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)

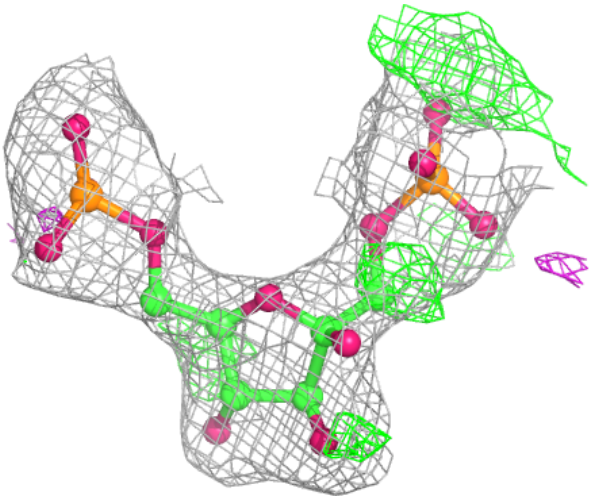
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

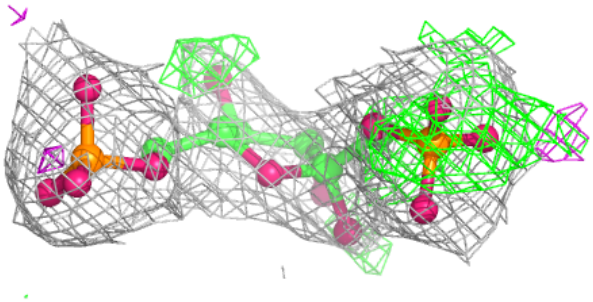
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FBP	B	402	20/20	0.88	0.31	26,36,58,61	13
3	FBP	F	402	20/20	0.89	0.30	24,33,62,69	13
3	FBP	E	402	20/20	0.93	0.35	19,23,38,41	13
2	SO4	F	401	5/5	0.94	0.14	68,68,73,77	0
2	SO4	B	401	5/5	0.94	0.13	58,58,59,70	0
2	SO4	C	401	5/5	0.96	0.12	57,62,66,71	0
2	SO4	E	401	5/5	0.96	0.10	52,54,64,64	0
2	SO4	A	401	5/5	0.96	0.12	64,65,71,73	0
2	SO4	D	401	5/5	0.97	0.11	48,52,53,54	0

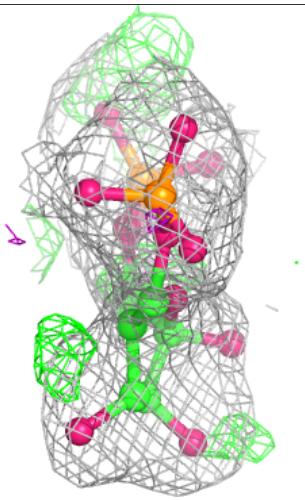
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP B 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

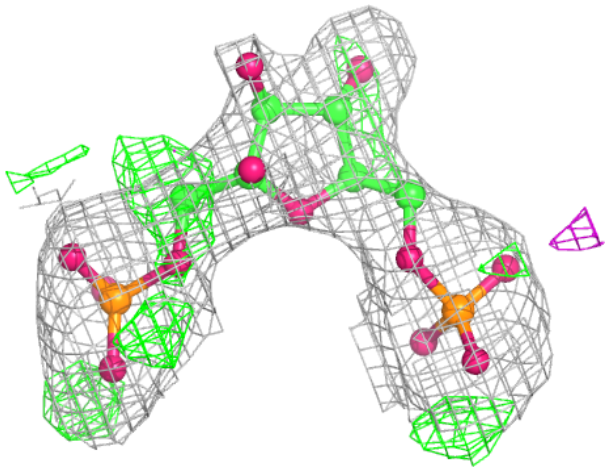


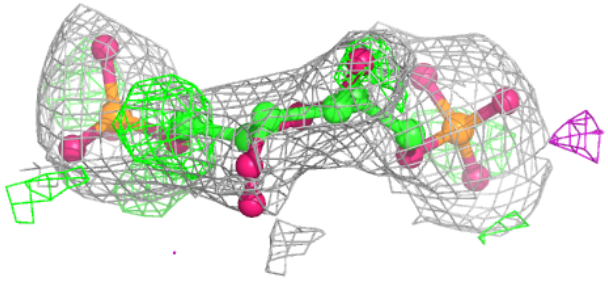


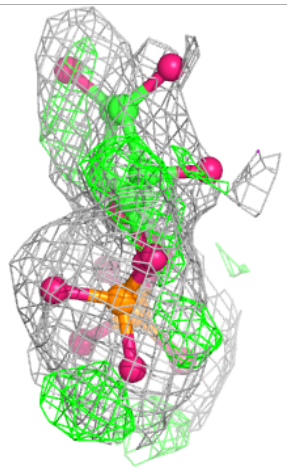


Electron density around FBP F 402:

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

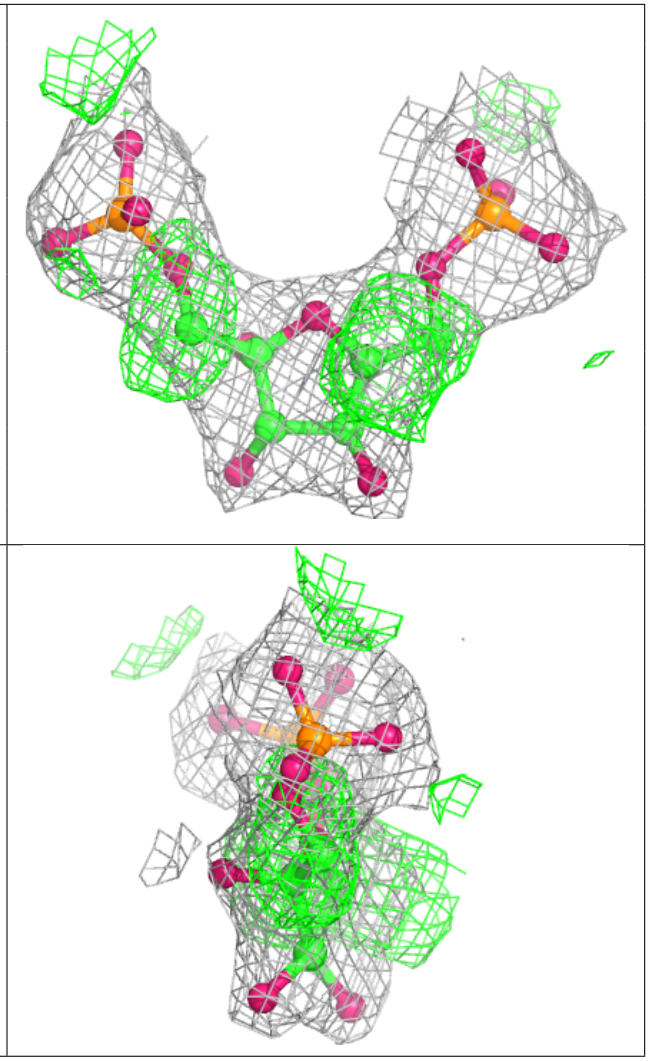






Electron density around FBP E 402:

$2mF_o$-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.