



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2025 – 12:15 pm GMT

PDB ID : 9FKF  
Title : Crystal structure of human Glucose-6-phosphate isomerase with phosphoenol pyruvate ligand  
Authors : Jonatansdottir, Y.Y.; Hjorleifsson, G.J.  
Deposited on : 2024-06-03  
Resolution : 1.60 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

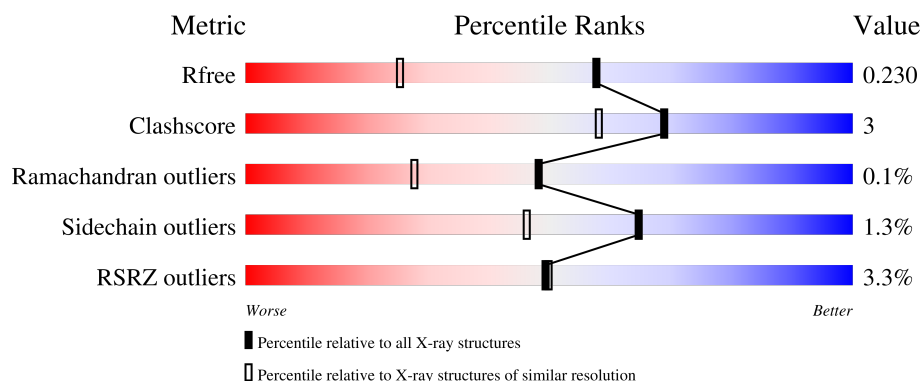
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

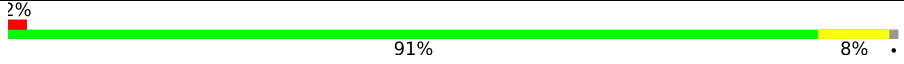
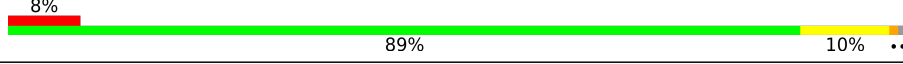
The reported resolution of this entry is 1.60 Å.

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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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	558	
1	B	558	
1	C	558	
1	D	558	

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	PEG	A	602	-	-	X	-
3	PEG	B	602	-	-	X	-
5	TRS	A	604	-	X	-	-

## 2 Entry composition [i](#)

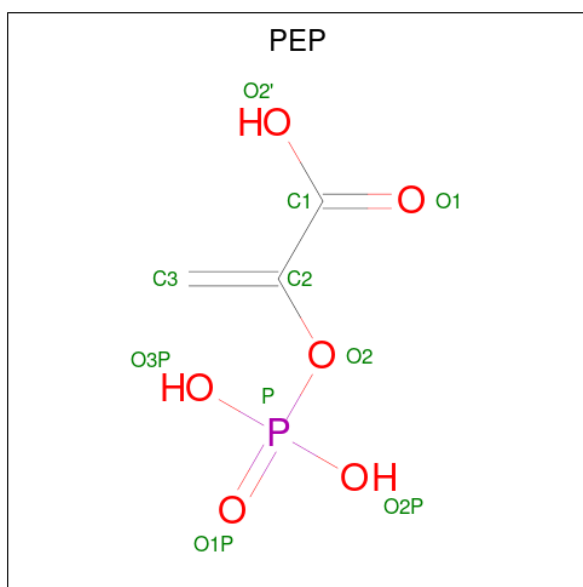
There are 6 unique types of molecules in this entry. The entry contains 36605 atoms, of which 17636 are hydrogens and 0 are deuteriums.

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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	555	Total	C	H	N	O	S	0	2	0
			8830	2827	4391	782	812	18			
1	B	555	Total	C	H	N	O	S	0	0	0
			8816	2822	4386	781	809	18			
1	C	556	Total	C	H	N	O	S	0	0	0
			8830	2827	4393	782	810	18			
1	D	555	Total	C	H	N	O	S	0	0	0
			8814	2822	4384	781	809	18			

- Molecule 2 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula:  $C_3H_5O_6P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			12	3	2	6	1		
2	B	1	Total	C	H	O	P	0	0
			12	3	2	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	O	P	0	0
			12	3	2	6	1		
2	D	1	Total	C	H	O	P	0	0
			12	3	2	6	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



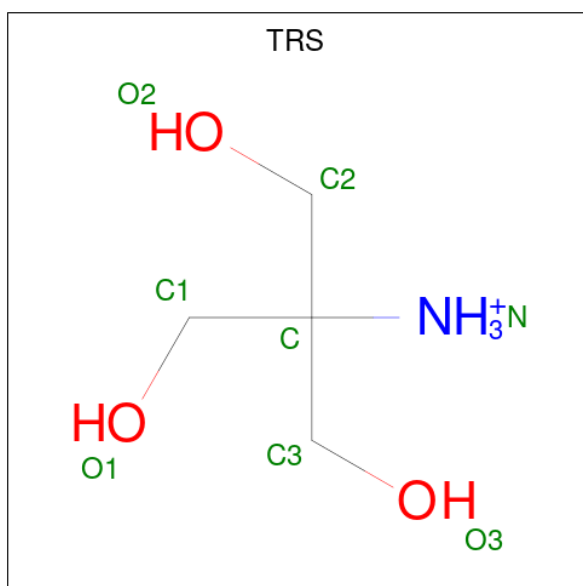
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		
4	A	1	Total	C	H	O	0	0
			24	6	14	4		
4	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

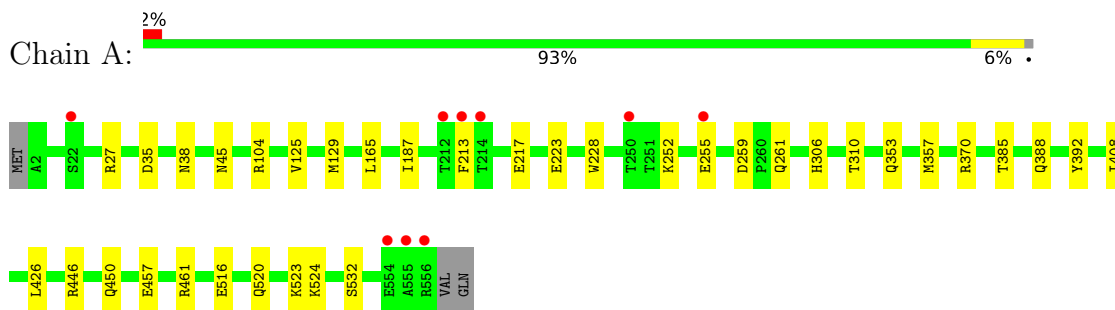
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	330	Total	O	0	0
			330	330		
6	B	253	Total	O	0	0
			253	253		
6	C	331	Total	O	0	0
			331	331		
6	D	227	Total	O	0	0
			227	227		

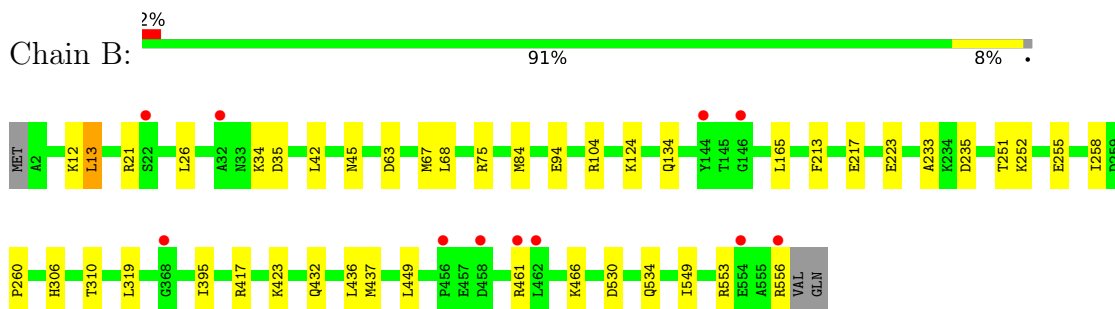
### 3 Residue-property plots [i](#)

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.

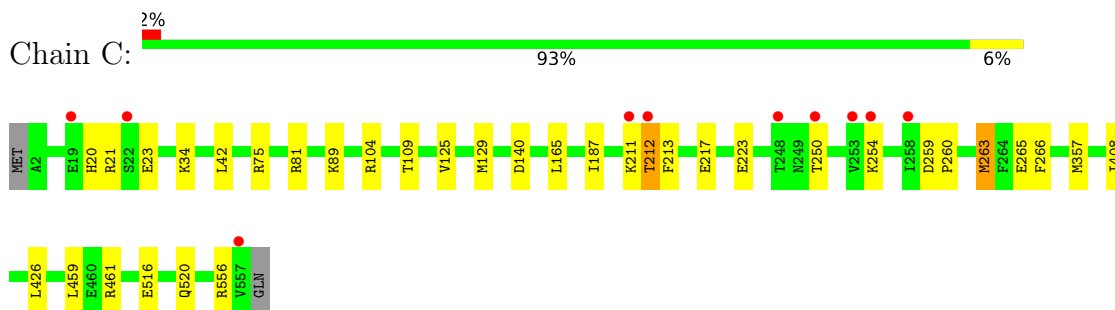
- Molecule 1: Glucose-6-phosphate isomerase



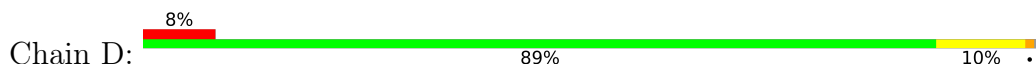
- Molecule 1: Glucose-6-phosphate isomerase



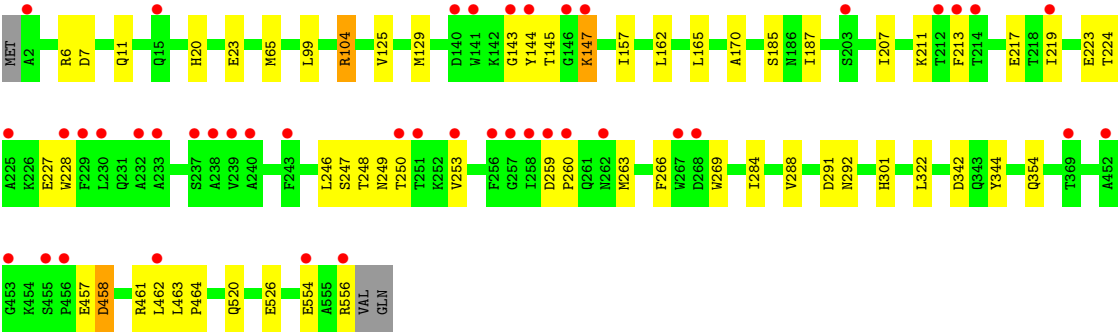
- Molecule 1: Glucose-6-phosphate isomerase



- Molecule 1: Glucose-6-phosphate isomerase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.84Å 107.48Å 271.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 1.60 48.42 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.42-1.60) 93.9 (48.42-1.60)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 1.60Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.187 , 0.224 0.194 , 0.230	Depositor DCC
$R_{free}$ test set	15759 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 37.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	36605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0581e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PEP, PGE, TRS, 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	0.71	0/4559	0.82	0/6172
1	B	0.68	0/4538	0.80	2/6144 (0.0%)
1	C	0.72	0/4545	0.83	3/6154 (0.0%)
1	D	0.67	0/4538	0.80	2/6144 (0.0%)
All	All	0.70	0/18180	0.81	7/24614 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	MET	CG-SD-CE	-7.88	87.59	100.20
1	C	357	MET	CG-SD-CE	5.78	109.44	100.20
1	D	65	MET	CG-SD-CE	5.19	108.50	100.20
1	C	81	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	13	LEU	CA-CB-CG	5.17	127.18	115.30
1	C	42	LEU	CA-CB-CG	5.06	126.93	115.30
1	D	342	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ARG	Sidechain
1	B	75	ARG	Sidechain
1	C	75	ARG	Sidechain
1	D	556	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	4439	4391	4380	32	0
1	B	4430	4386	4383	31	0
1	C	4437	4393	4392	22	0
1	D	4430	4384	4383	35	0
2	A	10	2	2	0	0
2	B	10	2	2	0	0
2	C	10	2	2	1	0
2	D	10	2	2	1	0
3	A	7	10	10	6	0
3	B	7	10	10	7	0
4	A	20	28	28	3	0
4	B	10	14	14	0	0
5	A	8	12	12	2	0
6	A	330	0	0	6	0
6	B	253	0	0	5	0
6	C	331	0	0	4	1
6	D	227	0	0	2	0
All	All	18969	17636	17620	119	1

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 3.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LYS:NZ	6:B:701:HOH:O	1.94	0.98
1:C:223:GLU:OE1	6:C:701:HOH:O	1.92	0.86
1:D:250:THR:HG23	1:D:263:MET:HE1	1.70	0.71
1:B:306:HIS:HD1	3:B:602:PEG:C2	2.04	0.71
1:A:223:GLU:OE1	6:A:701:HOH:O	2.09	0.69
1:A:38:ASN:OD1	6:A:702:HOH:O	2.10	0.69
1:B:223:GLU:OE1	6:B:702:HOH:O	2.12	0.66
1:A:217:GLU:OE1	6:A:703:HOH:O	2.14	0.66
1:D:7:ASP:OD2	6:D:701:HOH:O	2.13	0.65
1:D:125:VAL:O	1:D:129:MET:HG3	1.97	0.65
1:A:228:TRP:HB2	5:A:604:TRS:H22	1.82	0.62
1:B:94:GLU:OE1	6:B:703:HOH:O	2.16	0.61
1:A:353:GLN:O	1:A:357:MET:HB2	2.02	0.60
1:C:265:GLU:HG2	6:C:927:HOH:O	2.02	0.60
1:A:385:THR:O	1:A:388:GLN:HB2	2.03	0.59
1:B:217:GLU:HG3	6:B:801:HOH:O	2.02	0.59
1:D:143:GLY:CA	1:D:147:LYS:HZ1	2.15	0.59
1:A:310:THR:OG1	3:A:602:PEG:H42	2.02	0.59
1:C:250:THR:HA	1:C:263:MET:SD	2.42	0.59
1:A:45:ASN:HD22	3:B:602:PEG:H12	1.67	0.59
1:A:252:LYS:O	1:A:255[A]:GLU:HG3	2.04	0.58
1:B:251:THR:O	1:B:255:GLU:HG3	2.05	0.57
1:D:461:ARG:HG2	1:D:461:ARG:HH11	1.69	0.57
1:B:12:LYS:HB3	1:B:67:MET:CE	2.35	0.56
1:C:211:LYS:HB3	1:C:266:PHE:CZ	2.41	0.56
1:B:13:LEU:HD11	1:B:68:LEU:HD23	1.88	0.56
1:D:147:LYS:H	1:D:147:LYS:CE	2.19	0.55
1:A:45:ASN:ND2	3:B:602:PEG:H12	2.22	0.55
1:A:524:LYS:HE3	6:A:959:HOH:O	2.06	0.54
1:B:165:LEU:C	1:B:165:LEU:HD23	2.28	0.54
1:B:63:ASP:O	1:B:67:MET:HG3	2.08	0.54
1:A:252:LYS:HA	1:A:255[A]:GLU:HG3	1.90	0.54
1:B:306:HIS:HD1	3:B:602:PEG:H21	1.72	0.54
1:D:157:ILE:HD12	1:D:185:SER:O	2.07	0.54
1:C:259:ASP:OD1	1:C:260:PRO:HD2	2.08	0.53
1:B:432:GLN:O	1:B:436:LEU:HD22	2.08	0.53
1:D:259:ASP:OD1	1:D:260:PRO:HD2	2.07	0.53
3:A:602:PEG:H21	3:A:602:PEG:O4	2.08	0.53
1:A:187:ILE:HB	1:A:217:GLU:HG2	1.91	0.53
1:A:45:ASN:HD22	3:B:602:PEG:C1	2.21	0.53
1:C:250:THR:HG23	1:C:263:MET:HE1	1.91	0.53
1:D:165:LEU:C	1:D:165:LEU:HD23	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:HH22	4:A:605:PGE:H32	1.75	0.52
1:B:233:ALA:O	1:B:235:ASP:N	2.44	0.51
1:A:446:ARG:O	1:A:450:GLN:HG3	2.11	0.50
1:C:408:ILE:HD13	1:C:426:LEU:HD23	1.93	0.50
1:B:42:LEU:HD11	1:B:319:LEU:HD12	1.94	0.50
1:B:417:ARG:NH1	1:D:224:THR:OG1	2.40	0.50
1:B:12:LYS:HB3	1:B:67:MET:HE2	1.94	0.49
1:A:523:LYS:CE	6:A:915:HOH:O	2.59	0.49
1:C:211:LYS:O	1:C:212:THR:HG23	2.12	0.49
3:A:602:PEG:C4	1:B:45:ASN:HD22	2.25	0.49
1:D:219:ILE:O	1:D:223:GLU:HG2	2.12	0.49
1:A:524:LYS:CE	6:A:959:HOH:O	2.61	0.49
1:A:259:ASP:OD1	1:A:261:GLN:HG2	2.12	0.49
1:A:125:VAL:O	1:A:129:MET:HG3	2.13	0.48
1:C:109:THR:CG2	6:C:926:HOH:O	2.62	0.48
1:C:109:THR:HG22	6:C:926:HOH:O	2.13	0.48
1:D:457:GLU:HG3	1:D:458:ASP:N	2.28	0.48
1:D:99:LEU:HB2	1:D:269:TRP:CE3	2.48	0.48
1:B:534:GLN:NE2	6:B:706:HOH:O	2.38	0.47
1:A:228:TRP:HB2	5:A:604:TRS:C2	2.44	0.47
1:C:125:VAL:O	1:C:129:MET:HG3	2.14	0.47
1:D:104:ARG:O	1:D:301:HIS:HB2	2.14	0.47
1:C:187:ILE:HB	1:C:217:GLU:CG	2.45	0.47
1:A:187:ILE:HB	1:A:217:GLU:CG	2.45	0.46
1:A:35:ASP:OD2	1:B:35:ASP:OD2	2.33	0.46
1:D:249:ASN:O	1:D:253:VAL:HG23	2.16	0.46
1:D:463:LEU:HB3	1:D:464:PRO:HD3	1.96	0.46
1:C:20:HIS:O	1:C:23:GLU:HB3	2.15	0.46
1:D:223:GLU:O	1:D:227:GLU:HG3	2.16	0.46
1:D:144:TYR:CD1	1:D:145:THR:HG23	2.51	0.46
1:D:20:HIS:ND1	1:D:23:GLU:OE2	2.41	0.45
1:A:370:ARG:NH2	4:A:605:PGE:H32	2.30	0.45
1:B:310:THR:OG1	3:B:602:PEG:H11	2.16	0.45
1:B:423:LYS:HE3	1:D:526:GLU:O	2.17	0.45
1:A:165:LEU:C	1:A:165:LEU:HD23	2.37	0.45
1:A:306:HIS:HD1	3:A:602:PEG:C3	2.30	0.45
1:C:250:THR:HG23	1:C:263:MET:CE	2.46	0.45
1:B:449:LEU:HD21	1:B:466:LYS:HD3	1.98	0.44
1:D:143:GLY:HA3	1:D:147:LYS:HZ1	1.82	0.44
1:D:284:ILE:O	1:D:288:VAL:HG22	2.18	0.44
1:B:530:ASP:N	1:B:530:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ILE:O	1:B:553:ARG:HG3	2.17	0.44
1:C:254:LYS:O	1:C:254:LYS:HD3	2.17	0.44
1:D:7:ASP:O	1:D:11:GLN:HG3	2.18	0.44
1:B:233:ALA:C	1:B:235:ASP:H	2.20	0.43
2:D:601:PEP:C1	2:D:601:PEP:O2P	2.67	0.43
1:D:170:ALA:HA	1:D:344:TYR:HB3	1.99	0.43
1:C:461:ARG:HH11	1:C:461:ARG:HG2	1.83	0.43
1:C:459:LEU:C	1:C:459:LEU:HD23	2.38	0.43
1:A:516:GLU:O	1:A:520:GLN:HG3	2.19	0.42
1:A:252:LYS:HA	1:A:255[A]:GLU:CG	2.49	0.42
1:D:228:TRP:O	6:D:702:HOH:O	2.22	0.42
1:C:165:LEU:HD23	1:C:165:LEU:C	2.40	0.42
1:B:258:ILE:O	1:B:260:PRO:HD3	2.20	0.42
1:C:516:GLU:O	1:C:520:GLN:HG3	2.20	0.42
1:D:162:LEU:HD12	1:D:354:GLN:OE1	2.20	0.42
1:D:187:ILE:HB	1:D:217:GLU:CG	2.50	0.42
1:D:462:LEU:O	1:D:463:LEU:C	2.58	0.42
1:D:143:GLY:N	1:D:147:LYS:HZ1	2.18	0.42
3:A:602:PEG:H31	1:B:45:ASN:ND2	2.35	0.41
1:B:26:LEU:CB	1:B:437:MET:HG2	2.50	0.41
1:A:457:GLU:HG2	1:A:461:ARG:NH2	2.35	0.41
3:A:602:PEG:C3	1:B:45:ASN:HD22	2.34	0.41
1:B:306:HIS:HD1	3:B:602:PEG:C1	2.33	0.41
1:D:187:ILE:HB	1:D:217:GLU:HG3	2.02	0.41
1:A:370:ARG:HH22	4:A:605:PGE:C3	2.33	0.41
1:B:395:ILE:HG22	1:B:436:LEU:HD11	2.02	0.41
1:C:211:LYS:O	2:C:601:PEP:O1P	2.38	0.41
1:D:211:LYS:HA	1:D:266:PHE:CZ	2.56	0.41
1:A:388:GLN:HG3	1:A:392:TYR:CE2	2.55	0.41
1:D:291:ASP:OD1	1:D:292:ASN:N	2.54	0.41
1:D:145:THR:OG1	1:D:147:LYS:CD	2.69	0.41
1:D:247:SER:OG	1:D:248:THR:N	2.54	0.41
1:A:408:ILE:HD13	1:A:426:LEU:HD23	2.02	0.41
1:C:21:ARG:C	1:C:23:GLU:H	2.25	0.41
1:C:211:LYS:O	1:C:212:THR:CB	2.69	0.40
1:D:207:ILE:HG21	1:D:246:LEU:HD11	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:958:HOH:O	6:C:1004:HOH:O[1_655]	2.11	0.09

## 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	555/558 (100%)	537 (97%)	18 (3%)	0	100	100
1	B	553/558 (99%)	534 (97%)	18 (3%)	1 (0%)	44	25
1	C	554/558 (99%)	537 (97%)	16 (3%)	1 (0%)	44	25
1	D	553/558 (99%)	534 (97%)	19 (3%)	0	100	100
All	All	2215/2232 (99%)	2142 (97%)	71 (3%)	2 (0%)	48	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	212	THR
1	B	21	ARG

### 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	476/477 (100%)	473 (99%)	3 (1%)	84	74
1	B	474/477 (99%)	467 (98%)	7 (2%)	60	39
1	C	475/477 (100%)	468 (98%)	7 (2%)	60	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	474/477 (99%)	466 (98%)	8 (2%)	56	33
All	All	1899/1908 (100%)	1874 (99%)	25 (1%)	65	46

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	213	PHE
1	A	532	SER
1	B	34	LYS
1	B	104	ARG
1	B	134	GLN
1	B	213	PHE
1	B	252	LYS
1	B	461	ARG
1	B	556	ARG
1	C	34	LYS
1	C	89	LYS
1	C	104	ARG
1	C	140	ASP
1	C	213	PHE
1	C	263	MET
1	C	556	ARG
1	D	6	ARG
1	D	104	ARG
1	D	147	LYS
1	D	213	PHE
1	D	322	LEU
1	D	458	ASP
1	D	520	GLN
1	D	554	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	39	HIS
1	A	305	GLN
1	A	336	HIS
1	B	261	GLN
1	C	9	GLN

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Mol	Chain	Res	Type
1	C	11	GLN
1	C	305	GLN
1	D	11	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

10 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	$\# Z  > 2$
4	PGE	A	603	-	9,9,9	0.58	0	8,8,8	0.94	1 (12%)
2	PEP	A	601	-	9,9,9	1.66	2 (22%)	11,13,13	0.38	0
2	PEP	B	601	-	9,9,9	2.13	2 (22%)	11,13,13	0.59	0
5	TRS	A	604	-	7,7,7	0.35	0	9,9,9	1.65	2 (22%)
2	PEP	D	601	-	9,9,9	0.66	0	11,13,13	0.36	0
2	PEP	C	601	-	9,9,9	1.80	2 (22%)	11,13,13	0.45	0
4	PGE	B	603	-	9,9,9	0.34	0	8,8,8	0.55	0
4	PGE	A	605	-	9,9,9	0.49	0	8,8,8	0.74	0
3	PEG	A	602	-	6,6,6	0.62	0	5,5,5	0.72	0
3	PEG	B	602	-	6,6,6	0.41	0	5,5,5	0.51	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
4	PGE	A	603	-	-	5/7/7/7	-
2	PEP	A	601	-	-	4/9/9/9	-
2	PEP	B	601	-	-	4/9/9/9	-
5	TRS	A	604	-	-	8/9/9/9	-
2	PEP	D	601	-	-	6/9/9/9	-
2	PEP	C	601	-	-	4/9/9/9	-
4	PGE	B	603	-	-	3/7/7/7	-
4	PGE	A	605	-	-	5/7/7/7	-
3	PEG	A	602	-	-	2/4/4/4	-
3	PEG	B	602	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	PEP	C2-C1	4.81	1.54	1.49
2	A	601	PEP	P-O2	4.20	1.65	1.59
2	B	601	PEP	P-O2	3.94	1.65	1.59
2	C	601	PEP	P-O2	3.82	1.65	1.59
2	C	601	PEP	C2-C1	3.07	1.52	1.49
2	A	601	PEP	C2-C1	2.36	1.51	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	TRS	C3-C-N	3.36	118.01	107.98
5	A	604	TRS	C1-C-N	-2.26	101.24	107.98
4	A	603	PGE	C5-O3-C4	2.12	122.46	113.29

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PEP	O1-C1-C2-C3
2	A	601	PEP	O1-C1-C2-O2
2	A	601	PEP	O2'-C1-C2-C3

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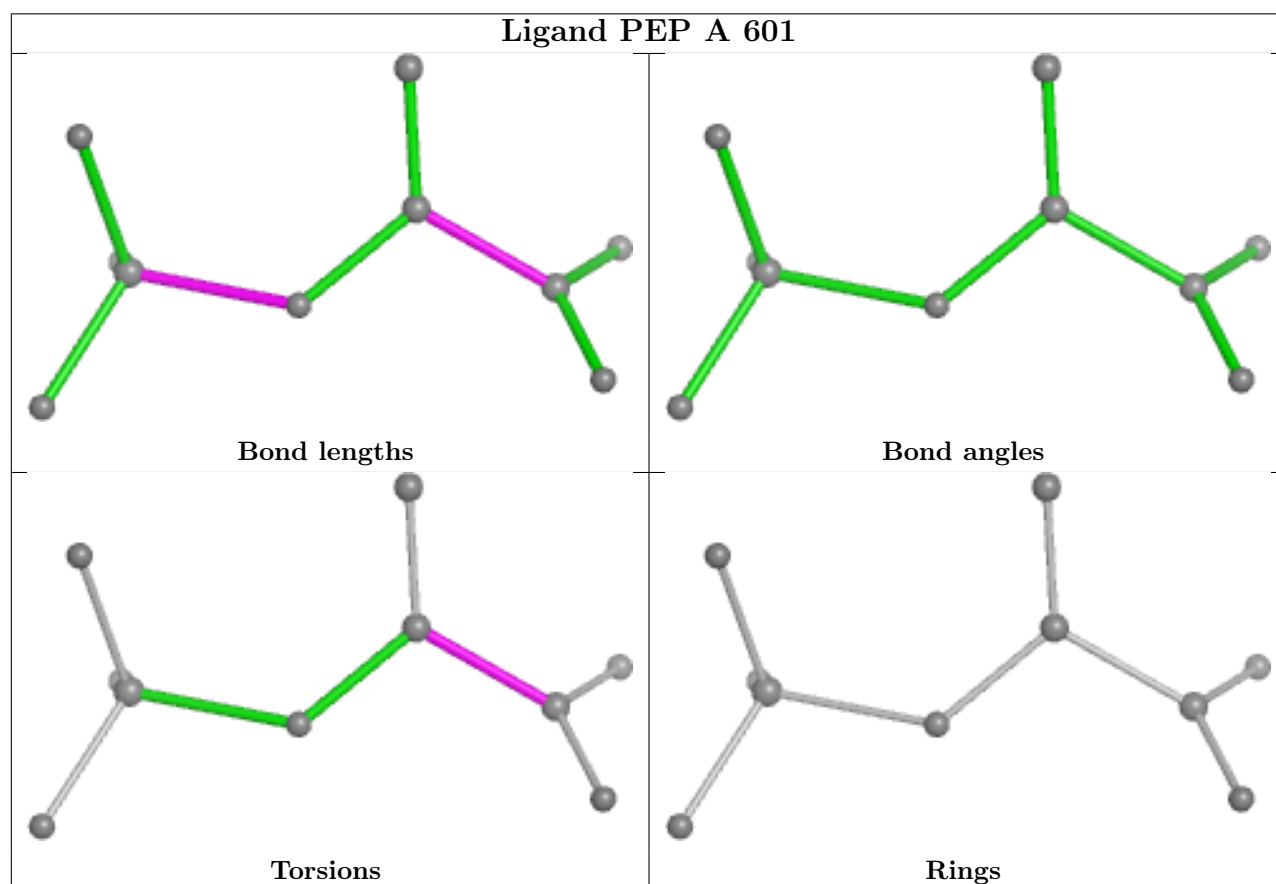
Mol	Chain	Res	Type	Atoms
2	A	601	PEP	O2'-C1-C2-O2
2	B	601	PEP	O1-C1-C2-C3
2	B	601	PEP	O1-C1-C2-O2
2	B	601	PEP	O2'-C1-C2-C3
2	B	601	PEP	O2'-C1-C2-O2
2	C	601	PEP	O1-C1-C2-C3
2	C	601	PEP	O1-C1-C2-O2
2	C	601	PEP	O2'-C1-C2-C3
2	C	601	PEP	O2'-C1-C2-O2
2	D	601	PEP	O1-C1-C2-C3
2	D	601	PEP	O2'-C1-C2-C3
2	D	601	PEP	O2'-C1-C2-O2
2	D	601	PEP	C1-C2-O2-P
2	D	601	PEP	C3-C2-O2-P
5	A	604	TRS	N-C-C1-O1
5	A	604	TRS	C1-C-C2-O2
5	A	604	TRS	C3-C-C2-O2
5	A	604	TRS	C2-C-C3-O3
5	A	604	TRS	N-C-C3-O3
3	A	602	PEG	C4-C3-O2-C2
4	A	603	PGE	O2-C3-C4-O3
4	B	603	PGE	O2-C3-C4-O3
4	A	603	PGE	O3-C5-C6-O4
4	A	603	PGE	O1-C1-C2-O2
4	A	605	PGE	O3-C5-C6-O4
3	A	602	PEG	O2-C3-C4-O4
3	B	602	PEG	C4-C3-O2-C2
4	A	605	PGE	C6-C5-O3-C4
4	B	603	PGE	C1-C2-O2-C3
4	B	603	PGE	C6-C5-O3-C4
5	A	604	TRS	C1-C-C3-O3
4	A	603	PGE	C6-C5-O3-C4
2	D	601	PEP	O1-C1-C2-O2
4	A	603	PGE	C4-C3-O2-C2
3	B	602	PEG	C1-C2-O2-C3
4	A	605	PGE	O2-C3-C4-O3
4	A	605	PGE	C4-C3-O2-C2
3	B	602	PEG	O2-C3-C4-O4
5	A	604	TRS	C3-C-C1-O1
5	A	604	TRS	N-C-C2-O2
4	A	605	PGE	C3-C4-O3-C5

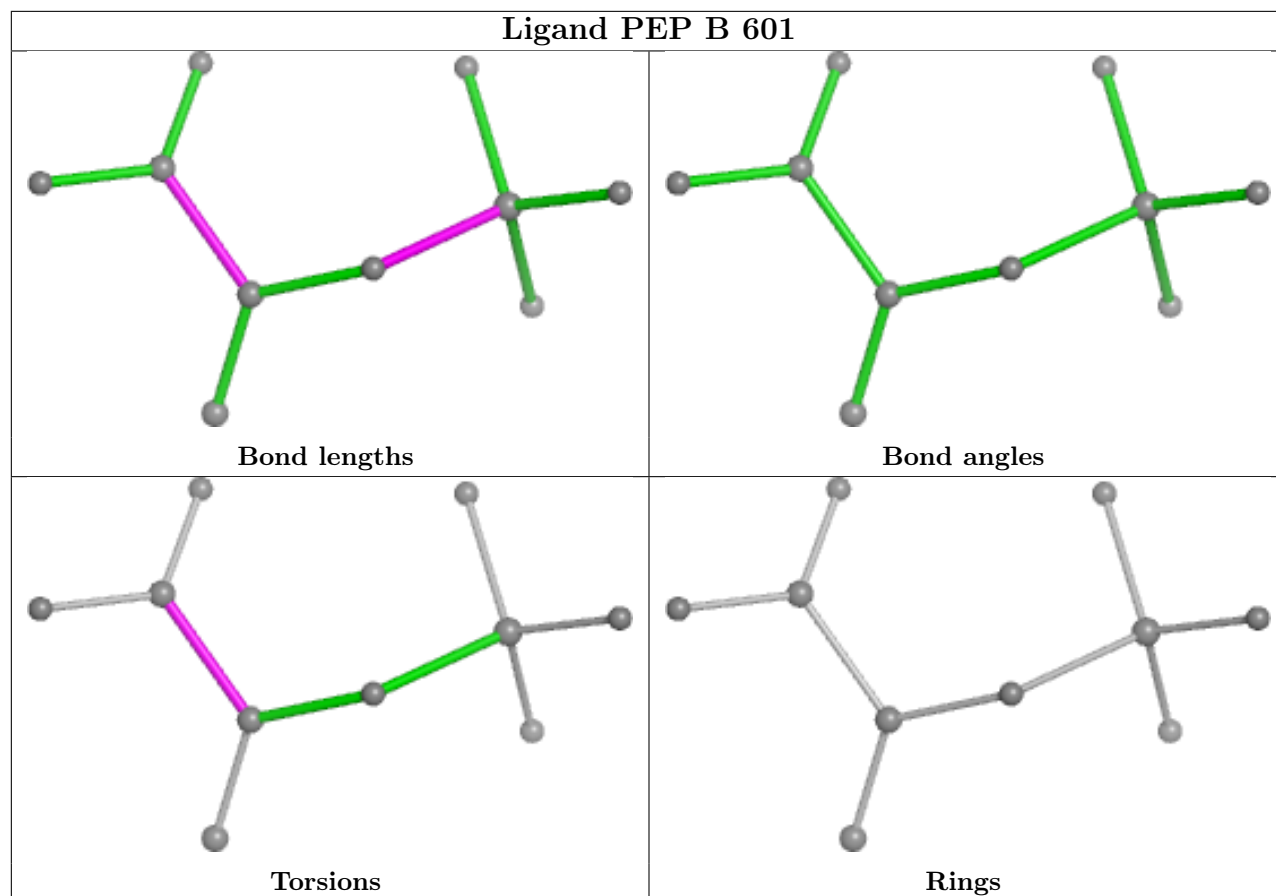
There are no ring outliers.

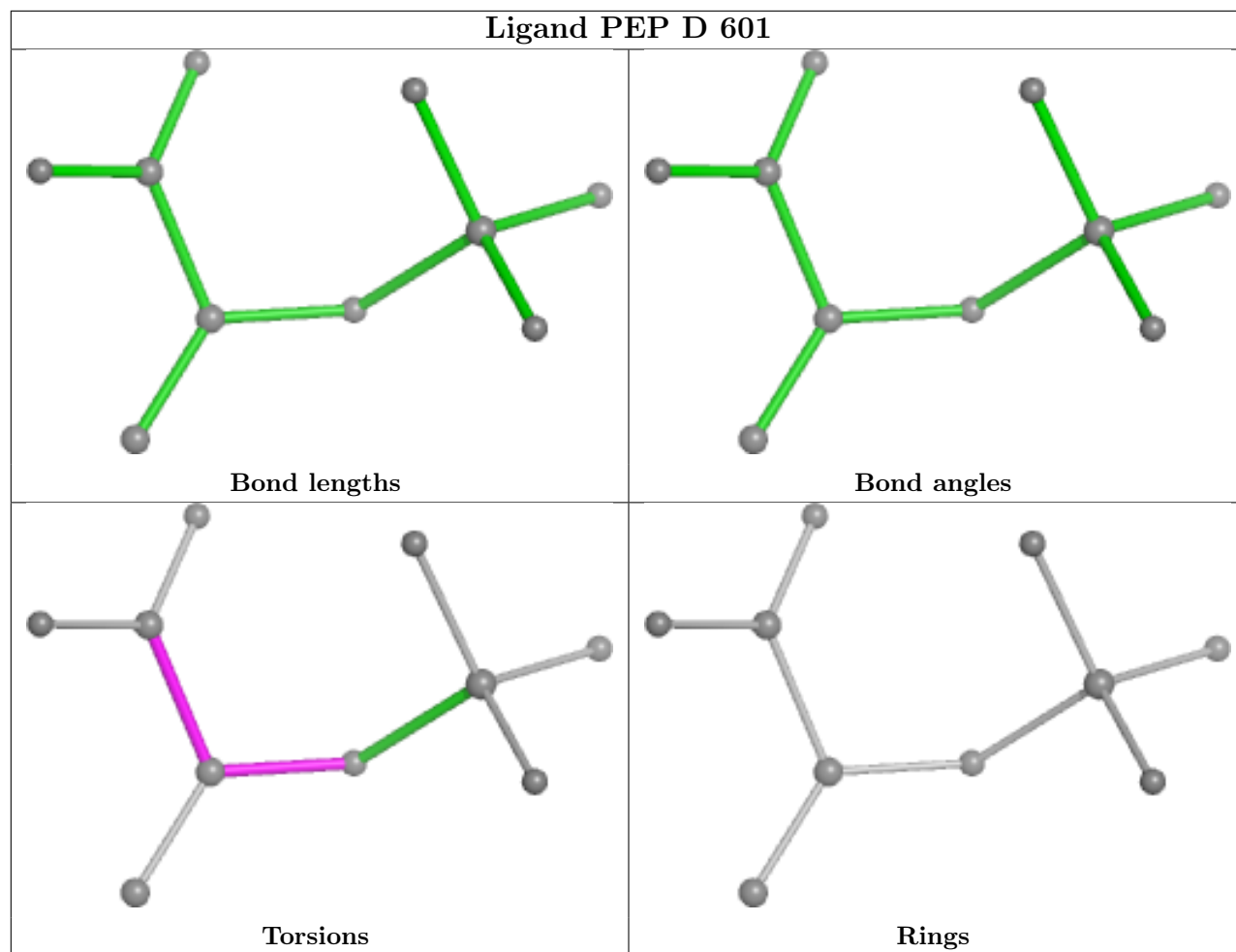
6 monomers are involved in 20 short contacts:

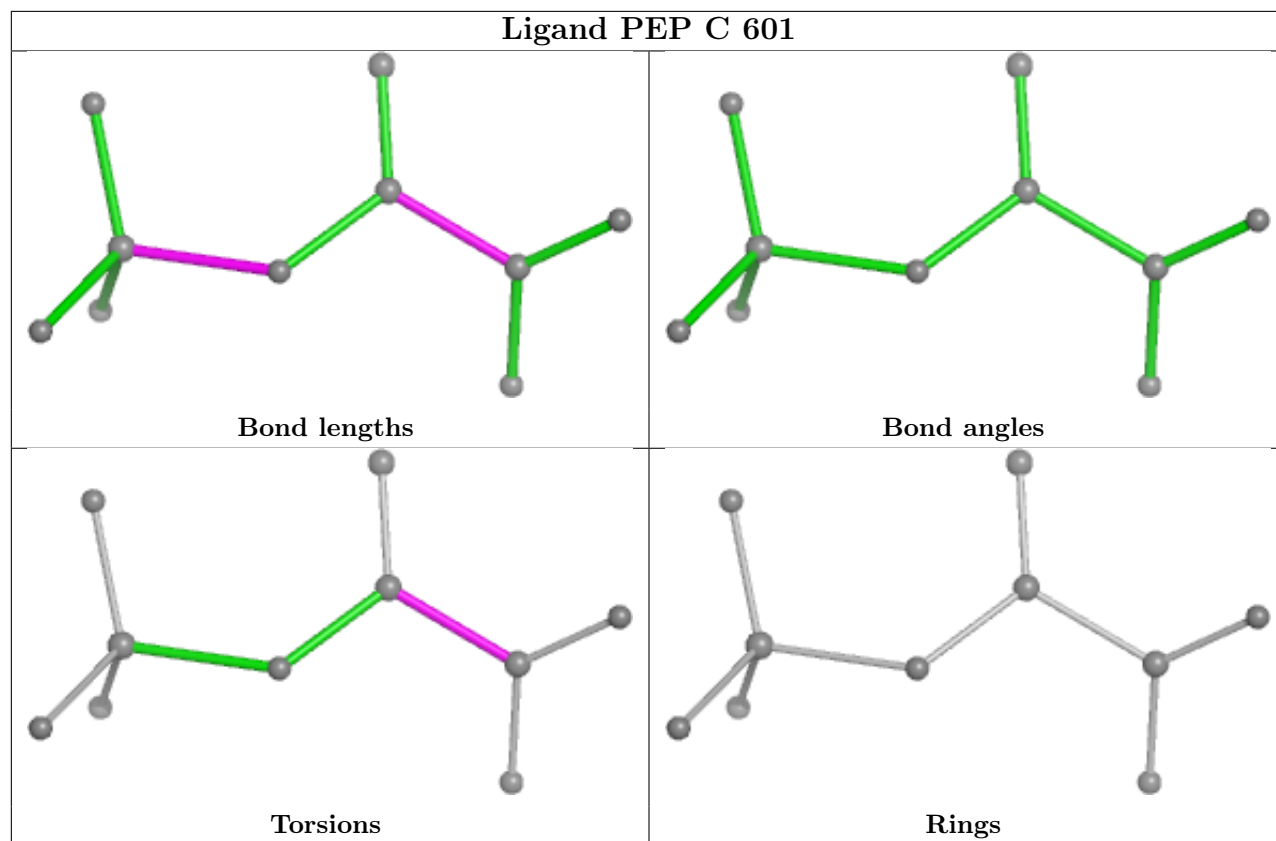
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	TRS	2	0
2	D	601	PEP	1	0
2	C	601	PEP	1	0
4	A	605	PGE	3	0
3	A	602	PEG	6	0
3	B	602	PEG	7	0

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	555/558 (99%)	-0.08	9 (1%) 70 73	14, 22, 46, 85	1 (0%)
1	B	555/558 (99%)	0.17	11 (1%) 64 67	15, 25, 51, 80	0
1	C	556/558 (99%)	0.00	10 (1%) 67 69	14, 23, 46, 70	0
1	D	555/558 (99%)	0.53	43 (7%) 21 20	16, 30, 60, 82	0
All	All	2221/2232 (99%)	0.16	73 (3%) 49 50	14, 25, 53, 85	1 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	THR	4.8
1	D	258	ILE	4.4
1	D	144	TYR	4.3
1	D	229	PHE	4.1
1	D	232	ALA	3.8
1	D	253	VAL	3.8
1	D	143	GLY	3.6
1	C	557	VAL	3.6
1	D	256	PHE	3.3
1	D	233	ALA	3.3
1	D	251	THR	3.2
1	D	237	SER	3.1
1	D	239	VAL	3.0
1	C	22	SER	3.0
1	D	2	ALA	2.9
1	D	147	LYS	2.9
1	B	556	ARG	2.8
1	A	255[A]	GLU	2.7
1	D	250	THR	2.7
1	D	260	PRO	2.6
1	C	211	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	250	THR	2.6
1	D	219	ILE	2.6
1	D	240	ALA	2.6
1	A	22	SER	2.5
1	D	213	PHE	2.5
1	D	141	TRP	2.5
1	D	259	ASP	2.5
1	D	462	LEU	2.5
1	D	554	GLU	2.5
1	A	214	THR	2.5
1	D	456	PRO	2.5
1	A	555	ALA	2.5
1	B	462	LEU	2.4
1	C	258	ILE	2.4
1	A	212	THR	2.4
1	A	556	ARG	2.4
1	D	556	ARG	2.4
1	A	554	GLU	2.4
1	D	452	ALA	2.4
1	A	213	PHE	2.4
1	D	212	THR	2.4
1	B	456	PRO	2.4
1	D	455	SER	2.3
1	D	238	ALA	2.3
1	D	262	ASN	2.3
1	D	214	THR	2.3
1	D	369	THR	2.3
1	D	453	GLY	2.3
1	B	554	GLU	2.3
1	B	22	SER	2.3
1	D	225	ALA	2.2
1	B	144	TYR	2.2
1	D	228	TRP	2.2
1	B	146	GLY	2.2
1	D	146	GLY	2.2
1	D	257	GLY	2.2
1	C	254	LYS	2.1
1	C	253	VAL	2.1
1	C	19	GLU	2.1
1	D	243	PHE	2.1
1	D	267	TRP	2.1
1	D	230	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	248	THR	2.1
1	B	368	GLY	2.1
1	D	203	SER	2.1
1	D	268	ASP	2.0
1	B	461	ARG	2.0
1	A	250	THR	2.0
1	B	32	ALA	2.0
1	D	15	GLN	2.0
1	B	458	ASP	2.0
1	D	140	ASP	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<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.

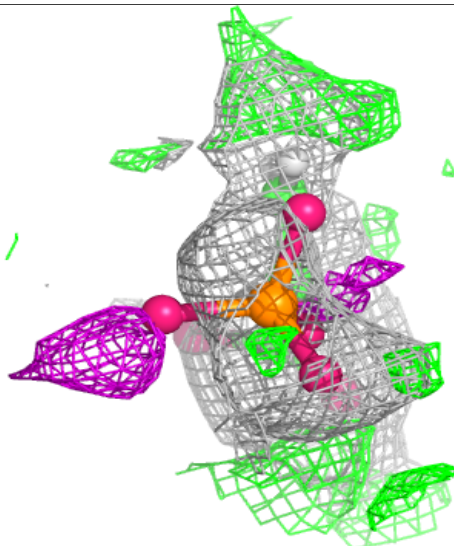
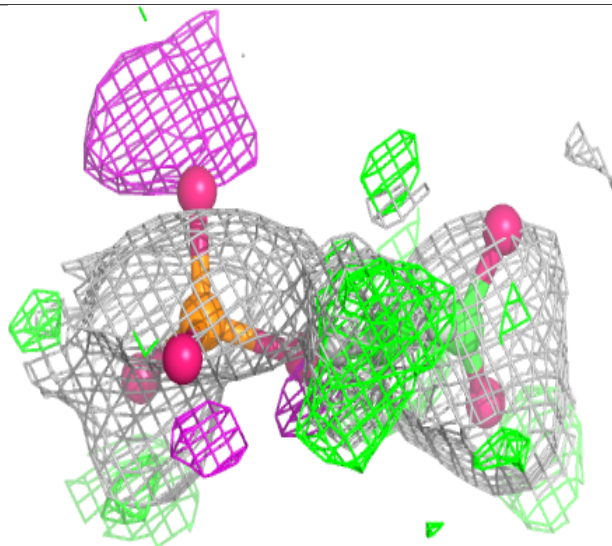
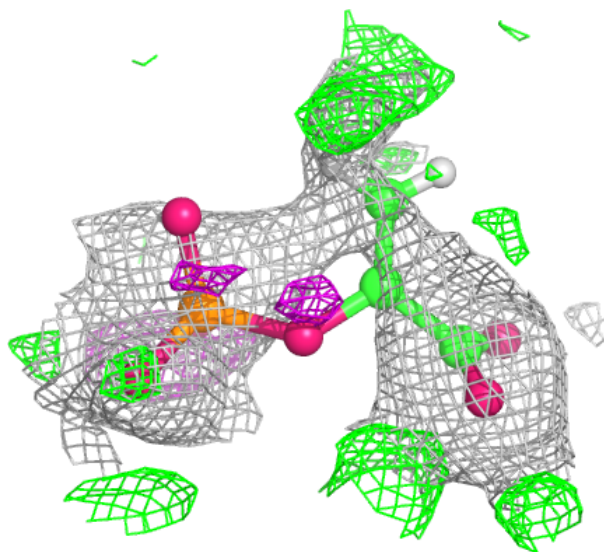
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PEP	A	601	10/10	0.57	0.23	40,70,90,93	0
2	PEP	C	601	10/10	0.71	0.21	39,54,69,86	0
2	PEP	D	601	10/10	0.74	0.17	47,67,85,85	0
4	PGE	A	605	10/10	0.80	0.17	34,47,57,62	0
2	PEP	B	601	10/10	0.81	0.14	43,60,75,76	0
4	PGE	A	603	10/10	0.84	0.13	32,41,51,51	0
5	TRS	A	604	8/8	0.84	0.14	32,42,54,56	0
3	PEG	B	602	7/7	0.86	0.15	13,39,52,52	0
4	PGE	B	603	10/10	0.88	0.11	35,46,64,66	0
3	PEG	A	602	7/7	0.89	0.12	19,32,49,58	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.

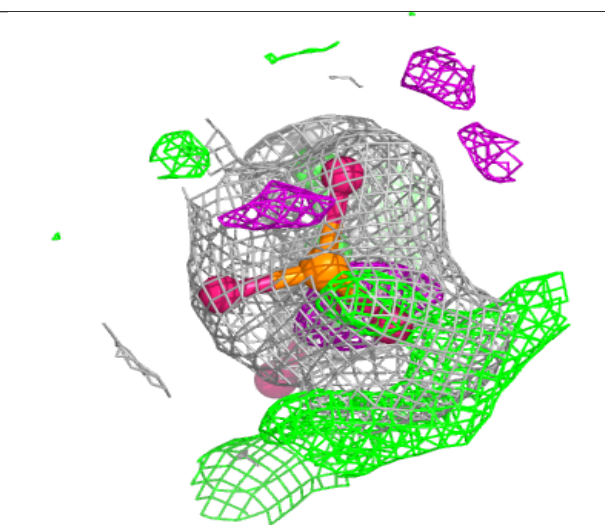
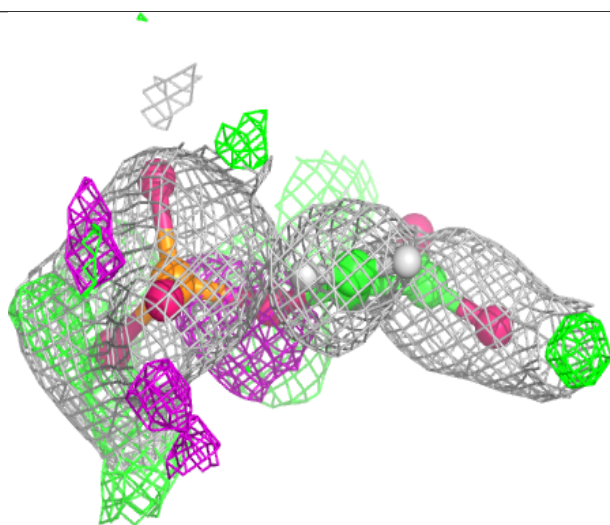
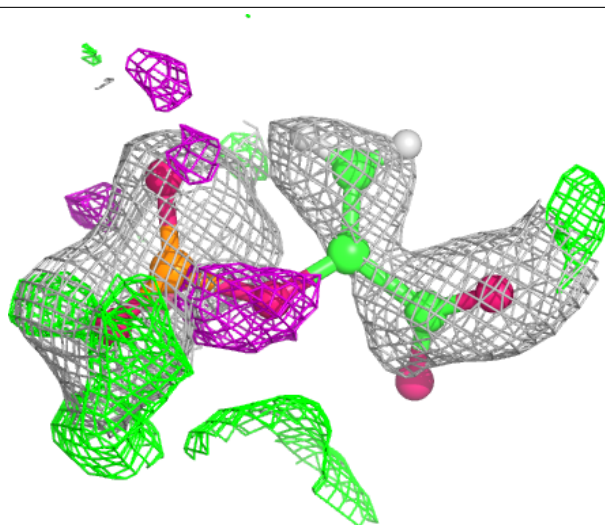
**Electron density around PEP A 601:**

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



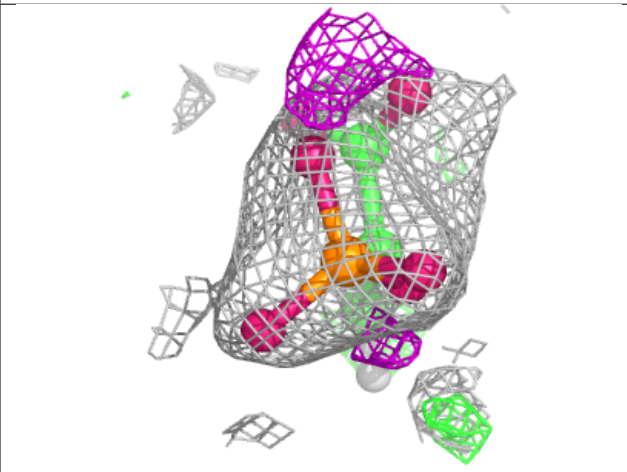
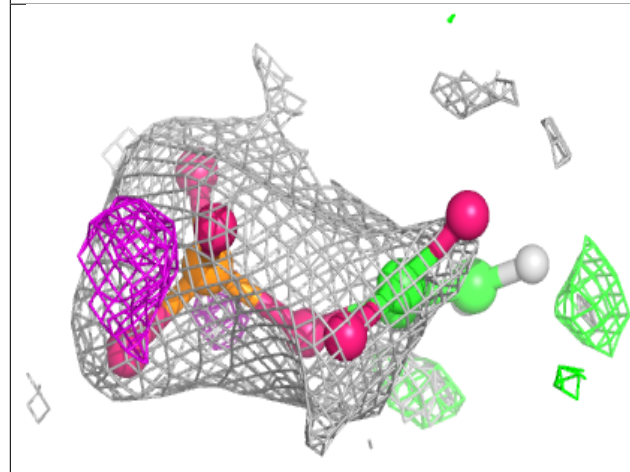
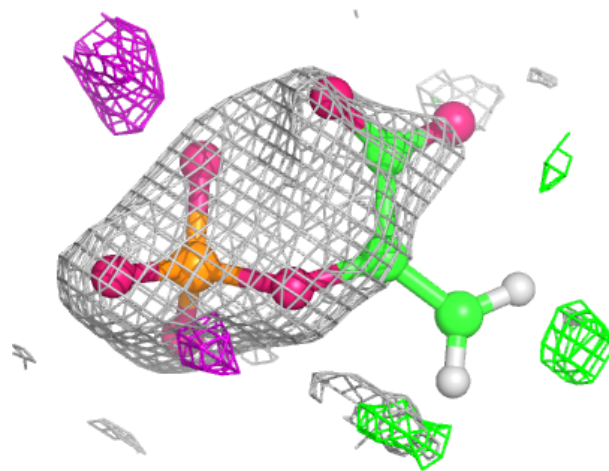
**Electron density around PEP C 601:**

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



**Electron density around PEP D 601:**

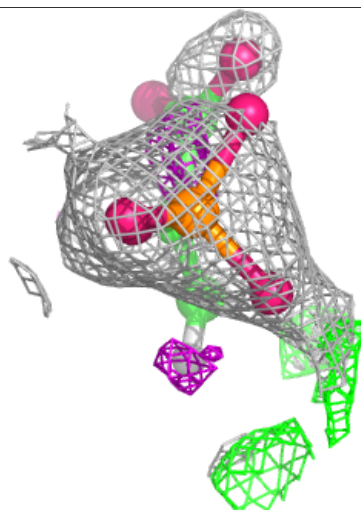
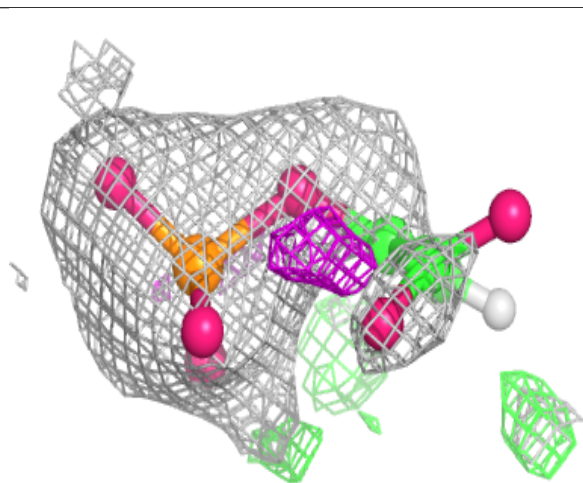
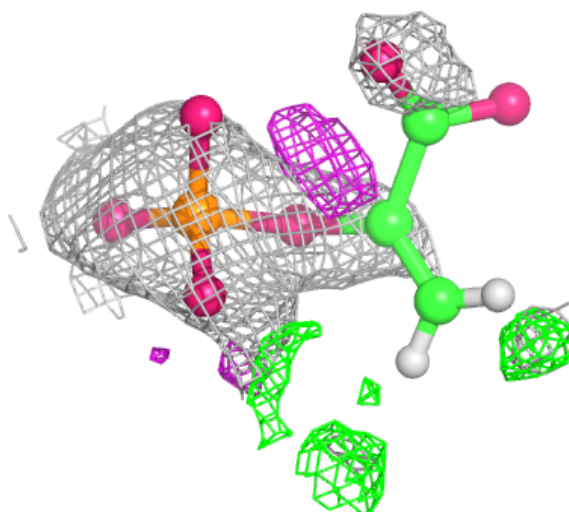
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PEP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.