wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 04:28 AM EDT

PDB ID	:	4JBW
Title	:	Crystal structure of E. coli maltose transporter MalFGK2 in complex with its regulatory protein EIIAglc
Authors	:	Chen, S.; Oldham, M.L.; Davidson, A.L.; Chen, J.
Deposited on	:	2013-02-20
Resolution	:	3.91 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 (i) symbol.

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

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

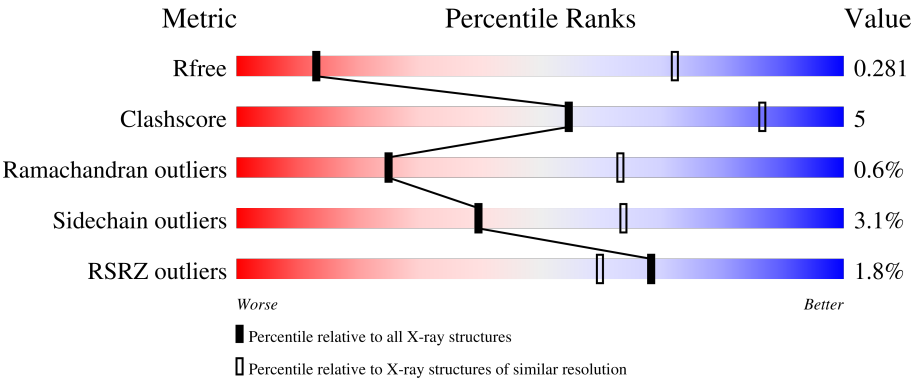
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	514	3% 82% 13%
1	H	514	4% 75% 16% 8%
2	G	296	% 77% 18%
2	I	296	5% 77% 18%
3	A	381	% 83% 13%

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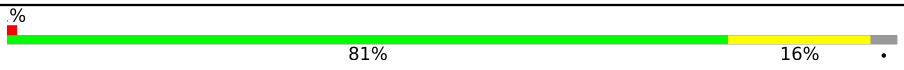
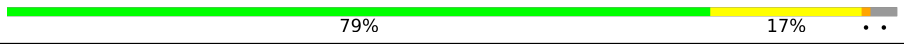
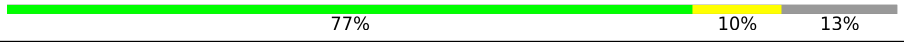
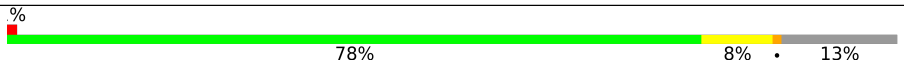
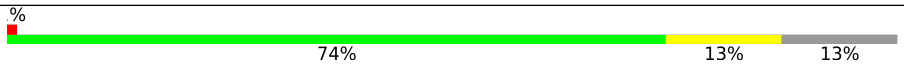
Mol	Chain	Length	Quality of chain
3	B	381	
3	C	381	
3	D	381	
4	M	172	
4	N	172	
4	O	172	
4	P	172	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27958 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 Maltose transport system permease protein MalF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	492	Total	C	N	O	S	0	0	0
			3805	2499	609	680	17			
1	H	472	Total	C	N	O	S	0	0	0
			3671	2416	582	656	17			

- Molecule 2 is a protein called Maltose transport system permease protein MalG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	286	Total	C	N	O	S	0	0	0
			2219	1487	354	369	9			
2	I	286	Total	C	N	O	S	0	0	0
			2219	1487	354	369	9			

- Molecule 3 is a protein called Maltose/maltodextrin import ATP-binding protein MalK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			
3	B	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			
3	C	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			
3	D	370	Total	C	N	O	S	0	0	0
			2871	1816	514	528	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	ALA	-	expression tag	UNP P68187
A	373	SER	-	expression tag	UNP P68187
A	374	ALA	-	expression tag	UNP P68187
A	375	SER	-	expression tag	UNP P68187

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Chain	Residue	Modelled	Actual	Comment	Reference
A	376	HIS	-	expression tag	UNP P68187
A	377	HIS	-	expression tag	UNP P68187
A	378	HIS	-	expression tag	UNP P68187
A	379	HIS	-	expression tag	UNP P68187
A	380	HIS	-	expression tag	UNP P68187
A	381	HIS	-	expression tag	UNP P68187
B	372	ALA	-	expression tag	UNP P68187
B	373	SER	-	expression tag	UNP P68187
B	374	ALA	-	expression tag	UNP P68187
B	375	SER	-	expression tag	UNP P68187
B	376	HIS	-	expression tag	UNP P68187
B	377	HIS	-	expression tag	UNP P68187
B	378	HIS	-	expression tag	UNP P68187
B	379	HIS	-	expression tag	UNP P68187
B	380	HIS	-	expression tag	UNP P68187
B	381	HIS	-	expression tag	UNP P68187
C	372	ALA	-	expression tag	UNP P68187
C	373	SER	-	expression tag	UNP P68187
C	374	ALA	-	expression tag	UNP P68187
C	375	SER	-	expression tag	UNP P68187
C	376	HIS	-	expression tag	UNP P68187
C	377	HIS	-	expression tag	UNP P68187
C	378	HIS	-	expression tag	UNP P68187
C	379	HIS	-	expression tag	UNP P68187
C	380	HIS	-	expression tag	UNP P68187
C	381	HIS	-	expression tag	UNP P68187
D	372	ALA	-	expression tag	UNP P68187
D	373	SER	-	expression tag	UNP P68187
D	374	ALA	-	expression tag	UNP P68187
D	375	SER	-	expression tag	UNP P68187
D	376	HIS	-	expression tag	UNP P68187
D	377	HIS	-	expression tag	UNP P68187
D	378	HIS	-	expression tag	UNP P68187
D	379	HIS	-	expression tag	UNP P68187
D	380	HIS	-	expression tag	UNP P68187
D	381	HIS	-	expression tag	UNP P68187

- Molecule 4 is a protein called Glucose-specific phosphotransferase enzyme IIA component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	150	Total	C	N	O	S	0	0	0
			1127	722	177	226	2			

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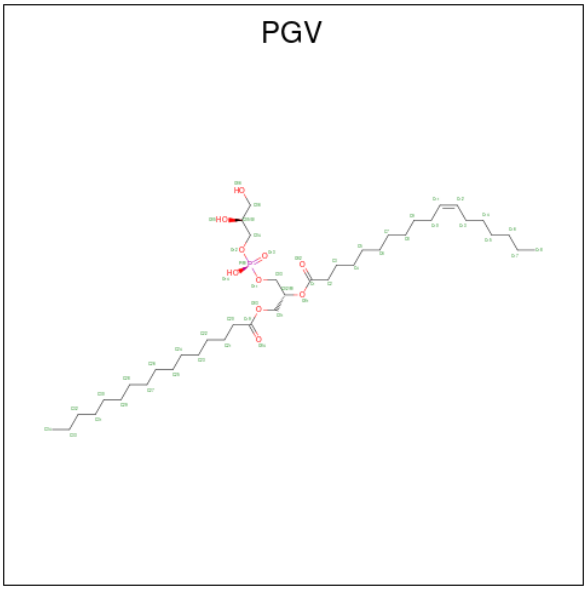
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	150	Total	C	N	O	S	0	0	0
			1127	722	177	226	2			
4	O	150	Total	C	N	O	S	0	0	0
			1127	722	177	226	2			
4	P	150	Total	C	N	O	S	0	0	0
			1127	722	177	226	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	SER	-	expression tag	UNP P69783
M	-2	ASN	-	expression tag	UNP P69783
M	-1	ALA	-	expression tag	UNP P69783
N	-3	SER	-	expression tag	UNP P69783
N	-2	ASN	-	expression tag	UNP P69783
N	-1	ALA	-	expression tag	UNP P69783
O	-3	SER	-	expression tag	UNP P69783
O	-2	ASN	-	expression tag	UNP P69783
O	-1	ALA	-	expression tag	UNP P69783
P	-3	SER	-	expression tag	UNP P69783
P	-2	ASN	-	expression tag	UNP P69783
P	-1	ALA	-	expression tag	UNP P69783

- Molecule 5 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



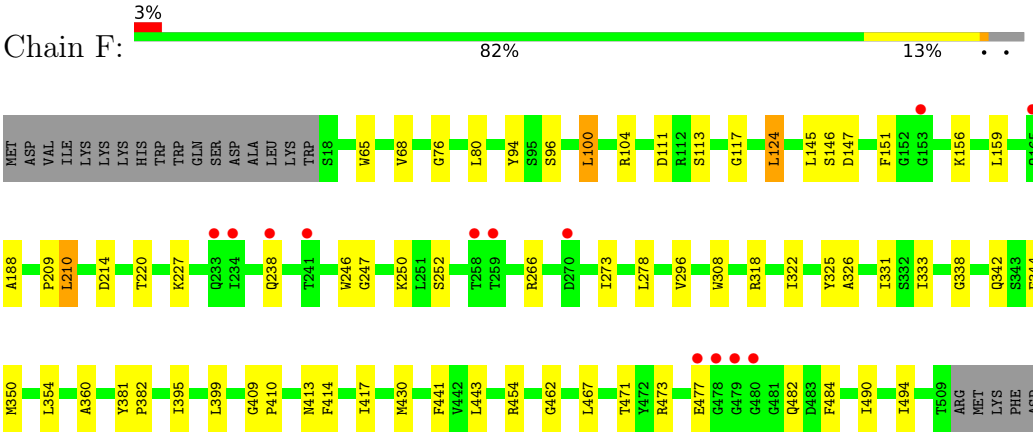
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	O	P	0	0
			26	15	10	1		
5	H	1	Total	C	O	P	0	0
			26	15	10	1		

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.

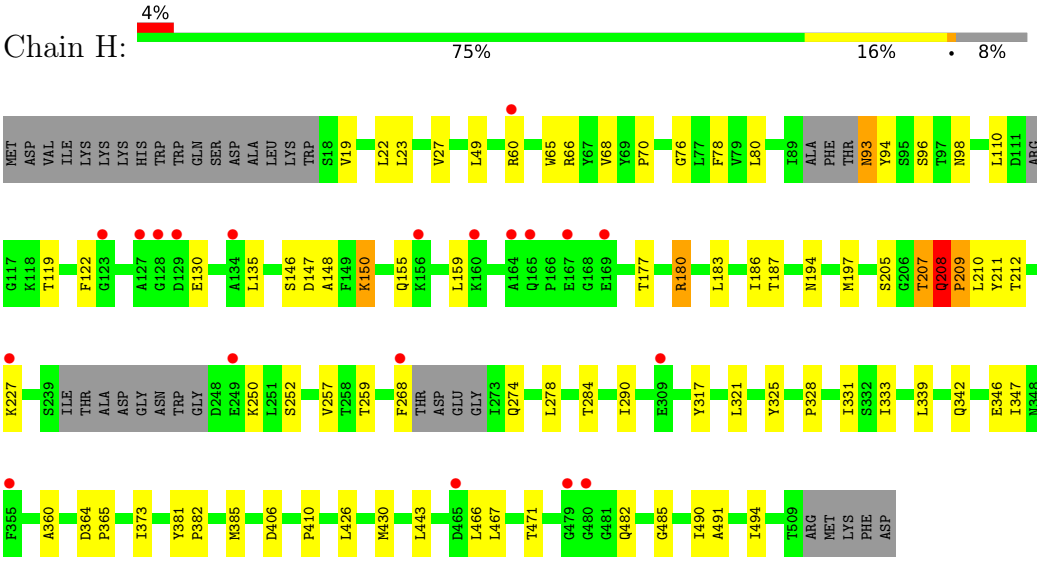
• Molecule 1: Maltose transport system permease protein MalF

Chain F:



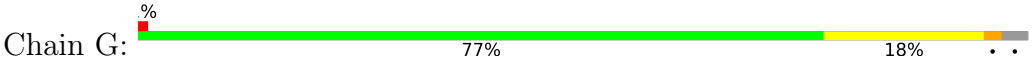
• Molecule 1: Maltose transport system permease protein MalF

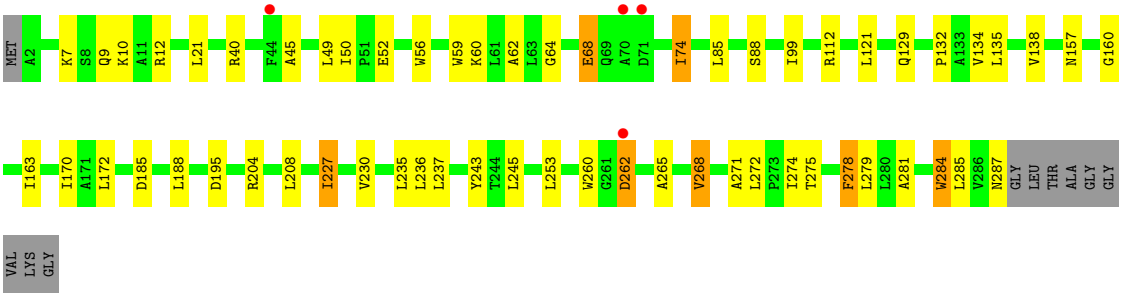
Chain H:



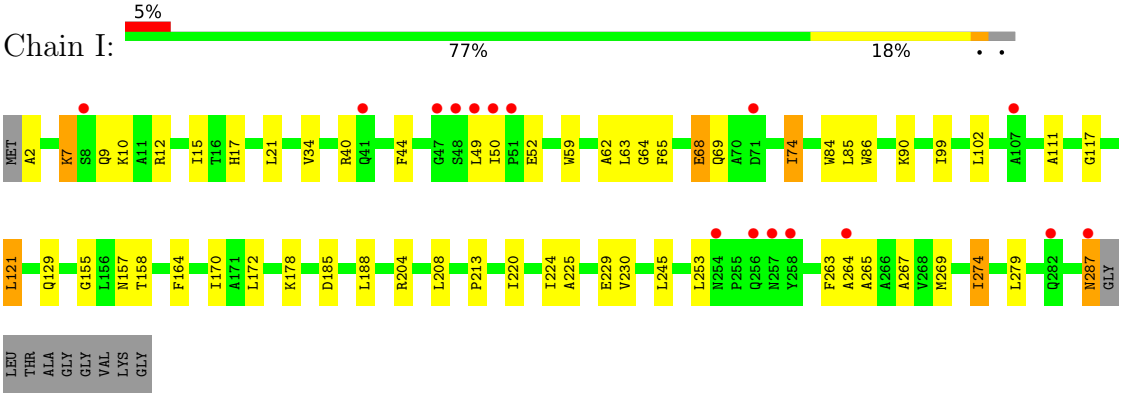
• Molecule 2: Maltose transport system permease protein MalG

Chain G:

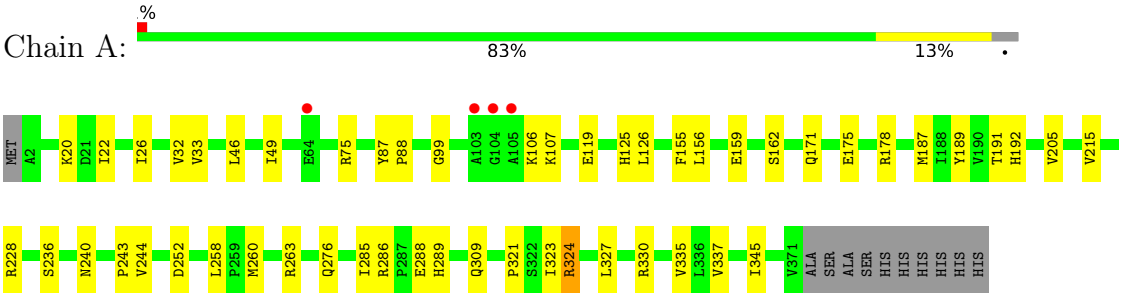




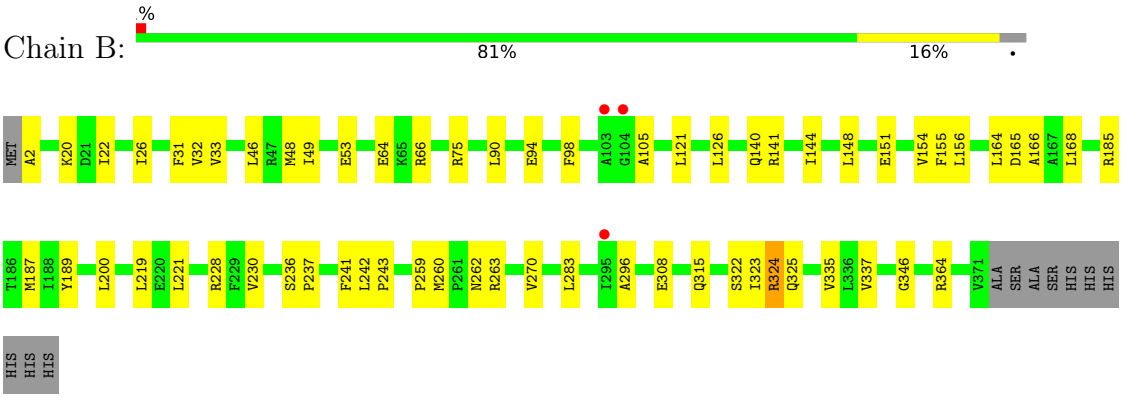
• Molecule 2: Maltose transport system permease protein MalG



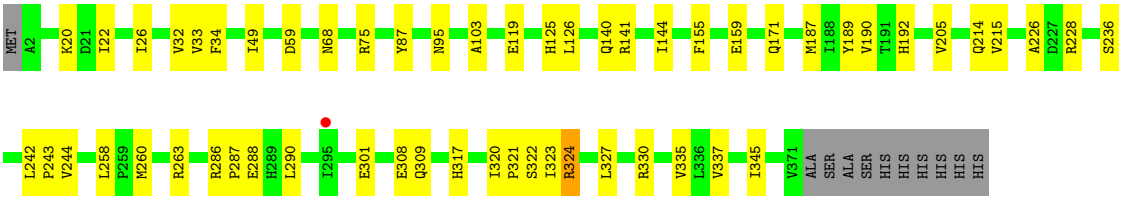
• Molecule 3: Maltose/maltodextrin import ATP-binding protein MalK



• Molecule 3: Maltose/maltodextrin import ATP-binding protein MalK



• Molecule 3: Maltose/maltodextrin import ATP-binding protein MalK

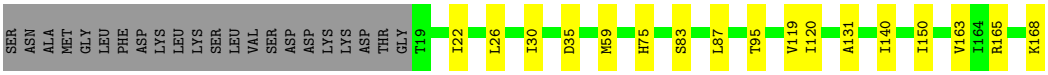


• Molecule 3: Maltose/maltodextrin import ATP-binding protein MalK

Chain D:

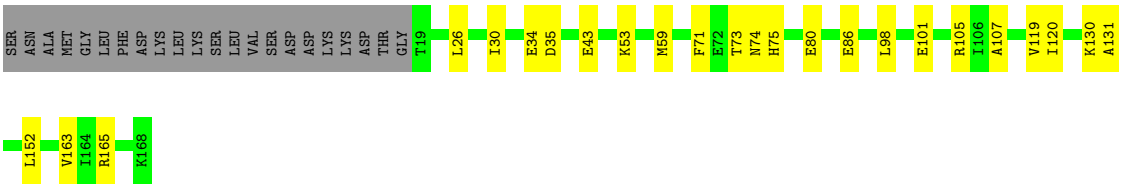
• Molecule 4: Glucose-specific phosphotransferase enzyme IIA component

Chain M:



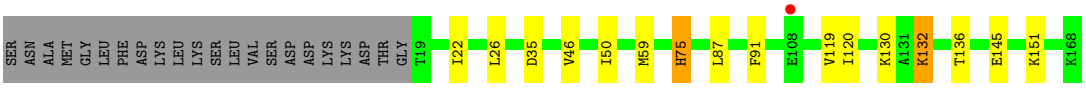
• Molecule 4: Glucose-specific phosphotransferase enzyme IIA component

Chain N:



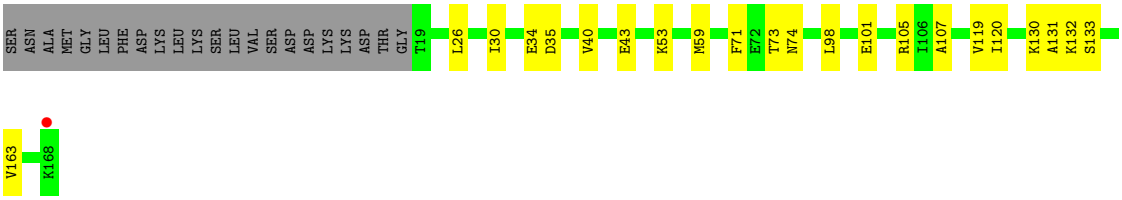
• Molecule 4: Glucose-specific phosphotransferase enzyme IIA component

Chain O:



• Molecule 4: Glucose-specific phosphotransferase enzyme IIA component

Chain P:


SER
ASN
ALA
MET
GLY
LEU
PHE
ASP
LYS
LEU
LYS
SER
LEU
VAL
SER
ASP
ASP
LYS
LYS
ASP
THR
GLY
T19
L26
I30
E34
D35
V40
E43
K53
M59
F71
E72
T73
N74
L98
E101
R105
I106
A107
V119
I120
K130
A131
K132
S133
V163
K168

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.53Å 208.45Å 347.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.91 19.98 – 3.91	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.98-3.91) 94.9 (19.98-3.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.226 , 0.281 0.225 , 0.281	Depositor DCC
R_{free} test set	3017 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	162.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27958	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGV

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	F	0.22	0/3898	0.39	0/5308
1	H	0.22	0/3756	0.39	0/5106
2	G	0.22	0/2281	0.41	0/3120
2	I	0.22	0/2281	0.39	0/3120
3	A	0.21	0/2921	0.39	0/3961
3	B	0.21	0/2921	0.39	0/3961
3	C	0.21	0/2921	0.39	0/3961
3	D	0.21	0/2921	0.39	0/3961
4	M	0.21	0/1142	0.41	0/1545
4	N	0.21	0/1142	0.41	0/1545
4	O	0.21	0/1142	0.41	0/1545
4	P	0.21	0/1142	0.41	0/1545
All	All	0.21	0/28468	0.39	0/38678

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	208	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3805	0	3837	43	0
1	H	3671	0	3727	46	0
2	G	2219	0	2307	32	0
2	I	2219	0	2307	28	0
3	A	2871	0	2937	29	0
3	B	2871	0	2937	33	0
3	C	2871	0	2937	33	0
3	D	2871	0	2937	43	0
4	M	1127	0	1155	9	0
4	N	1127	0	1155	13	0
4	O	1127	0	1155	10	0
4	P	1127	0	1155	16	0
5	F	26	0	22	4	0
5	H	26	0	22	2	0
All	All	27958	0	28590	296	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 5.

The worst 5 of 296 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:H:93:ASN:N	1:H:259:THR:HG1	1.63	0.97
3:D:33:VAL:HG22	3:D:189:TYR:HB3	1.57	0.87
3:B:33:VAL:HG22	3:B:189:TYR:HB3	1.57	0.86
3:C:33:VAL:HG22	3:C:189:TYR:HB3	1.56	0.84
3:A:33:VAL:HG22	3:A:189:TYR:HB3	1.62	0.82

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	F	490/514 (95%)	460 (94%)	28 (6%)	2 (0%)	34	71
1	H	462/514 (90%)	426 (92%)	29 (6%)	7 (2%)	10	45
2	G	284/296 (96%)	265 (93%)	16 (6%)	3 (1%)	14	51
2	I	284/296 (96%)	263 (93%)	17 (6%)	4 (1%)	11	46
3	A	368/381 (97%)	343 (93%)	24 (6%)	1 (0%)	41	75
3	B	368/381 (97%)	344 (94%)	24 (6%)	0	100	100
3	C	368/381 (97%)	342 (93%)	24 (6%)	2 (0%)	29	67
3	D	368/381 (97%)	341 (93%)	25 (7%)	2 (0%)	29	67
4	M	148/172 (86%)	141 (95%)	7 (5%)	0	100	100
4	N	148/172 (86%)	141 (95%)	7 (5%)	0	100	100
4	O	148/172 (86%)	141 (95%)	7 (5%)	0	100	100
4	P	148/172 (86%)	141 (95%)	7 (5%)	0	100	100
All	All	3584/3832 (94%)	3348 (93%)	215 (6%)	21 (1%)	25	63

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	117	GLY
3	A	263	ARG
1	H	208	GLN
1	H	209	PRO
3	C	263	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	F	397/424 (94%)	385 (97%)	12 (3%)	41	64
1	H	389/424 (92%)	376 (97%)	13 (3%)	38	63
2	G	232/237 (98%)	214 (92%)	18 (8%)	12	41
2	I	232/237 (98%)	213 (92%)	19 (8%)	11	39
3	A	314/323 (97%)	308 (98%)	6 (2%)	57	75
3	B	314/323 (97%)	309 (98%)	5 (2%)	62	79
3	C	314/323 (97%)	309 (98%)	5 (2%)	62	79
3	D	314/323 (97%)	307 (98%)	7 (2%)	52	71
4	M	127/148 (86%)	126 (99%)	1 (1%)	81	89
4	N	127/148 (86%)	125 (98%)	2 (2%)	62	79
4	O	127/148 (86%)	124 (98%)	3 (2%)	49	69
4	P	127/148 (86%)	124 (98%)	3 (2%)	49	69
All	All	3014/3206 (94%)	2920 (97%)	94 (3%)	40	64

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	7	LYS
2	I	253	LEU
2	I	10	LYS
2	I	52	GLU
2	I	287	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	264	GLN
3	D	140	GLN
3	B	255	GLN
3	B	265	GLN
1	H	348	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
5	PGV	H	601	-	25,25,50	1.24	2 (8%)	28,31,56	1.39	3 (10%)
5	PGV	F	4001	-	25,25,50	1.24	2 (8%)	28,31,56	1.38	3 (10%)

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
5	PGV	H	601	-	-	17/30/30/55	-
5	PGV	F	4001	-	-	14/30/30/55	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	601	PGV	O01-C02	-3.48	1.37	1.46
5	F	4001	PGV	O01-C02	-3.42	1.38	1.46
5	F	4001	PGV	O03-C01	-2.99	1.38	1.45
5	H	601	PGV	O03-C01	-2.93	1.38	1.45

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	4001	PGV	O01-C1-C2	4.16	120.47	111.50
5	H	601	PGV	O01-C1-C2	4.08	120.29	111.50
5	H	601	PGV	O03-C01-C02	3.46	118.50	108.43
5	F	4001	PGV	O03-C01-C02	3.30	118.04	108.43
5	F	4001	PGV	O03-C19-C20	2.64	120.19	111.91

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	4001	PGV	C04-O12-P-O13
5	F	4001	PGV	C04-O12-P-O14
5	F	4001	PGV	O12-C04-C05-C06
5	F	4001	PGV	C2-C1-O01-C02
5	H	601	PGV	C04-O12-P-O11

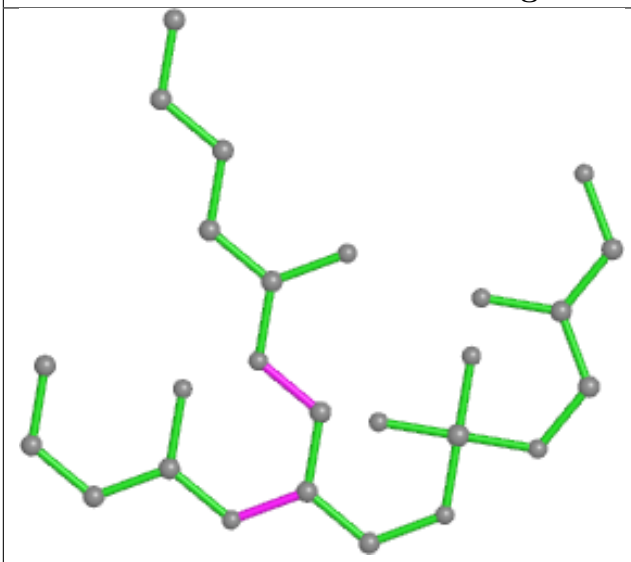
There are no ring outliers.

2 monomers are involved in 6 short contacts:

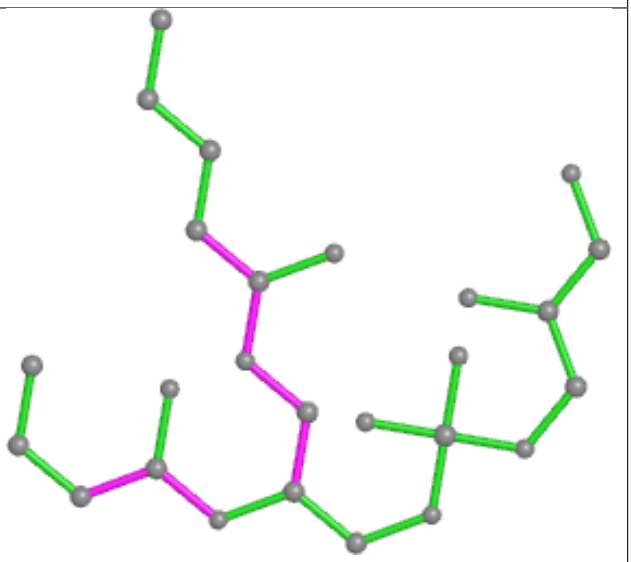
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	601	PGV	2	0
5	F	4001	PGV	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

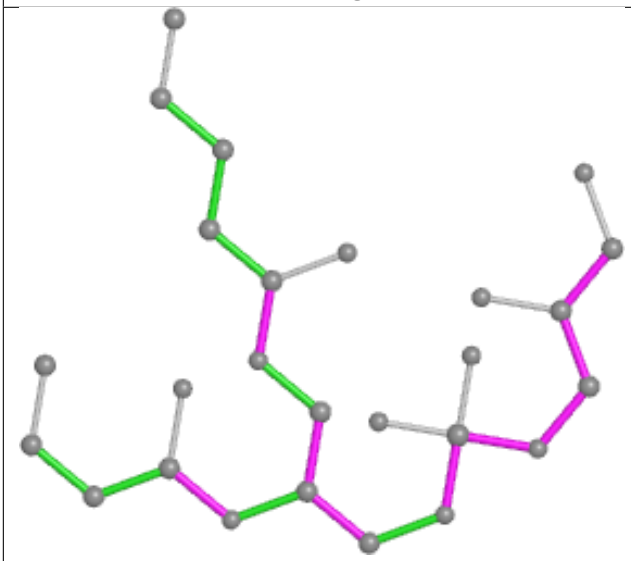
Ligand PGV H 601



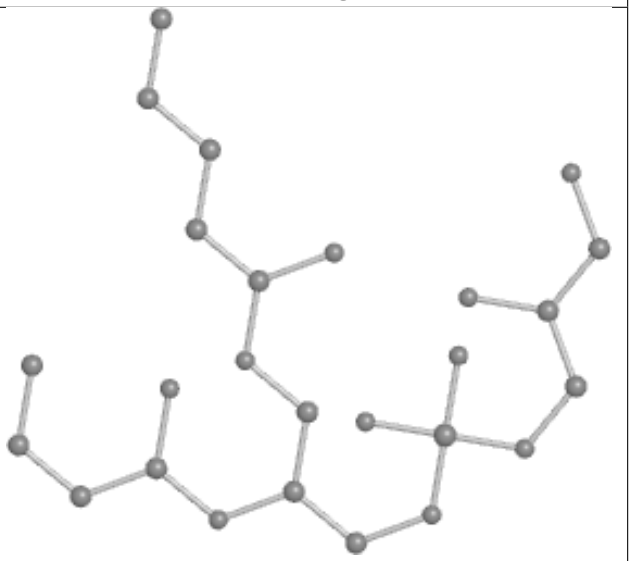
Bond lengths



Bond angles

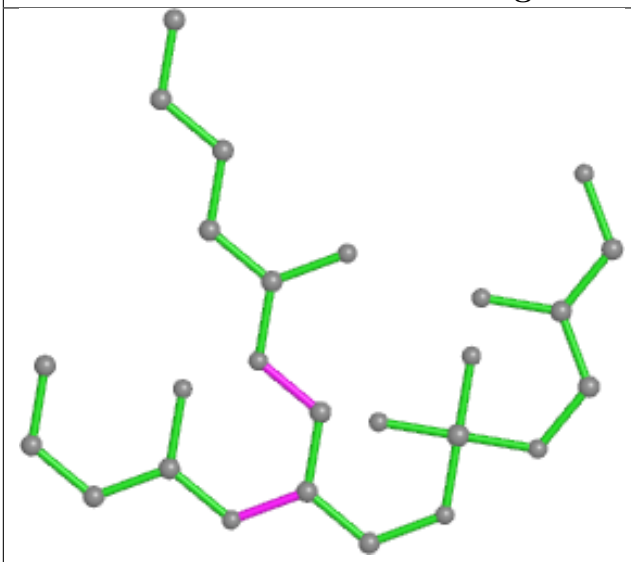


Torsions

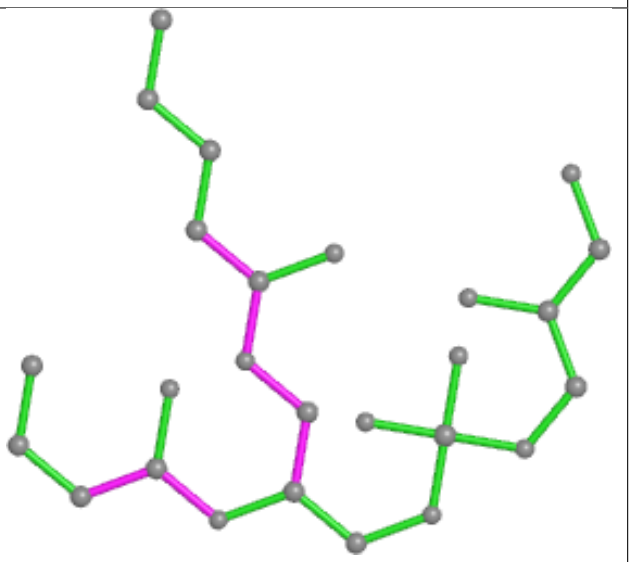


Rings

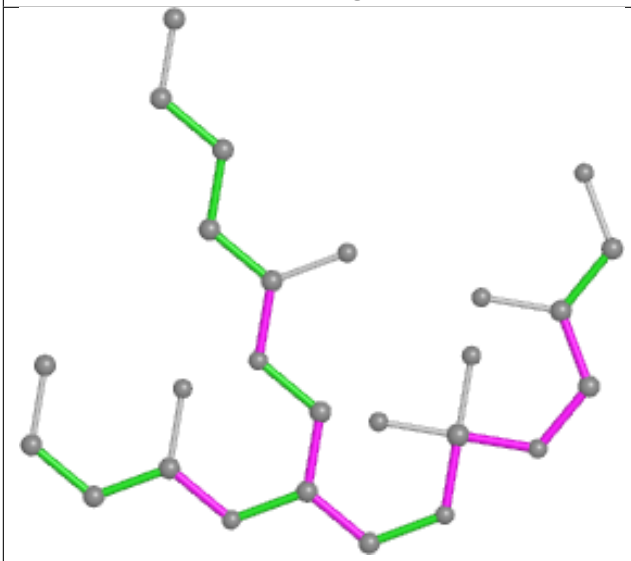
Ligand PGV F 4001



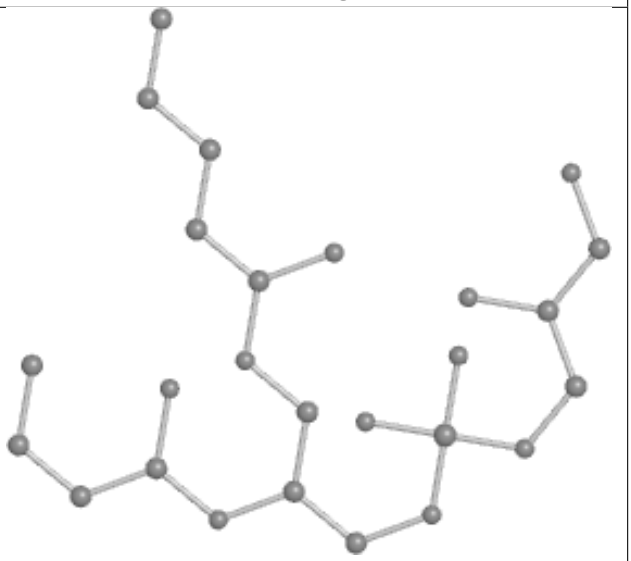
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	F	492/514 (95%)	-0.34	13 (2%) 56 46	81, 137, 189, 239	0
1	H	472/514 (91%)	-0.08	21 (4%) 34 29	94, 164, 203, 229	0
2	G	286/296 (96%)	-0.36	4 (1%) 75 66	87, 136, 189, 214	0
2	I	286/296 (96%)	-0.05	16 (5%) 24 21	100, 169, 217, 240	0
3	A	370/381 (97%)	-0.46	4 (1%) 80 73	71, 121, 164, 198	0
3	B	370/381 (97%)	-0.53	3 (0%) 86 80	55, 104, 152, 208	0
3	C	370/381 (97%)	-0.54	1 (0%) 94 90	65, 115, 163, 201	0
3	D	370/381 (97%)	-0.58	0 100 100	55, 105, 150, 203	0
4	M	150/172 (87%)	-0.43	0 100 100	86, 136, 174, 187	0
4	N	150/172 (87%)	-0.46	0 100 100	90, 128, 162, 186	0
4	O	150/172 (87%)	-0.46	1 (0%) 87 82	86, 141, 179, 189	0
4	P	150/172 (87%)	-0.32	1 (0%) 87 82	73, 123, 166, 194	0
All	All	3616/3832 (94%)	-0.37	64 (1%) 68 60	55, 131, 190, 240	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	51	PRO	6.4
2	I	50	ILE	6.4
1	H	134	ALA	6.2
3	A	103	ALA	5.1
1	H	128	GLY	5.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

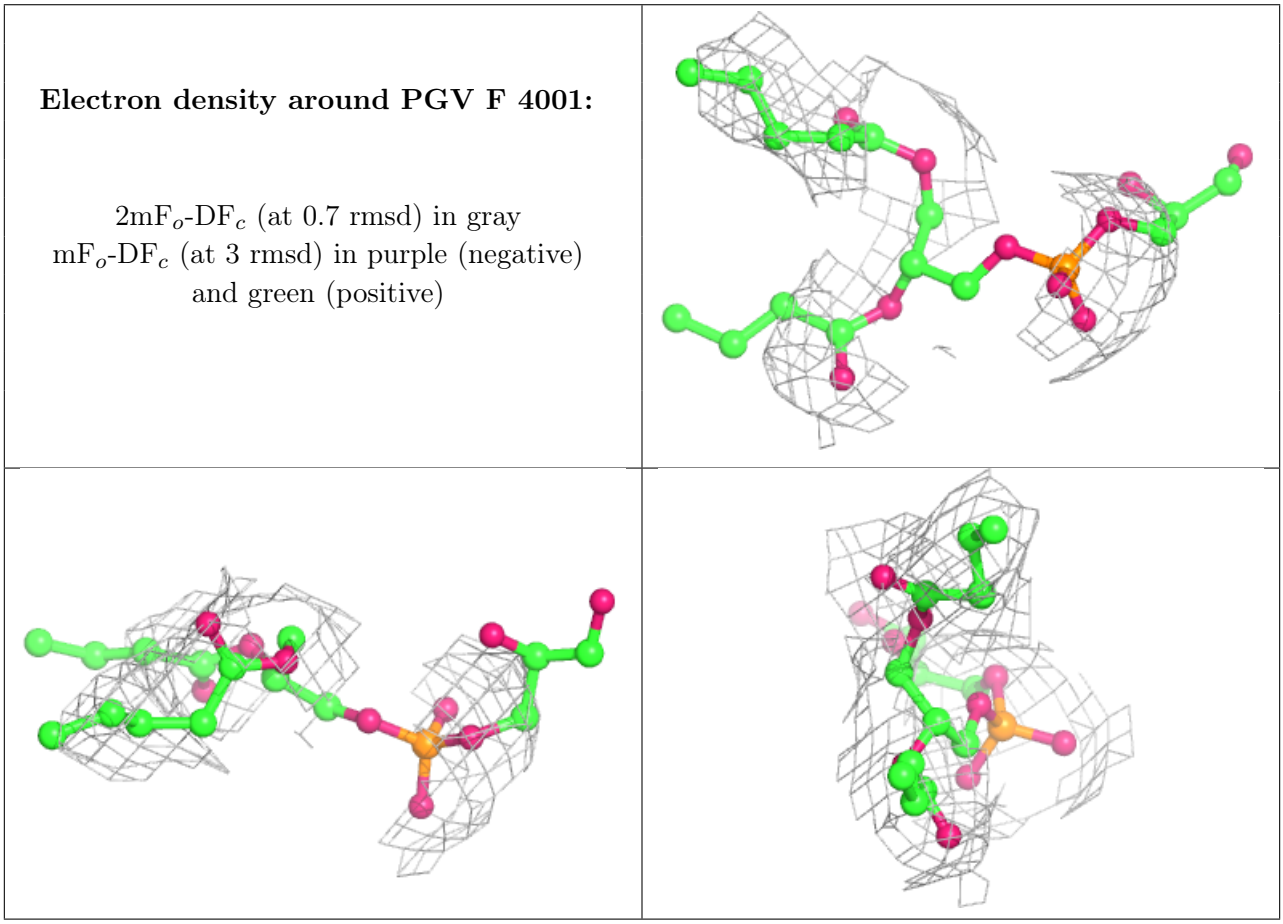
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGV	F	4001	26/51	0.86	0.33	42,107,135,141	0
5	PGV	H	601	26/51	0.86	0.36	66,147,171,182	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.

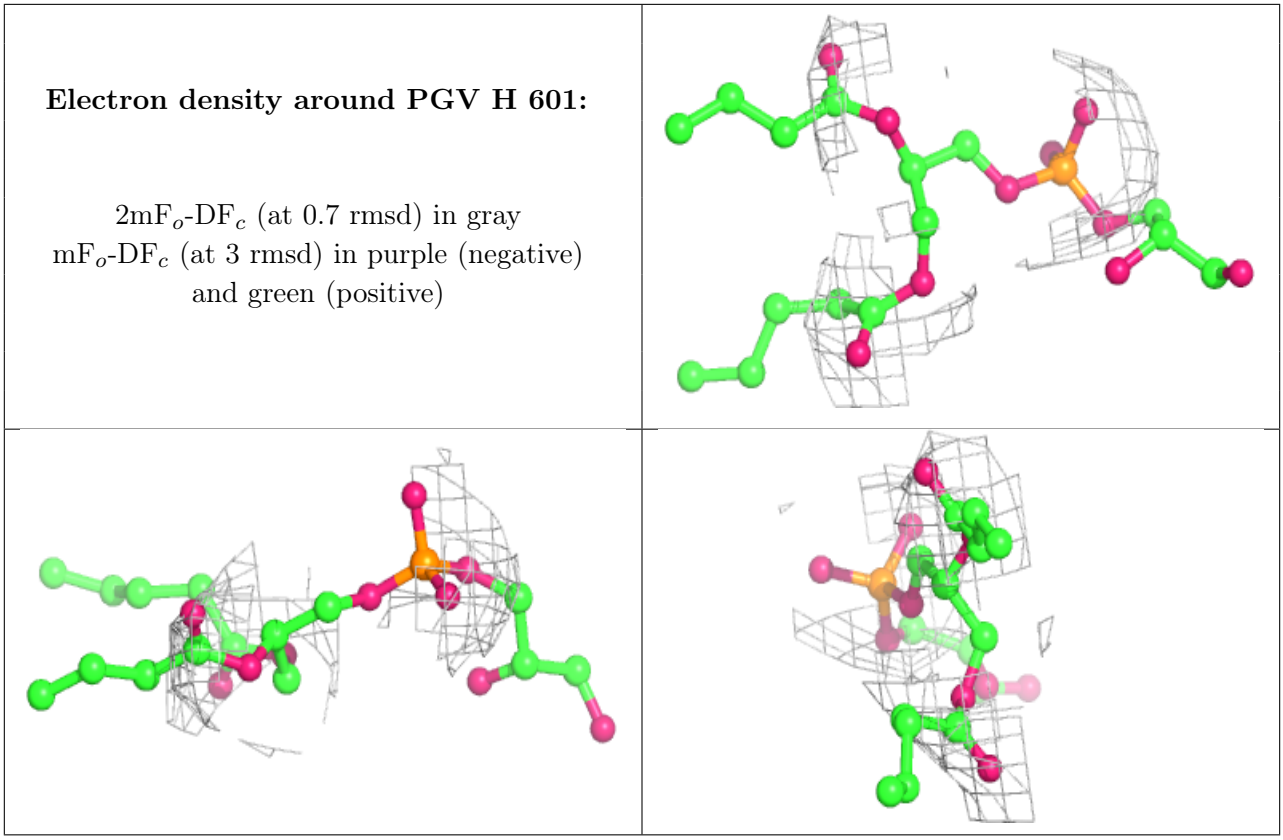
Electron density around PGV F 4001:

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



Electron density around PGV H 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.