



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 12:34 AM BST

PDB ID : 1BO5
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN ESCHERICHIA COLI GLYCEROL KINASE AND THE ALLOSTERIC REGULATOR FRUCTOSE 1,6-BISPHOSPHATE.
Authors : Ormo, M.; Bystrom, C.E.; Remington, S.J.
Deposited on : 1998-08-10
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

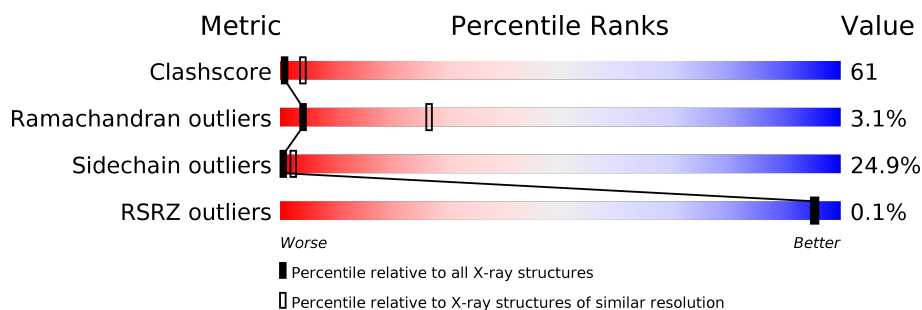
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

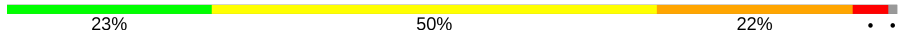
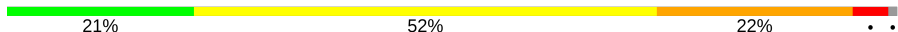
The reported resolution of this entry is 3.20 Å.

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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	501	
1	Z	501	

2 Entry composition [i](#)

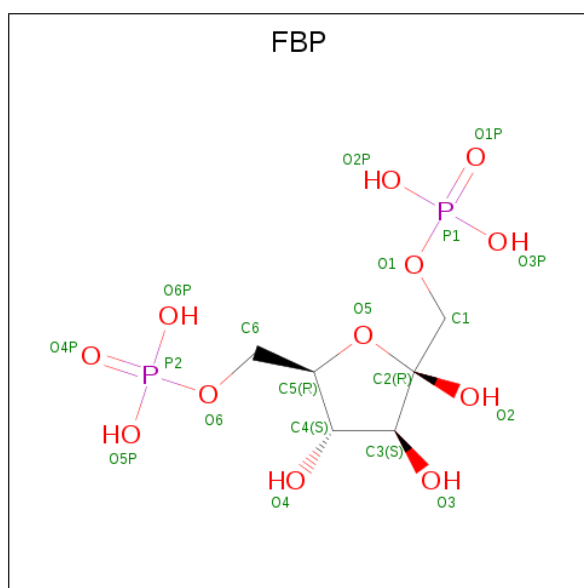
There are 3 unique types of molecules in this entry. The entry contains 7818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (GLYCEROL KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	498	Total	C	N	O	S	0	0	0
			3878	2453	671	735	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3888	2456	674	739	19			

- Molecule 2 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
2	O	1	Total	C	O	P	0	1
			40	12	24	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

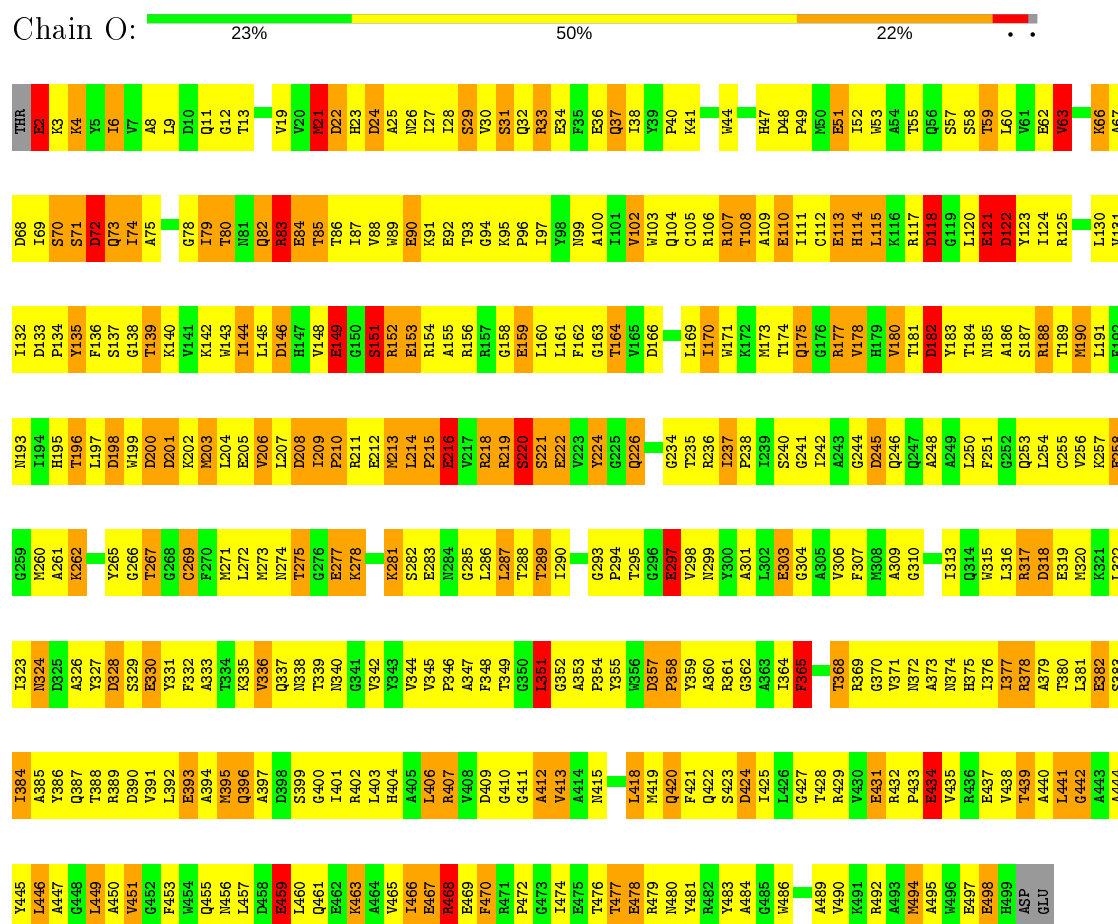


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			6	3	3		
3	Z	1	Total	C	O	0	0
			6	3	3		

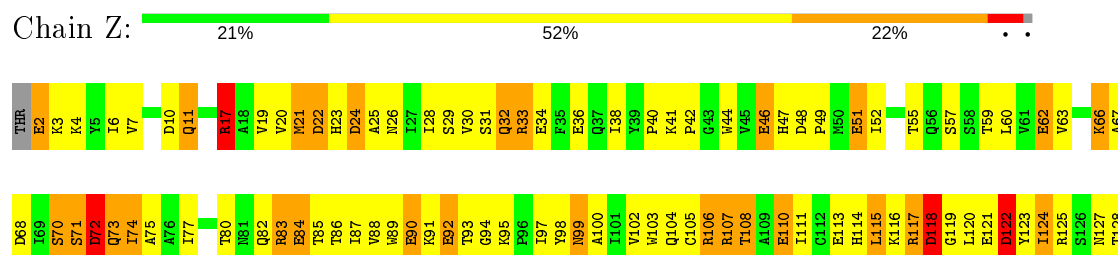
3 Residue-property plots

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

• Molecule 1: PROTEIN (GLYCEROL KINASE)



• Molecule 1: PROTEIN (GLYCEROL KINASE)



L441	G442	A443	A444	Y445	L446	A447	G448	L449	A450	V451	G452	F453	Y454	Q455	Y456	L457	Y458	F459	L460	Q461	F462	K463	A464	Y465	L466	E467	R468	E469	F470	R471	P472	E475	T476	T477	E478	R479	N480	Y481	R482	Y483	A484	G485	Y486	A489	V490	R491	R492	A493	N494	Y495	Y496	F497	F498	H499	ASP	GLU							
A379	T380	L381	E382	S383	L384	A385	Y386	Q387	T388	R389	D390	Y391	L392	E393	A394	N395	Q396	A397	D398	S399	G400	I401	R402	L403	L406	R407	Y408	D409	Q410	F411	A412	V413	N415	L418	N419	Q420	F421	Q422	Y483	N484	D424	G485	Y486	L426	Q427	T428	R429	V430	E431	R432	A433	E434	T435	R436	E437	V438	T439	A440					
R317	C318	E319	N320	K321	L322	I323	N324	D325	A326	Y327	D328	S329	E330	F331	C332	A333	T334	K335	V336	Q337	R338	T339	N340	G341	V342	T343	V344	V345	P346	A347	F348	T349	G350	L351	G352	A353	P354	Y355	Y356	D357	P358	Y359	A360	R361	G362	I363	F365	T368	V371	N372	A373	N374	H375	I376	T377	R378							
C254	L191	V256	K257	E258	G259	K260	A261	R262	N263	T264	Y265	G266	T267	G268	C269	F270	M271	L272	M273	N274	E277	V280	K281	S282	E283	L286	L287	T288	T289	I290	A291	G292	G293	P294	T295	G296	E297	V298	N299	Y300	A301	L302	E303	G304	A305	V306	F307	M308	G309	G310	A311	S312	I313	Q314	L316								
L130	L191	F192	M193	K194	H195	T196	L197	D198	W199	D200	T201	K202	M203	L204	E205	I206	L207	D208	I209	P210	R211	E212	M213	L214	P215	E216	V217	R218	R219	S220	S221	E222	Y223	Y224	G225	Q226	K227	G228	G229	T230	R231	I232	P233	I234	S235	G236	G237	T238	D239	G240	I241	I242	A243	G244	D245	Q246	Q247	A248	A249	L250	F251	G252	Q253
G129	L130	V131	I132	D133	I194	P134	Y135	F136	S137	G138	T139	K140	V141	K142	W143	I144	L145	D146	H147	V148	E149	G150	S151	R152	E153	R154	A155	R156	R157	G158	E159	L160	L161	F162	G163	T164	V165	D166	L169	I170	W171	K172	M173	T174	Q175	G176	R177	V178	H179	V180	T181	D182	Y183	T184	N185	A186	S187	R188	T189				

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.41Å 169.41Å 204.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-3.20) 90.3 (19.97-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.98Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.211 , (Not available) 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7818	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	O	1.17	35/3958 (0.9%)	1.51	55/5373 (1.0%)
1	Z	1.18	32/3968 (0.8%)	1.53	55/5387 (1.0%)
All	All	1.18	67/7926 (0.8%)	1.52	110/10760 (1.0%)

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	O	1	1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	51	GLU	CD-OE1	8.97	1.35	1.25
1	Z	92	GLU	CD-OE1	8.22	1.34	1.25
1	Z	382	GLU	CD-OE2	8.19	1.34	1.25
1	O	51	GLU	CD-OE1	8.05	1.34	1.25
1	Z	212	GLU	CD-OE2	7.96	1.34	1.25

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	22	ASP	CB-CG-OD1	8.79	126.21	118.30
1	O	201	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	Z	10	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	Z	409	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	O	24	ASP	CB-CG-OD1	-7.97	111.12	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	O	21	MET	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	351	LEU	Mainchain

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	O	3878	0	3774	472	0
1	Z	3888	0	3778	463	0
2	O	40	0	20	3	0
3	O	6	0	8	2	0
3	Z	6	0	8	0	0
All	All	7818	0	7588	935	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 61.

The worst 5 of 935 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:O:83:ARG:HH11	1:O:83:ARG:HG3	1.04	1.11
1:O:145:LEU:HD11	1:O:213:MET:HE1	1.30	1.11
1:Z:438:VAL:HA	1:Z:441:LEU:HD12	1.30	1.06
1:Z:71:SER:HB2	1:Z:235:THR:HG21	1.32	1.05
1:O:255:CYS:HB3	1:O:260:MET:HB3	1.39	1.03

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	O	496/501 (99%)	406 (82%)	74 (15%)	16 (3%)	4	26
1	Z	496/501 (99%)	414 (84%)	67 (14%)	15 (3%)	4	28
All	All	992/1002 (99%)	820 (83%)	141 (14%)	31 (3%)	4	26

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	99	ASN
1	O	121	GLU
1	O	151	SER
1	Z	149	GLU
1	O	72	ASP

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	O	396/412 (96%)	301 (76%)	95 (24%)	0	3
1	Z	398/412 (97%)	295 (74%)	103 (26%)	0	2
All	All	794/824 (96%)	596 (75%)	198 (25%)	0	2

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	466	ILE

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Mol	Chain	Res	Type
1	Z	74	ILE
1	Z	455	GLN
1	O	477	THR
1	Z	29	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	11	GLN
1	Z	179	HIS
1	Z	461	GLN
1	Z	147	HIS
1	Z	228	ASN

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 ⓘ

4 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	GOL	O	601	-	5,5,5	0.38	0	5,5,5	0.51	0
2	FBP	O	502[B]	-	18,20,20	0.96	0	23,32,32	1.21	2 (8%)
2	FBP	O	502[A]	-	18,20,20	1.04	0	23,32,32	1.44	2 (8%)
3	GOL	Z	601	-	5,5,5	0.34	0	5,5,5	0.39	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	GOL	O	601	-	-	2/4/4/4	-
2	FBP	O	502[B]	-	-	9/13/32/32	0/1/1/1
2	FBP	O	502[A]	-	-	10/13/32/32	0/1/1/1
3	GOL	Z	601	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	502[A]	FBP	O3P-P1-O2P	4.86	126.22	107.64
2	O	502[A]	FBP	O6P-P2-O5P	3.11	119.54	107.64
2	O	502[B]	FBP	O6P-P2-O5P	3.06	119.34	107.64
2	O	502[B]	FBP	O3P-P1-O2P	2.96	118.94	107.64

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	O	601	GOL	O1-C1-C2-C3
2	O	502[B]	FBP	C1-O1-P1-O1P
2	O	502[B]	FBP	C1-O1-P1-O2P
2	O	502[B]	FBP	C1-O1-P1-O3P
2	O	502[B]	FBP	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	601	GOL	2	0

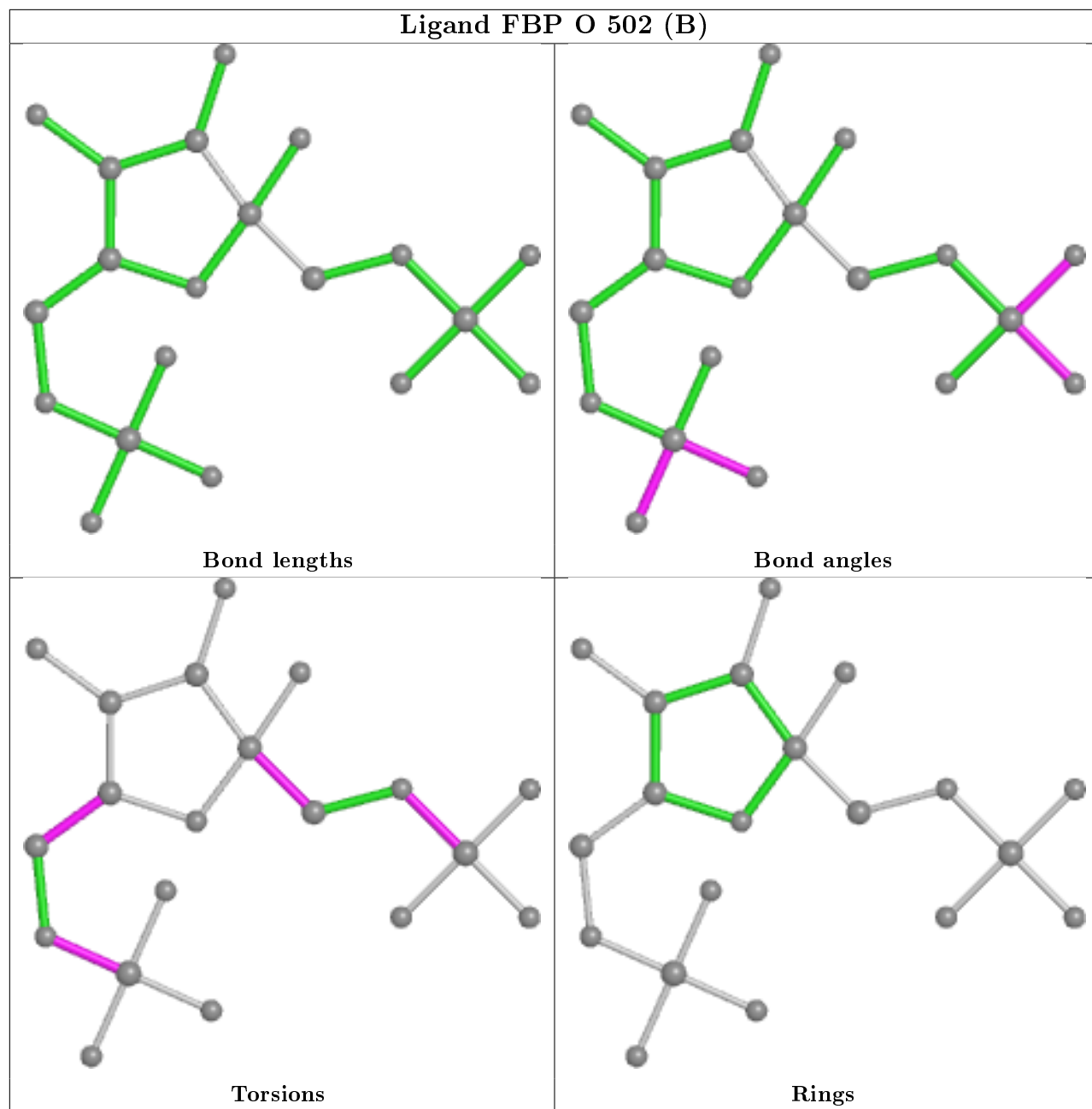
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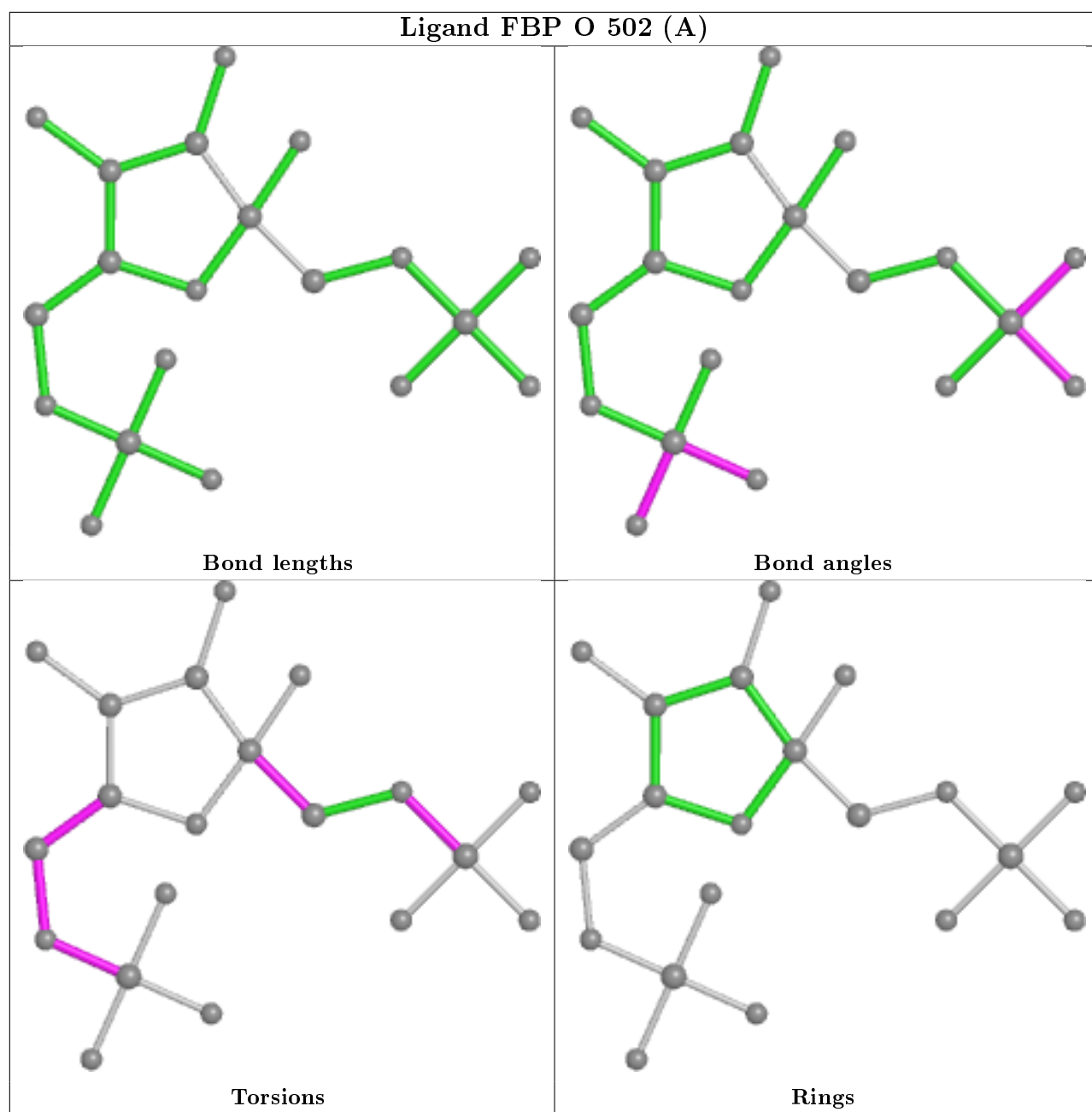
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	502[B]	FBP	1	0
2	O	502[A]	FBP	2	0

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

Ligand FBP O 502 (B)





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	O	498/501 (99%)	-0.85	0 100 100	12, 28, 62, 90	0
1	Z	498/501 (99%)	-0.89	1 (0%) 95 94	10, 26, 60, 89	0
All	All	996/1002 (99%)	-0.87	1 (0%) 95 95	10, 27, 61, 90	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	325	ASP	2.3

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](#)

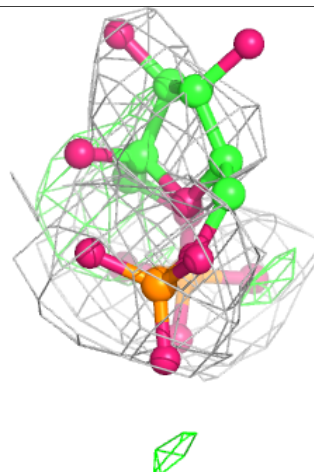
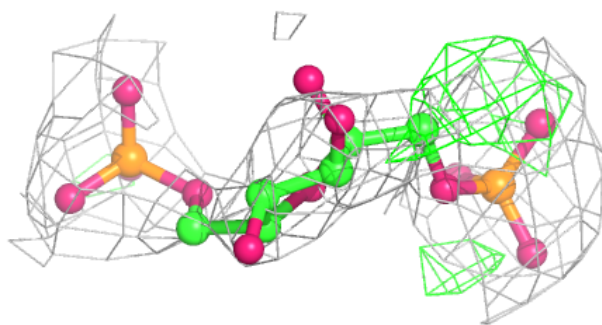
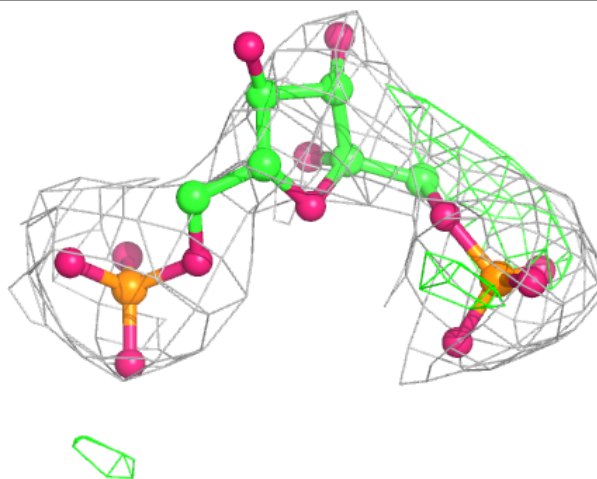
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FBP	O	502[B]	20/20	0.87	0.26	49,49,49,49	20
2	FBP	O	502[A]	20/20	0.87	0.26	49,49,49,49	20
3	GOL	O	601	6/6	0.97	0.15	10,18,32,41	0
3	GOL	Z	601	6/6	0.97	0.14	10,11,15,34	0

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

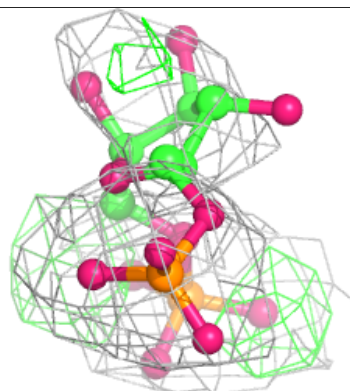
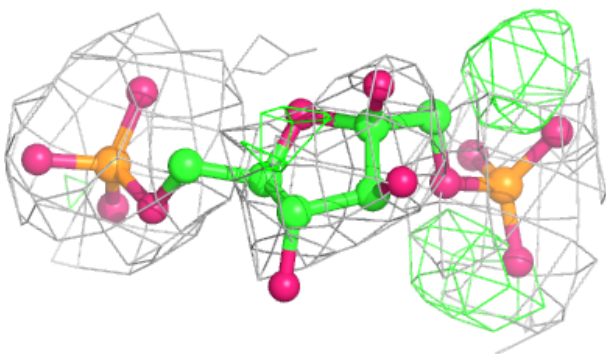
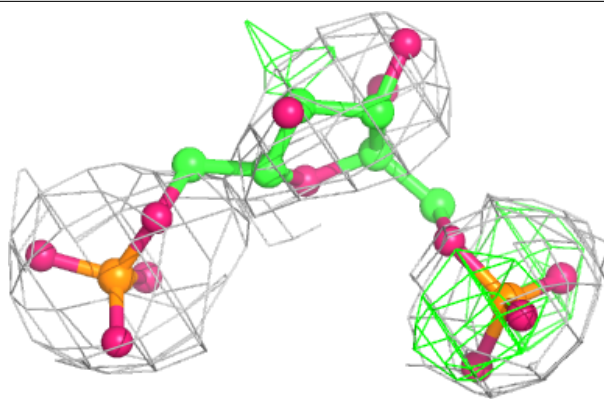
Electron density around FBP O 502 (B):

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



Electron density around FBP O 502 (A):

$2mF_o - DF_c$ (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.