



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 08:30 AM EDT

PDB ID : 6ECK  
Title : Pyruvate Kinase Isoform L-type with phosphorylated Ser113 (pS113) in complex with FBP  
Authors : Padyana, A.; Tong, S.  
Deposited on : 2018-08-08  
Resolution : 2.36 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

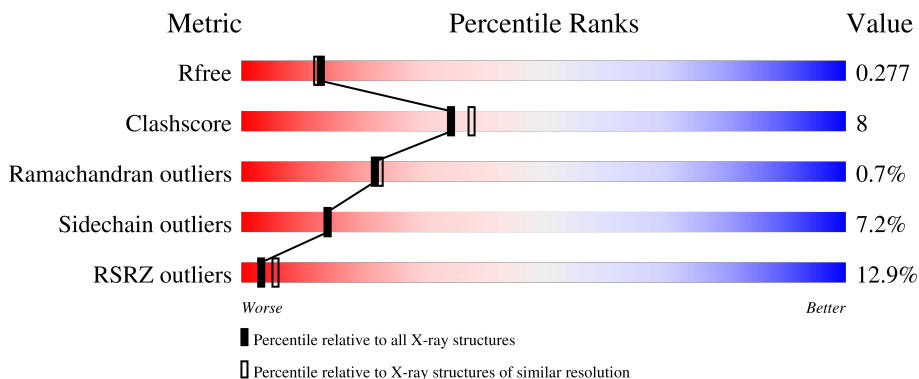
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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	A	550	
1	B	550	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	602	-	X	X	-
5	EDO	A	606	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8633 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.

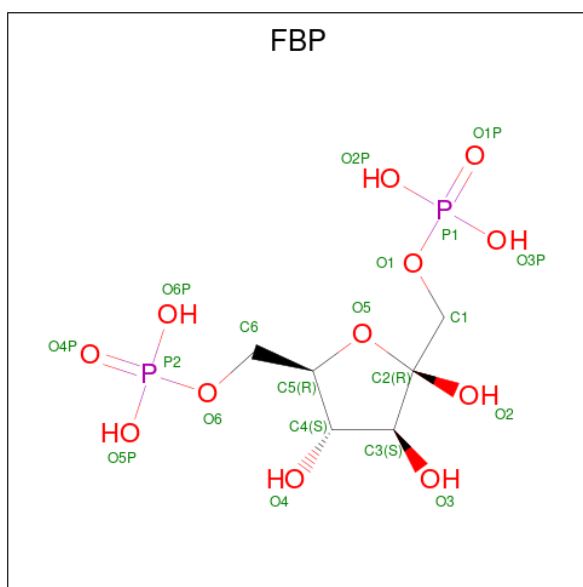
- Molecule 1 is a protein called Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	529	4054	2547	725	762	1	19	0	2	0
1	B	532	4085	2563	734	768	1	19	0	3	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P12928
A	544	HIS	-	expression tag	UNP P12928
A	546	HIS	-	expression tag	UNP P12928
A	547	HIS	-	expression tag	UNP P12928
A	548	HIS	-	expression tag	UNP P12928
A	549	HIS	-	expression tag	UNP P12928
A	550	HIS	-	expression tag	UNP P12928
B	0	HIS	-	expression tag	UNP P12928
B	544	HIS	-	expression tag	UNP P12928
B	545	HIS	-	expression tag	UNP P12928
B	546	HIS	-	expression tag	UNP P12928
B	547	HIS	-	expression tag	UNP P12928
B	548	HIS	-	expression tag	UNP P12928
B	549	HIS	-	expression tag	UNP P12928

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



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

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



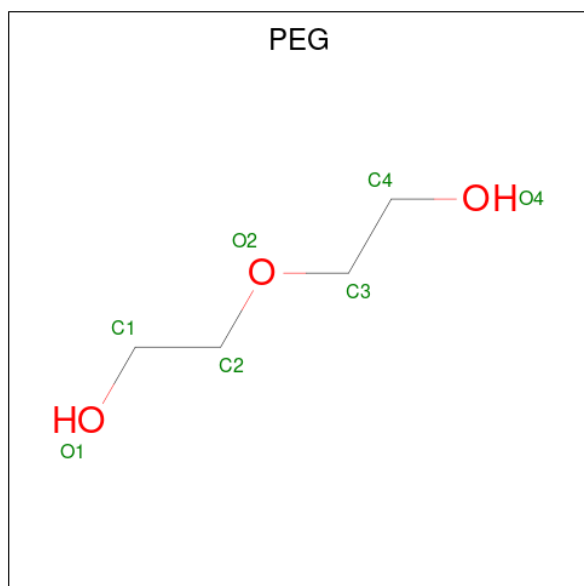
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



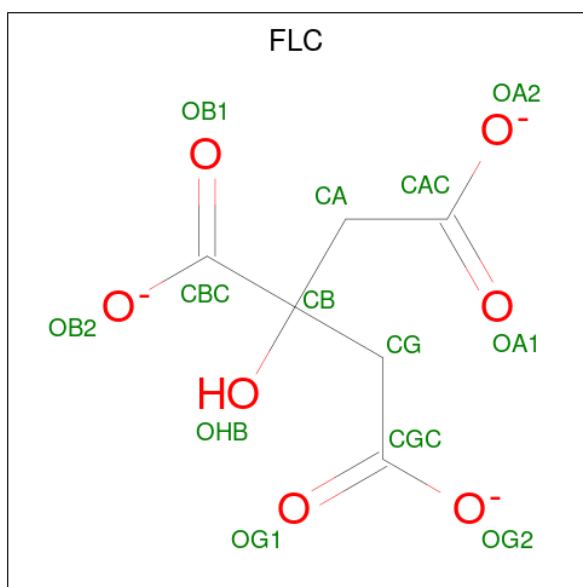
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0
4	B	1	7	4	3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



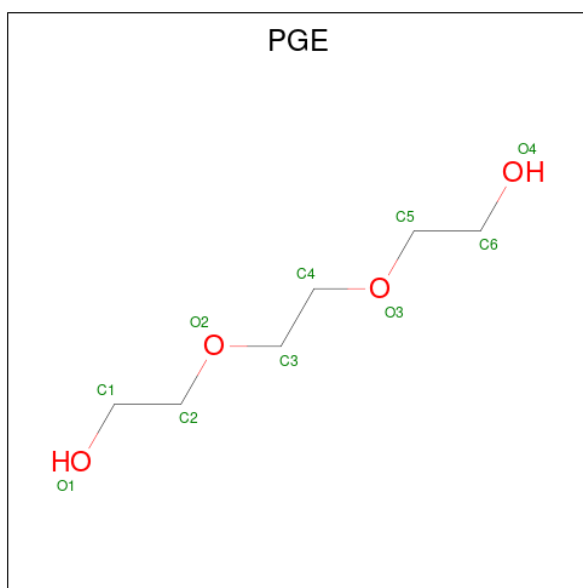
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			4	2 2		
5	A	1	Total	C O	0	0
			4	2 2		
5	A	1	Total	C O	0	0
			4	2 2		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



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

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	C O	0	0
			10	6 4		

- Molecule 8 is water.

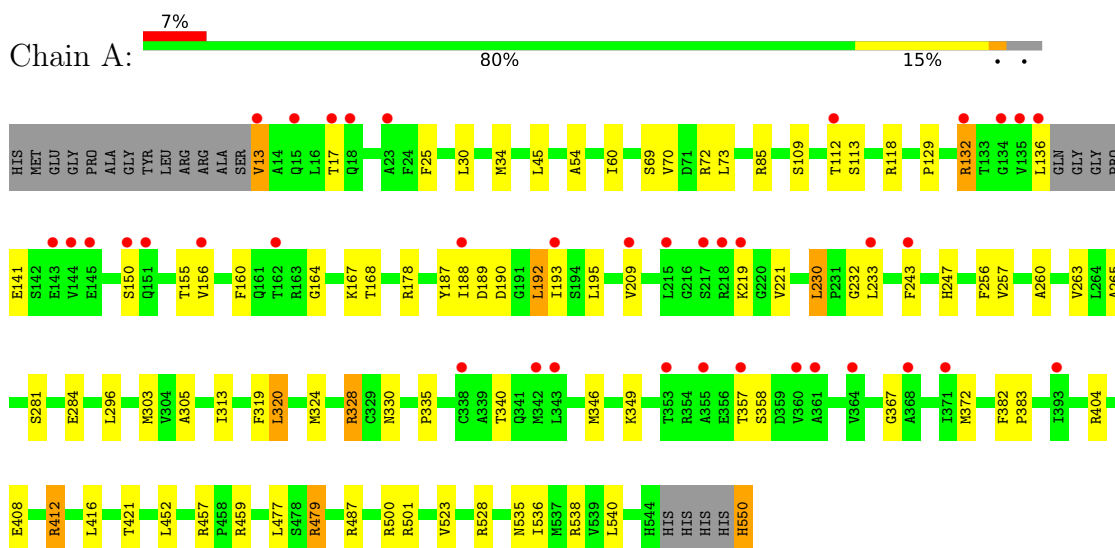
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	229	Total	O	0	0
			229	229		
8	B	158	Total	O	0	0
			158	158		



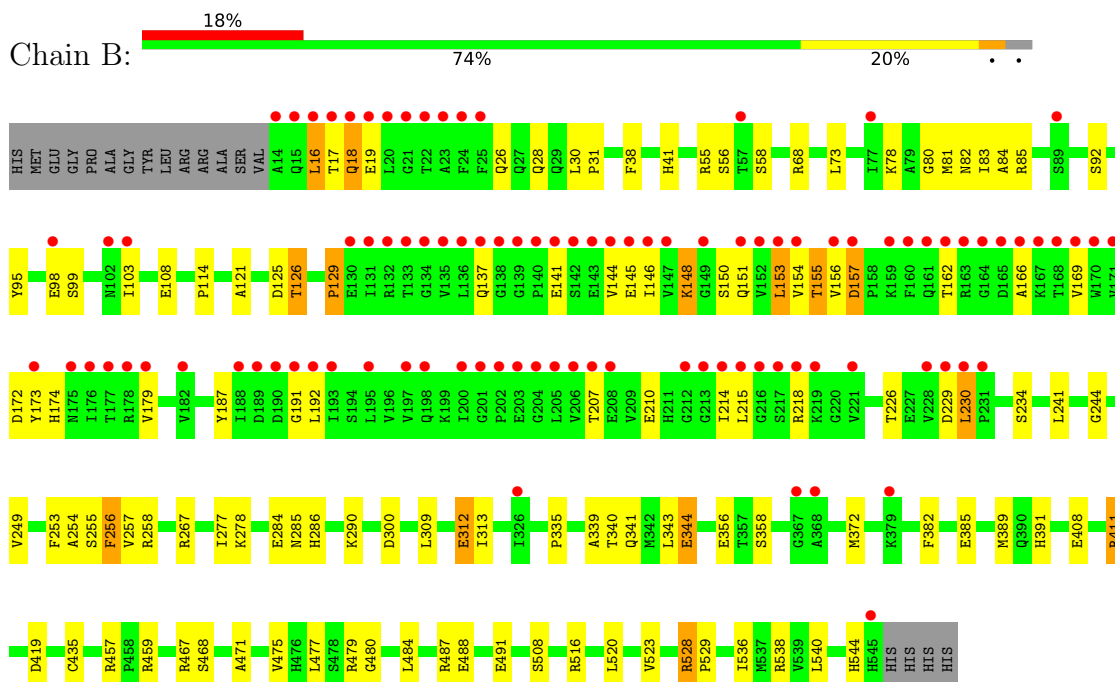
### 3 Residue-property plots i

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 PKLR



- Molecule 1: Pyruvate kinase PKLR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.77Å 111.84Å 127.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.36 48.54 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.59-2.36) 97.6 (48.54-2.36)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.203 , 0.275 0.209 , 0.277	Depositor DCC
$R_{free}$ test set	2815 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, PGE, EDO, GOL, FLC, SEP, PEG

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	0.65	0/4109	0.77	0/5560
1	B	0.62	0/4140	0.76	0/5604
All	All	0.63	0/8249	0.77	0/11164

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	A	412	ARG	Sidechain
1	A	528	ARG	Sidechain
1	B	339	ALA	Peptide
1	B	467	ARG	Sidechain

## 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	4054	0	4123	61	0
1	B	4085	0	4149	81	0
2	A	20	0	10	2	0
2	B	20	0	10	0	0
3	A	12	0	16	1	0
3	B	6	0	8	12	0
4	A	7	0	10	3	0
4	B	7	0	10	3	0
5	A	12	0	18	1	0
6	B	13	0	5	2	0
7	B	10	0	14	0	0
8	A	229	0	0	7	0
8	B	158	0	0	3	0
All	All	8633	0	8373	138	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 8.

All (138) 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:A:188:ILE:HD12	1:A:193:ILE:HD11	1.54	0.89
1:B:58:SER:OG	3:B:602:GOL:H12	1.83	0.79
1:B:55:ARG:HD3	1:B:391:HIS:ND1	2.00	0.77
1:A:136:LEU:HB2	8:A:860:HOH:O	1.90	0.71
1:B:58:SER:CB	3:B:602:GOL:H12	2.21	0.70
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.74	0.69
1:B:137:GLN:HE22	1:B:144:VAL:CG2	2.08	0.67
1:B:538[B]:ARG:HH11	1:B:540:LEU:HD11	1.60	0.67
1:A:178:ARG:NE	8:A:701:HOH:O	2.26	0.66
1:A:412:ARG:NH2	1:B:408:GLU:OE1	2.30	0.65
1:B:528:ARG:HD2	1:B:529:PRO:O	1.98	0.64
1:A:257:VAL:HG21	1:A:281:SER:HB3	1.79	0.62
1:A:319:PHE:CE2	1:A:320:LEU:HD13	2.35	0.62
1:B:81:MET:CE	1:B:84:ALA:HB2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:HA	5:A:606:EDO:O1	2.00	0.61
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.83	0.60
1:B:16:LEU:O	1:B:18:GLN:N	2.35	0.60
1:B:114:PRO:HB3	1:B:487:ARG:HH11	1.67	0.60
1:A:188:ILE:CD1	1:A:193:ILE:HD11	2.28	0.59
1:B:58:SER:CA	3:B:602:GOL:H31	2.33	0.59
1:B:56:SER:O	3:B:602:GOL:H2	2.02	0.59
1:A:536:ILE:HG12	1:B:538[A]:ARG:HG2	1.84	0.58
1:B:382:PHE:HB3	1:B:385:GLU:HG2	1.86	0.57
1:B:156:VAL:HG13	1:B:174:HIS:CD2	2.39	0.57
1:A:132:ARG:HA	1:A:219:LYS:O	2.05	0.57
1:B:141:GLU:HB3	8:B:706:HOH:O	2.04	0.57
1:B:58:SER:HA	3:B:602:GOL:H31	1.87	0.56
1:A:232:GLY:C	1:A:233:LEU:HD12	2.26	0.56
3:B:602:GOL:H32	8:B:740:HOH:O	2.06	0.56
1:A:330:ASN:HD21	1:A:367:GLY:HA3	1.72	0.55
1:A:85:ARG:HH22	3:A:603:GOL:H32	1.73	0.54
1:A:118:ARG:NE	8:A:704:HOH:O	2.32	0.54
1:A:60:ILE:HG21	1:A:372:MET:HE2	1.89	0.53
1:A:457:ARG:HH11	1:A:479:ARG:NE	2.05	0.53
1:A:538[A]:ARG:HG2	1:B:536:ILE:HG12	1.90	0.53
1:B:81:MET:HE1	1:B:84:ALA:HB2	1.89	0.53
1:B:85:ARG:NE	1:B:125:ASP:OD2	2.37	0.53
1:A:550:HIS:HB2	8:A:925:HOH:O	2.08	0.53
1:B:150:SER:OG	1:B:151:GLN:N	2.42	0.53
1:A:538[B]:ARG:HG2	1:B:536:ILE:HG12	1.90	0.52
1:A:70:VAL:HG12	8:A:845:HOH:O	2.09	0.52
1:A:187:TYR:O	1:A:221:VAL:HA	2.09	0.52
1:A:457:ARG:NH1	1:A:479:ARG:NE	2.58	0.52
1:B:129:PRO:HG2	1:B:258:ARG:NH2	2.25	0.52
1:A:408:GLU:OE1	1:B:411:ARG:NH2	2.42	0.52
1:A:188:ILE:HB	1:A:193:ILE:CG1	2.39	0.51
1:B:241:LEU:O	1:B:244:GLY:N	2.42	0.51
1:B:341:GLN:HG2	1:B:344:GLU:HG2	1.93	0.51
1:B:344:GLU:HA	1:B:344:GLU:OE1	2.11	0.51
1:B:538[B]:ARG:NH1	1:B:540:LEU:HD11	2.25	0.51
1:B:309:LEU:O	1:B:313:ILE:HG12	2.11	0.51
1:A:457:ARG:NH1	1:A:479:ARG:CB	2.74	0.50
1:B:343:LEU:HD23	1:B:356:GLU:HB3	1.93	0.50
1:B:419:ASP:OD1	1:B:419:ASP:C	2.50	0.50
1:B:528:ARG:HD3	1:B:529:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:O	1:A:190:ASP:C	2.49	0.50
1:A:540:LEU:CD2	4:A:604:PEG:H41	2.41	0.50
1:B:179:VAL:HG12	1:B:226:THR:CG2	2.41	0.50
1:B:267:ARG:NH2	1:B:300:ASP:OD2	2.45	0.50
1:B:56:SER:O	3:B:602:GOL:C2	2.61	0.49
1:B:58:SER:N	3:B:602:GOL:H11	2.27	0.49
1:A:195:LEU:CD2	1:A:209:VAL:HG22	2.42	0.49
1:A:188:ILE:HB	1:A:193:ILE:HG13	1.95	0.49
1:B:335:PRO:HB3	1:B:477:LEU:O	2.12	0.49
1:A:17:THR:HG22	1:A:25:PHE:CD2	2.47	0.49
1:B:254:ALA:O	1:B:257:VAL:HG23	2.14	0.48
1:A:178:ARG:NH1	8:A:711:HOH:O	2.45	0.48
1:A:136:LEU:HA	1:A:164:GLY:HA3	1.94	0.48
1:A:501:ARG:NH2	2:A:601:FBP:O2P	2.47	0.48
6:B:603:FLC:OA1	6:B:603:FLC:OHB	2.30	0.48
1:A:523:VAL:HG21	1:A:540:LEU:HD12	1.94	0.48
1:B:523:VAL:HG21	1:B:540:LEU:HD12	1.95	0.48
1:A:501:ARG:HH22	2:A:601:FBP:P1	2.35	0.48
1:B:83:ILE:HG12	1:B:121:ALA:HB3	1.95	0.48
1:B:92:SER:O	1:B:95:TYR:HB3	2.14	0.48
1:B:108:GLU:HA	1:B:108:GLU:OE1	2.14	0.47
1:B:56:SER:O	3:B:602:GOL:H11	2.15	0.46
1:B:187:TYR:HB3	1:B:191:GLY:HA2	1.97	0.46
1:B:154:VAL:HA	1:B:169:VAL:O	2.16	0.46
1:B:341:GLN:HG2	1:B:344:GLU:CG	2.45	0.46
1:A:156:VAL:HG12	1:A:156:VAL:O	2.16	0.45
1:A:538[B]:ARG:CG	1:B:536:ILE:HG12	2.46	0.45
1:A:487:ARG:HH11	1:A:487:ARG:HG2	1.81	0.45
1:B:58:SER:N	3:B:602:GOL:C1	2.80	0.45
1:A:233:LEU:HD12	1:A:233:LEU:N	2.31	0.45
1:A:538[B]:ARG:HH21	4:A:604:PEG:H41	1.81	0.45
1:B:253:PHE:CE2	1:B:372:MET:HE1	2.52	0.45
1:A:13:VAL:O	1:A:17:THR:HG23	2.16	0.45
1:B:153:LEU:HD13	1:B:155:THR:HG23	1.97	0.45
1:B:480:GLY:HA3	4:B:604:PEG:H42	1.98	0.45
1:B:256:PHE:N	1:B:284:GLU:OE1	2.42	0.45
1:B:28:GLN:O	1:B:459[A]:ARG:NH1	2.50	0.45
1:A:233:LEU:HD13	1:A:265:ALA:HB1	1.99	0.44
1:B:249:VAL:O	1:B:277:ILE:HD13	2.16	0.44
1:B:38:PHE:O	1:B:41:HIS:HB3	2.17	0.44
1:B:144:VAL:CG1	1:B:166:ALA:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:TYR:CE1	1:B:229:ASP:HB3	2.52	0.44
1:B:484:LEU:HD13	1:B:508:SER:CB	2.47	0.44
1:B:30:LEU:N	1:B:31:PRO:CD	2.81	0.44
1:B:126:THR:HG22	1:B:255:SER:HB2	2.00	0.44
1:B:468:SER:HB3	1:B:471:ALA:HB3	1.99	0.44
1:B:58:SER:OG	3:B:602:GOL:C3	2.65	0.44
1:A:346:MET:HA	1:A:349:LYS:O	2.18	0.43
1:A:160:PHE:HD2	1:A:168:THR:HG21	1.84	0.43
1:B:230:LEU:O	1:B:258:ARG:NH1	2.49	0.43
1:B:85:ARG:NH2	1:B:125:ASP:OD2	2.50	0.43
1:A:459:ARG:NH2	8:A:721:HOH:O	2.51	0.43
1:A:324:MET:SD	1:A:328:ARG:HD2	2.59	0.42
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.87	0.42
1:A:30:LEU:O	1:A:34:MET:HG2	2.18	0.42
1:A:284:GLU:HG2	1:A:305:ALA:HB3	2.00	0.42
1:A:540:LEU:HD22	4:A:604:PEG:H41	2.00	0.42
1:B:157:ASP:HB3	8:B:727:HOH:O	2.19	0.42
1:B:457:ARG:HA	4:B:604:PEG:H32	2.00	0.42
1:B:56:SER:HB2	1:B:480:GLY:CA	2.48	0.42
1:A:260:ALA:O	1:A:263:VAL:N	2.47	0.42
1:B:56:SER:CB	1:B:480:GLY:HA2	2.50	0.42
1:A:156:VAL:O	1:A:156:VAL:CG1	2.68	0.41
1:A:335:PRO:HB3	1:A:477:LEU:O	2.20	0.41
1:B:479:ARG:HA	3:B:602:GOL:O1	2.20	0.41
1:B:153:LEU:CD1	1:B:155:THR:HG23	2.49	0.41
1:A:189:ASP:O	1:A:192:LEU:HB2	2.21	0.41
1:A:408:GLU:OE2	1:B:408:GLU:HG3	2.20	0.41
1:B:73:LEU:HD13	1:B:103:ILE:HA	2.02	0.41
1:A:243:PHE:CE2	1:A:247:HIS:NE2	2.89	0.41
1:A:382:PHE:N	1:A:383:PRO:CD	2.84	0.41
1:B:285:ASN:HB2	1:B:312:GLU:CD	2.42	0.41
1:A:136:LEU:HD23	1:A:164:GLY:HA3	2.02	0.41
1:B:148:LYS:H	1:B:148:LYS:HG3	1.75	0.41
1:B:435:CYS:HB2	1:B:520:LEU:HD12	2.03	0.40
1:B:341:GLN:HA	1:B:344:GLU:HG2	2.03	0.40
1:B:479:ARG:CG	4:B:604:PEG:H31	2.51	0.40
1:A:303:MET:HE2	1:A:372:MET:HE3	2.03	0.40
1:A:535:ASN:OD1	1:A:536:ILE:HG13	2.21	0.40
1:B:55:ARG:NH2	1:B:82:ASN:OD1	2.54	0.40
1:B:286:HIS:NE2	1:B:290:LYS:HE2	2.36	0.40
6:B:603:FLC:OHB	6:B:603:FLC:OG1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:VAL:CG1	1:B:174:HIS:NE2	2.84	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	525/550 (96%)	500 (95%)	23 (4%)	2 (0%)	34	38
1	B	532/550 (97%)	490 (92%)	37 (7%)	5 (1%)	17	17
All	All	1057/1100 (96%)	990 (94%)	60 (6%)	7 (1%)	22	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	340	THR
1	A	129	PRO
1	A	340	THR
1	B	234	SER
1	B	129	PRO
1	B	80	GLY

### 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	433/446 (97%)	408 (94%)	25 (6%)	20	22
1	B	435/446 (98%)	398 (92%)	37 (8%)	10	10
All	All	868/892 (97%)	806 (93%)	62 (7%)	14	15

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	45	LEU
1	A	69	SER
1	A	72	ARG
1	A	73	LEU
1	A	109	SER
1	A	112	THR
1	A	132	ARG
1	A	141	GLU
1	A	150	SER
1	A	155	THR
1	A	167	LYS
1	A	192	LEU
1	A	230	LEU
1	A	256	PHE
1	A	296	LEU
1	A	313	ILE
1	A	320	LEU
1	A	357	THR
1	A	358	SER
1	A	404	ARG
1	A	416	LEU
1	A	479	ARG
1	A	500	ARG
1	A	550	HIS
1	B	16	LEU
1	B	18	GLN
1	B	19	GLU
1	B	26	GLN
1	B	68	ARG
1	B	78	LYS
1	B	98	GLU
1	B	99	SER
1	B	126	THR
1	B	145	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	146	ILE
1	B	148	LYS
1	B	153	LEU
1	B	155	THR
1	B	157	ASP
1	B	162	THR
1	B	172	ASP
1	B	192	LEU
1	B	207	THR
1	B	210	GLU
1	B	214	ILE
1	B	215	LEU
1	B	218	ARG
1	B	230	LEU
1	B	256	PHE
1	B	278	LYS
1	B	312	GLU
1	B	344	GLU
1	B	358	SER
1	B	389	MET
1	B	411	ARG
1	B	475	VAL
1	B	488	GLU
1	B	491	GLU
1	B	516	ARG
1	B	528	ARG
1	B	544	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	330	ASN
1	B	15	GLN
1	B	18	GLN
1	B	26	GLN
1	B	87	ASN
1	B	96	HIS
1	B	137	GLN
1	B	151	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](#)

2 non-standard protein/DNA/RNA residues 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
1	SEP	A	113	1	8,9,10	0.69	0	8,12,14	1.92	2 (25%)
1	SEP	B	113	1	8,9,10	0.66	0	8,12,14	1.22	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
1	SEP	A	113	1	-	4/5/8/10	-
1	SEP	B	113	1	-	1/5/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	SEP	O3P-P-O2P	3.37	120.52	107.64
1	A	113	SEP	O2P-P-OG	-3.34	97.86	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	113	SEP	N-CA-CB-OG
1	A	113	SEP	CB-OG-P-O2P

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Mol	Chain	Res	Type	Atoms
1	A	113	SEP	CB-OG-P-O3P
1	B	113	SEP	CB-OG-P-O1P
1	A	113	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	B	602	-	5,5,5	1.32	1 (20%)	5,5,5	2.06	3 (60%)
5	EDO	A	605	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	A	606	-	3,3,3	0.71	0	2,2,2	0.29	0
3	GOL	A	602	-	5,5,5	1.08	0	5,5,5	1.20	0
5	EDO	A	607	-	3,3,3	0.60	0	2,2,2	0.24	0
7	PGE	B	605	-	9,9,9	0.66	0	8,8,8	0.68	0
2	FBP	B	601	-	18,20,20	1.04	1 (5%)	23,32,32	1.71	7 (30%)
4	PEG	A	604	-	6,6,6	0.99	0	5,5,5	1.18	0
2	FBP	A	601	-	18,20,20	1.07	2 (11%)	23,32,32	1.88	7 (30%)
4	PEG	B	604	-	6,6,6	0.60	0	5,5,5	0.84	0
6	FLC	B	603	-	12,12,12	1.41	1 (8%)	17,17,17	1.76	3 (17%)
3	GOL	A	603	-	5,5,5	0.61	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	B	602	-	-	3/4/4/4	-
5	EDO	A	605	-	-	0/1/1/1	-
5	EDO	A	606	-	-	0/1/1/1	-
3	GOL	A	602	-	-	4/4/4/4	-
5	EDO	A	607	-	-	1/1/1/1	-
7	PGE	B	605	-	-	5/7/7/7	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
4	PEG	A	604	-	-	1/4/4/4	-
2	FBP	A	601	-	-	1/13/32/32	0/1/1/1
4	PEG	B	604	-	-	1/4/4/4	-
6	FLC	B	603	-	-	10/16/16/16	-
3	GOL	A	603	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	603	FLC	CB-CBC	2.88	1.56	1.53
2	A	601	FBP	C4-C5	-2.39	1.46	1.53
2	A	601	FBP	P1-O2P	-2.30	1.46	1.54
2	B	601	FBP	O5-C5	2.27	1.48	1.43
3	B	602	GOL	O2-C2	2.13	1.49	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	603	FLC	OB2-CBC-CB	5.79	123.10	113.05
2	B	601	FBP	O6P-P2-O5P	4.02	123.01	107.64
2	A	601	FBP	O5-C5-C6	3.43	117.00	109.45
2	A	601	FBP	O3P-P1-O1	-3.37	97.77	106.73
2	A	601	FBP	O6P-P2-O4P	3.12	122.88	110.68
3	B	602	GOL	O1-C1-C2	2.97	124.43	110.20
2	B	601	FBP	O3P-P1-O2P	2.95	118.92	107.64
2	A	601	FBP	O3P-P1-O1P	2.83	121.76	110.68
2	B	601	FBP	O1-P1-O1P	2.68	114.00	106.47
2	A	601	FBP	P1-O1-C1	2.68	125.67	118.30
2	B	601	FBP	O6-C6-C5	2.60	117.92	108.99
6	B	603	FLC	OB2-CBC-OB1	-2.58	115.61	123.82
2	B	601	FBP	O6P-P2-O6	-2.48	100.14	106.73
3	B	602	GOL	O2-C2-C3	2.44	119.89	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FBP	O6-P2-O4P	-2.34	99.90	106.47
2	B	601	FBP	O5-C5-C6	2.16	114.22	109.45
2	A	601	FBP	O1-P1-O1P	-2.16	100.42	106.47
6	B	603	FLC	CA-CB-CBC	2.14	114.70	110.11
2	B	601	FBP	O3P-P1-O1	-2.13	101.08	106.73
3	B	602	GOL	O3-C3-C2	2.01	119.86	110.20

There are no chirality outliers.

All (30) torsion outliers are listed below:

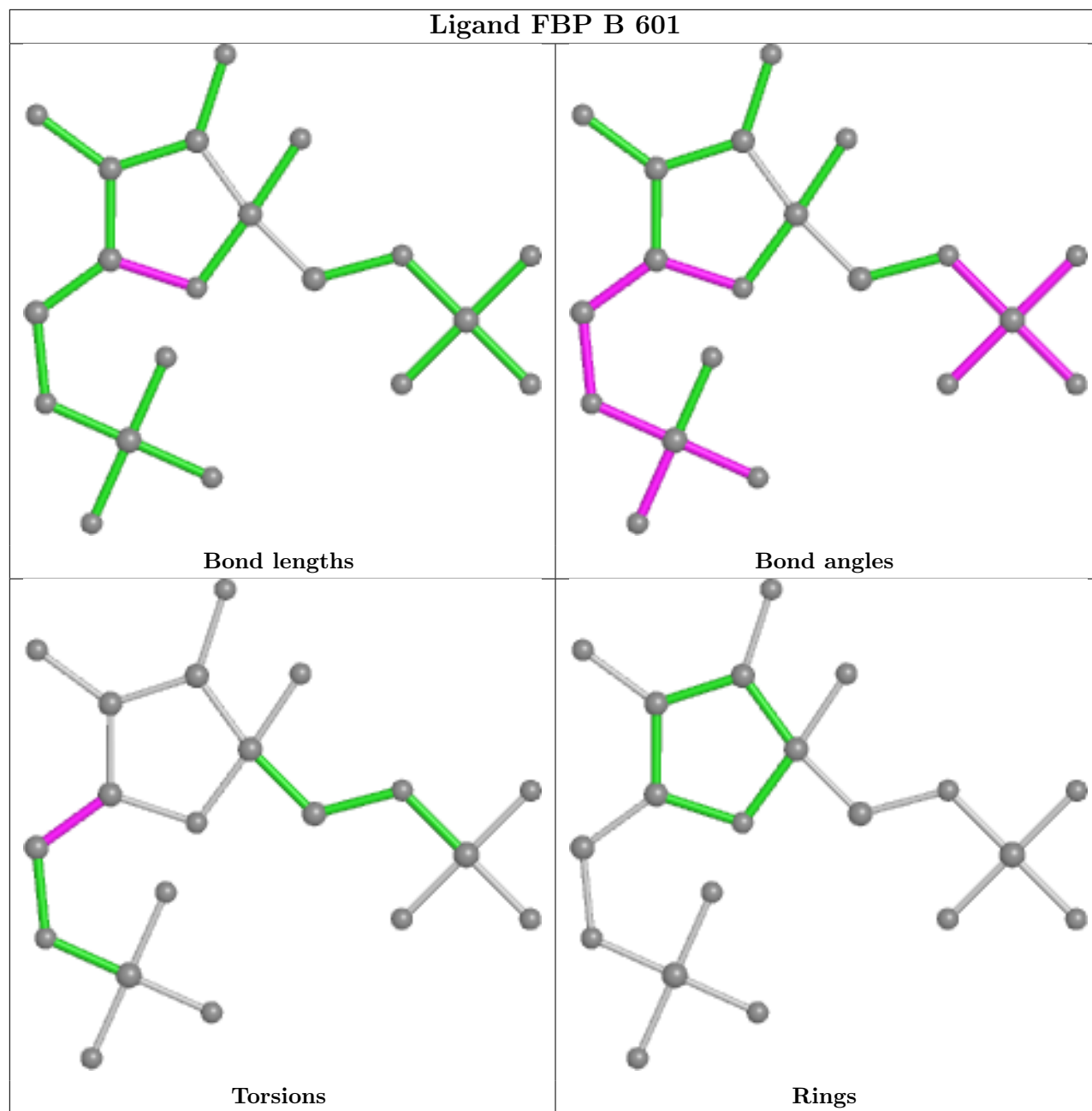
Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
6	B	603	FLC	CAC-CA-CB-CBC
6	B	603	FLC	CAC-CA-CB-CG
6	B	603	FLC	CAC-CA-CB-OHB
6	B	603	FLC	CA-CB-CBC-OB1
6	B	603	FLC	CA-CB-CBC-OB2
6	B	603	FLC	OHB-CB-CBC-OB1
6	B	603	FLC	OHB-CB-CBC-OB2
4	A	604	PEG	O1-C1-C2-O2
2	B	601	FBP	C4-C5-C6-O6
7	B	605	PGE	O3-C5-C6-O4
3	A	603	GOL	C1-C2-C3-O3
7	B	605	PGE	O1-C1-C2-O2
3	A	602	GOL	O2-C2-C3-O3
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
7	B	605	PGE	C1-C2-O2-C3
7	B	605	PGE	C4-C3-O2-C2
4	B	604	PEG	C4-C3-O2-C2
5	A	607	EDO	O1-C1-C2-O2
6	B	603	FLC	CA-CB-CG-CGC
7	B	605	PGE	C3-C4-O3-C5
6	B	603	FLC	CG-CB-CBC-OB2
3	A	603	GOL	O2-C2-C3-O3
3	B	602	GOL	O1-C1-C2-O2
6	B	603	FLC	OHB-CB-CG-CGC

There are no ring outliers.

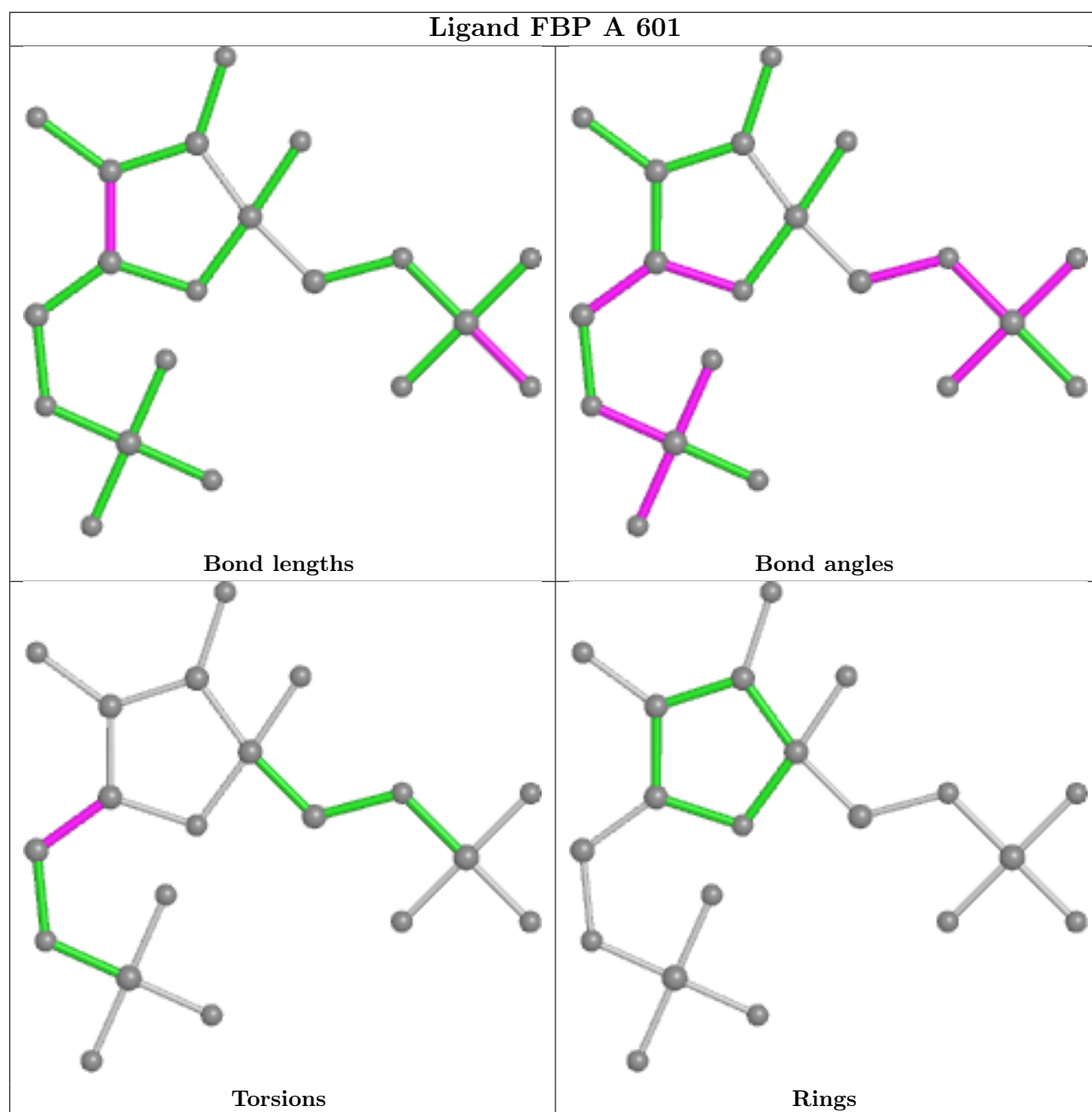
7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	12	0
5	A	606	EDO	1	0
4	A	604	PEG	3	0
2	A	601	FBP	2	0
4	B	604	PEG	3	0
6	B	603	FLC	2	0
3	A	603	GOL	1	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.







## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	528/550 (96%)	0.37	38 (7%) 15 23	27, 48, 96, 135	0
1	B	531/550 (96%)	0.88	99 (18%) 1 2	30, 56, 136, 206	0
All	All	1059/1100 (96%)	0.63	137 (12%) 3 5	27, 53, 126, 206	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	LEU	11.7
1	B	17	THR	10.7
1	B	139	GLY	8.7
1	B	214	ILE	8.5
1	B	138	GLY	7.6
1	B	545	HIS	6.3
1	B	140	PRO	6.3
1	B	169	VAL	6.3
1	B	147	VAL	6.2
1	B	134	GLY	6.1
1	B	201	GLY	6.1
1	B	137	GLN	5.9
1	B	152	VAL	5.3
1	B	142	SER	5.3
1	A	13	VAL	5.3
1	B	20	LEU	5.2
1	B	135	VAL	5.2
1	A	162	THR	5.2
1	B	164	GLY	5.1
1	B	144	VAL	4.9
1	A	17	THR	4.8
1	B	200	ILE	4.8
1	B	159	LYS	4.8
1	B	173	TYR	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	168	THR	4.5
1	B	146	ILE	4.5
1	B	212	GLY	4.4
1	B	229	ASP	4.4
1	B	136	LEU	4.3
1	B	163	ARG	4.2
1	B	204	GLY	4.2
1	B	219	LYS	4.2
1	A	144	VAL	4.1
1	B	153	LEU	4.1
1	B	18	GLN	4.1
1	B	192	LEU	4.1
1	A	132	ARG	4.0
1	B	179	VAL	4.0
1	B	216	GLY	4.0
1	B	228	VAL	4.0
1	B	19	GLU	3.9
1	B	16	LEU	3.9
1	B	203	GLU	3.8
1	B	213	GLY	3.7
1	B	176	ILE	3.7
1	B	177	THR	3.7
1	B	193	ILE	3.7
1	B	178	ARG	3.7
1	B	182	VAL	3.6
1	B	154	VAL	3.5
1	B	22	THR	3.5
1	B	14	ALA	3.5
1	B	171	VAL	3.4
1	A	218	ARG	3.4
1	B	170	TRP	3.3
1	B	175	ASN	3.3
1	B	191	GLY	3.3
1	B	188	ILE	3.3
1	A	233	LEU	3.2
1	B	149	GLY	3.2
1	B	156	VAL	3.2
1	B	145	GLU	3.2
1	B	202	PRO	3.2
1	B	24	PHE	3.1
1	B	15	GLN	3.1
1	B	231	PRO	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	217	SER	3.1
1	B	21	GLY	3.1
1	A	151	GLN	3.1
1	B	218	ARG	3.0
1	A	217	SER	3.0
1	B	25	PHE	3.0
1	A	150	SER	3.0
1	B	205	LEU	2.9
1	A	364	VAL	2.9
1	A	355	ALA	2.9
1	B	198	GLN	2.9
1	B	151	GLN	2.9
1	B	206	VAL	2.9
1	B	165	ASP	2.9
1	A	18	GLN	2.9
1	B	23	ALA	2.9
1	A	193	ILE	2.8
1	B	143	GLU	2.8
1	B	190	ASP	2.8
1	A	145	GLU	2.8
1	B	133	THR	2.8
1	A	243	PHE	2.8
1	A	156	VAL	2.8
1	A	136	LEU	2.8
1	B	195	LEU	2.8
1	A	357	THR	2.7
1	A	15	GLN	2.7
1	B	98	GLU	2.6
1	A	134	GLY	2.6
1	B	221	VAL	2.6
1	B	208	GLU	2.6
1	A	353	THR	2.6
1	A	393	ILE	2.6
1	B	230	LEU	2.5
1	A	135	VAL	2.5
1	B	161	GLN	2.5
1	A	360	VAL	2.5
1	A	368	ALA	2.5
1	A	342	MET	2.4
1	A	23	ALA	2.4
1	A	338	CYS	2.4
1	A	112	THR	2.4

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	162	THR	2.4
1	B	207	THR	2.4
1	B	368	ALA	2.4
1	A	209	VAL	2.4
1	A	371	ILE	2.3
1	B	326	ILE	2.3
1	B	197	VAL	2.3
1	A	361	ALA	2.3
1	B	167	LYS	2.3
1	A	143	GLU	2.3
1	B	103	ILE	2.3
1	B	131	ILE	2.3
1	B	160	PHE	2.2
1	B	141	GLU	2.2
1	B	102	ASN	2.2
1	B	57	THR	2.2
1	A	215	LEU	2.2
1	A	188	ILE	2.1
1	B	89	SER	2.1
1	B	130	GLU	2.1
1	B	379	LYS	2.1
1	B	77	ILE	2.1
1	A	219	LYS	2.1
1	B	189	ASP	2.1
1	A	343	LEU	2.1
1	B	166	ALA	2.1
1	B	157	ASP	2.0
1	B	132	ARG	2.0
1	B	367	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	B	113	10/11	0.89	0.14	81,88,111,130	0
1	SEP	A	113	10/11	0.96	0.15	57,69,84,84	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

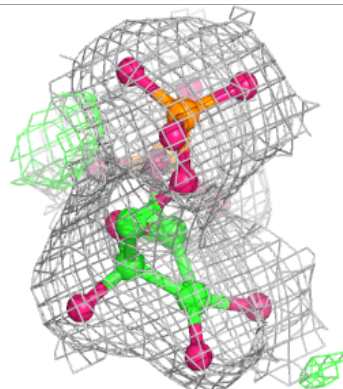
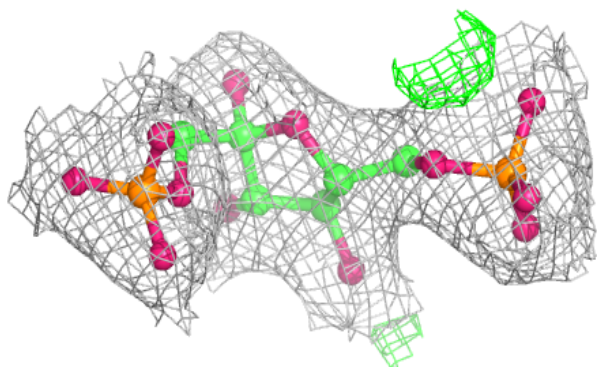
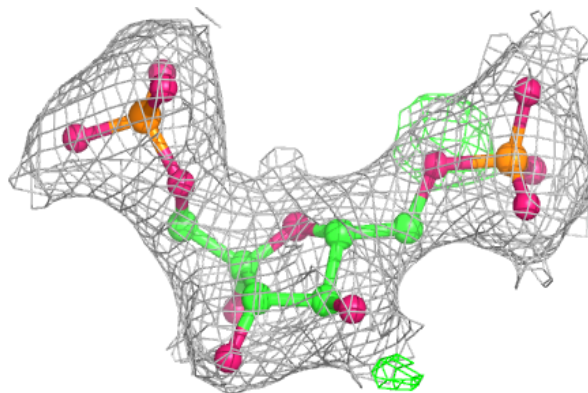
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	A	606	4/4	0.64	0.41	76,77,81,81	0
4	PEG	A	604	7/7	0.78	0.25	62,70,80,83	0
3	GOL	A	603	6/6	0.79	0.35	61,70,75,78	0
3	GOL	A	602	6/6	0.83	0.24	62,73,74,77	0
7	PGE	B	605	10/10	0.84	0.30	67,73,76,77	0
4	PEG	B	604	7/7	0.88	0.31	66,75,82,85	0
5	EDO	A	607	4/4	0.89	0.35	68,70,74,80	0
5	EDO	A	605	4/4	0.89	0.23	72,79,80,83	0
6	FLC	B	603	13/13	0.90	0.14	67,77,84,95	0
3	GOL	B	602	6/6	0.94	0.18	44,45,52,52	0
2	FBP	B	601	20/20	0.98	0.11	30,36,43,43	0
2	FBP	A	601	20/20	0.99	0.11	28,33,42,44	0

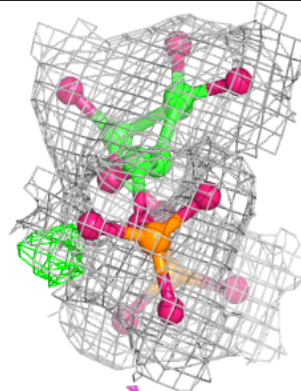
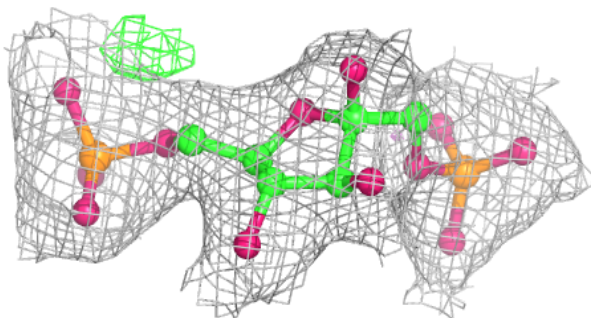
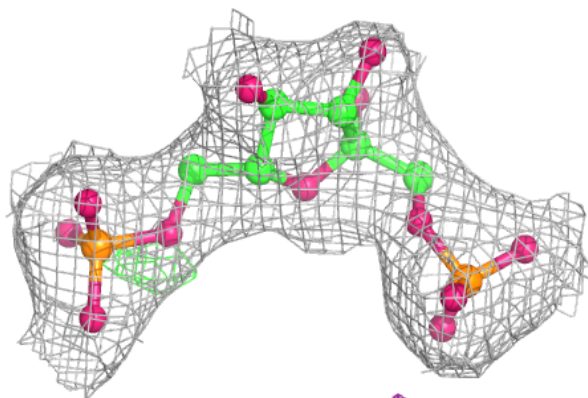
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FBP B 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 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.