wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 10:20 am BST

PDB ID	:	7PQ9
Title	:	Crystal structure of Bacillus clausii pdxR at 2.8 Angstroms resolution
Authors	:	Vivoli Vega, M.; Isupov, M.N.; Harmer, N.
Deposited on	:	2021-09-16
Resolution	:	2.80 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:

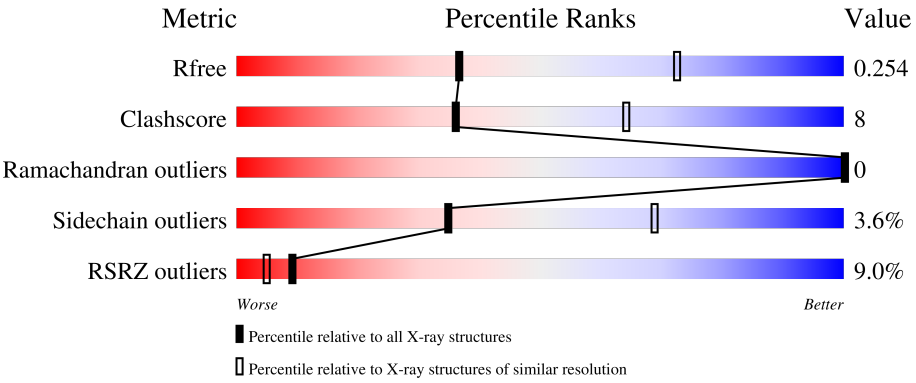
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	AAA	478	6% 63% 12% • 23%
1	BBB	478	7% 62% 13% • 23%
1	CCC	478	2% 62% 13% • 23%
1	DDD	478	6% 64% 11% • 23%
1	EEE	478	9% 65% 10% • 24%

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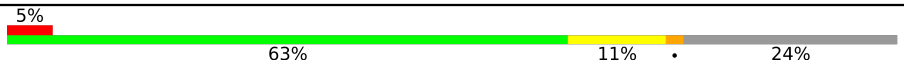
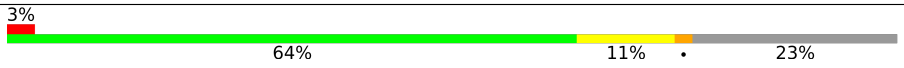
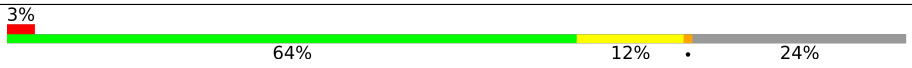
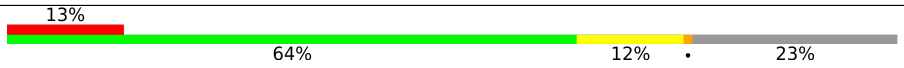
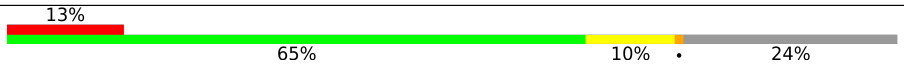
Mol	Chain	Length	Quality of chain
1	FFF	478	
1	GGG	478	
1	HHH	478	
1	III	478	
1	JJJ	478	
1	KKK	478	

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	CL	AAA	503	-	-	-	X
3	CL	AAA	504	-	-	-	X
5	EDO	GGG	501	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 30729 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 PLP-dependent aminotransferase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	367	Total	C	N	O	S	0	0	0
			2999	1928	520	542	9			
1	BBB	368	Total	C	N	O	S	0	0	0
			3005	1931	521	544	9			
1	CCC	367	Total	C	N	O	S	0	0	0
			2999	1928	520	542	9			
1	DDD	366	Total	C	N	O	S	0	0	0
			2995	1926	519	541	9			
1	EEE	364	Total	C	N	O	S	0	0	0
			2977	1915	514	539	9			
1	FFF	365	Total	C	N	O	S	0	0	0
			2984	1920	515	540	9			
1	GGG	368	Total	C	N	O	S	0	0	0
			3005	1931	521	544	9			
1	HHH	364	Total	C	N	O	S	0	0	0
			2976	1916	514	537	9			
1	III	367	Total	C	N	O	S	0	0	0
			2997	1927	520	541	9			
1	JJJ	364	Total	C	N	O	S	0	0	0
			2976	1916	514	537	9			
1	KKK	81	Total	C	N	O	S	0	0	0
			658	425	108	124	1			

There are 154 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	465	LEU	-	expression tag	UNP A0A7Y3RUA1
AAA	466	VAL	-	expression tag	UNP A0A7Y3RUA1
AAA	467	PRO	-	expression tag	UNP A0A7Y3RUA1
AAA	468	ARG	-	expression tag	UNP A0A7Y3RUA1
AAA	469	GLY	-	expression tag	UNP A0A7Y3RUA1
AAA	470	SER	-	expression tag	UNP A0A7Y3RUA1
AAA	471	LEU	-	expression tag	UNP A0A7Y3RUA1

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	472	GLU	-	expression tag	UNP A0A7Y3RUA1
AAA	473	HIS	-	expression tag	UNP A0A7Y3RUA1
AAA	474	HIS	-	expression tag	UNP A0A7Y3RUA1
AAA	475	HIS	-	expression tag	UNP A0A7Y3RUA1
AAA	476	HIS	-	expression tag	UNP A0A7Y3RUA1
AAA	477	HIS	-	expression tag	UNP A0A7Y3RUA1
AAA	478	HIS	-	expression tag	UNP A0A7Y3RUA1
BBB	465	LEU	-	expression tag	UNP A0A7Y3RUA1
BBB	466	VAL	-	expression tag	UNP A0A7Y3RUA1
BBB	467	PRO	-	expression tag	UNP A0A7Y3RUA1
BBB	468	ARG	-	expression tag	UNP A0A7Y3RUA1
BBB	469	GLY	-	expression tag	UNP A0A7Y3RUA1
BBB	470	SER	-	expression tag	UNP A0A7Y3RUA1
BBB	471	LEU	-	expression tag	UNP A0A7Y3RUA1
BBB	472	GLU	-	expression tag	UNP A0A7Y3RUA1
BBB	473	HIS	-	expression tag	UNP A0A7Y3RUA1
BBB	474	HIS	-	expression tag	UNP A0A7Y3RUA1
BBB	475	HIS	-	expression tag	UNP A0A7Y3RUA1
BBB	476	HIS	-	expression tag	UNP A0A7Y3RUA1
BBB	477	HIS	-	expression tag	UNP A0A7Y3RUA1
BBB	478	HIS	-	expression tag	UNP A0A7Y3RUA1
CCC	465	LEU	-	expression tag	UNP A0A7Y3RUA1
CCC	466	VAL	-	expression tag	UNP A0A7Y3RUA1
CCC	467	PRO	-	expression tag	UNP A0A7Y3RUA1
CCC	468	ARG	-	expression tag	UNP A0A7Y3RUA1
CCC	469	GLY	-	expression tag	UNP A0A7Y3RUA1
CCC	470	SER	-	expression tag	UNP A0A7Y3RUA1
CCC	471	LEU	-	expression tag	UNP A0A7Y3RUA1
CCC	472	GLU	-	expression tag	UNP A0A7Y3RUA1
CCC	473	HIS	-	expression tag	UNP A0A7Y3RUA1
CCC	474	HIS	-	expression tag	UNP A0A7Y3RUA1
CCC	475	HIS	-	expression tag	UNP A0A7Y3RUA1
CCC	476	HIS	-	expression tag	UNP A0A7Y3RUA1
CCC	477	HIS	-	expression tag	UNP A0A7Y3RUA1
CCC	478	HIS	-	expression tag	UNP A0A7Y3RUA1
DDD	465	LEU	-	expression tag	UNP A0A7Y3RUA1
DDD	466	VAL	-	expression tag	UNP A0A7Y3RUA1
DDD	467	PRO	-	expression tag	UNP A0A7Y3RUA1
DDD	468	ARG	-	expression tag	UNP A0A7Y3RUA1
DDD	469	GLY	-	expression tag	UNP A0A7Y3RUA1
DDD	470	SER	-	expression tag	UNP A0A7Y3RUA1
DDD	471	LEU	-	expression tag	UNP A0A7Y3RUA1

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	472	GLU	-	expression tag	UNP A0A7Y3RUA1
DDD	473	HIS	-	expression tag	UNP A0A7Y3RUA1
DDD	474	HIS	-	expression tag	UNP A0A7Y3RUA1
DDD	475	HIS	-	expression tag	UNP A0A7Y3RUA1
DDD	476	HIS	-	expression tag	UNP A0A7Y3RUA1
DDD	477	HIS	-	expression tag	UNP A0A7Y3RUA1
DDD	478	HIS	-	expression tag	UNP A0A7Y3RUA1
EEE	465	LEU	-	expression tag	UNP A0A7Y3RUA1
EEE	466	VAL	-	expression tag	UNP A0A7Y3RUA1
EEE	467	PRO	-	expression tag	UNP A0A7Y3RUA1
EEE	468	ARG	-	expression tag	UNP A0A7Y3RUA1
EEE	469	GLY	-	expression tag	UNP A0A7Y3RUA1
EEE	470	SER	-	expression tag	UNP A0A7Y3RUA1
EEE	471	LEU	-	expression tag	UNP A0A7Y3RUA1
EEE	472	GLU	-	expression tag	UNP A0A7Y3RUA1
EEE	473	HIS	-	expression tag	UNP A0A7Y3RUA1
EEE	474	HIS	-	expression tag	UNP A0A7Y3RUA1
EEE	475	HIS	-	expression tag	UNP A0A7Y3RUA1
EEE	476	HIS	-	expression tag	UNP A0A7Y3RUA1
EEE	477	HIS	-	expression tag	UNP A0A7Y3RUA1
EEE	478	HIS	-	expression tag	UNP A0A7Y3RUA1
FFF	465	LEU	-	expression tag	UNP A0A7Y3RUA1
FFF	466	VAL	-	expression tag	UNP A0A7Y3RUA1
FFF	467	PRO	-	expression tag	UNP A0A7Y3RUA1
FFF	468	ARG	-	expression tag	UNP A0A7Y3RUA1
FFF	469	GLY	-	expression tag	UNP A0A7Y3RUA1
FFF	470	SER	-	expression tag	UNP A0A7Y3RUA1
FFF	471	LEU	-	expression tag	UNP A0A7Y3RUA1
FFF	472	GLU	-	expression tag	UNP A0A7Y3RUA1
FFF	473	HIS	-	expression tag	UNP A0A7Y3RUA1
FFF	474	HIS	-	expression tag	UNP A0A7Y3RUA1
FFF	475	HIS	-	expression tag	UNP A0A7Y3RUA1
FFF	476	HIS	-	expression tag	UNP A0A7Y3RUA1
FFF	477	HIS	-	expression tag	UNP A0A7Y3RUA1
FFF	478	HIS	-	expression tag	UNP A0A7Y3RUA1
GGG	465	LEU	-	expression tag	UNP A0A7Y3RUA1
GGG	466	VAL	-	expression tag	UNP A0A7Y3RUA1
GGG	467	PRO	-	expression tag	UNP A0A7Y3RUA1
GGG	468	ARG	-	expression tag	UNP A0A7Y3RUA1
GGG	469	GLY	-	expression tag	UNP A0A7Y3RUA1
GGG	470	SER	-	expression tag	UNP A0A7Y3RUA1
GGG	471	LEU	-	expression tag	UNP A0A7Y3RUA1

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Chain	Residue	Modelled	Actual	Comment	Reference
GGG	472	GLU	-	expression tag	UNP A0A7Y3RUA1
GGG	473	HIS	-	expression tag	UNP A0A7Y3RUA1
GGG	474	HIS	-	expression tag	UNP A0A7Y3RUA1
GGG	475	HIS	-	expression tag	UNP A0A7Y3RUA1
GGG	476	HIS	-	expression tag	UNP A0A7Y3RUA1
GGG	477	HIS	-	expression tag	UNP A0A7Y3RUA1
GGG	478	HIS	-	expression tag	UNP A0A7Y3RUA1
HHH	465	LEU	-	expression tag	UNP A0A7Y3RUA1
HHH	466	VAL	-	expression tag	UNP A0A7Y3RUA1
HHH	467	PRO	-	expression tag	UNP A0A7Y3RUA1
HHH	468	ARG	-	expression tag	UNP A0A7Y3RUA1
HHH	469	GLY	-	expression tag	UNP A0A7Y3RUA1
HHH	470	SER	-	expression tag	UNP A0A7Y3RUA1
HHH	471	LEU	-	expression tag	UNP A0A7Y3RUA1
HHH	472	GLU	-	expression tag	UNP A0A7Y3RUA1
HHH	473	HIS	-	expression tag	UNP A0A7Y3RUA1
HHH	474	HIS	-	expression tag	UNP A0A7Y3RUA1
HHH	475	HIS	-	expression tag	UNP A0A7Y3RUA1
HHH	476	HIS	-	expression tag	UNP A0A7Y3RUA1
HHH	477	HIS	-	expression tag	UNP A0A7Y3RUA1
HHH	478	HIS	-	expression tag	UNP A0A7Y3RUA1
III	465	LEU	-	expression tag	UNP A0A7Y3RUA1
III	466	VAL	-	expression tag	UNP A0A7Y3RUA1
III	467	PRO	-	expression tag	UNP A0A7Y3RUA1
III	468	ARG	-	expression tag	UNP A0A7Y3RUA1
III	469	GLY	-	expression tag	UNP A0A7Y3RUA1
III	470	SER	-	expression tag	UNP A0A7Y3RUA1
III	471	LEU	-	expression tag	UNP A0A7Y3RUA1
III	472	GLU	-	expression tag	UNP A0A7Y3RUA1
III	473	HIS	-	expression tag	UNP A0A7Y3RUA1
III	474	HIS	-	expression tag	UNP A0A7Y3RUA1
III	475	HIS	-	expression tag	UNP A0A7Y3RUA1
III	476	HIS	-	expression tag	UNP A0A7Y3RUA1
III	477	HIS	-	expression tag	UNP A0A7Y3RUA1
III	478	HIS	-	expression tag	UNP A0A7Y3RUA1
JJJ	465	LEU	-	expression tag	UNP A0A7Y3RUA1
JJJ	466	VAL	-	expression tag	UNP A0A7Y3RUA1
JJJ	467	PRO	-	expression tag	UNP A0A7Y3RUA1
JJJ	468	ARG	-	expression tag	UNP A0A7Y3RUA1
JJJ	469	GLY	-	expression tag	UNP A0A7Y3RUA1
JJJ	470	SER	-	expression tag	UNP A0A7Y3RUA1
JJJ	471	LEU	-	expression tag	UNP A0A7Y3RUA1

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Chain	Residue	Modelled	Actual	Comment	Reference
JJJ	472	GLU	-	expression tag	UNP A0A7Y3RUA1
JJJ	473	HIS	-	expression tag	UNP A0A7Y3RUA1
JJJ	474	HIS	-	expression tag	UNP A0A7Y3RUA1
JJJ	475	HIS	-	expression tag	UNP A0A7Y3RUA1
JJJ	476	HIS	-	expression tag	UNP A0A7Y3RUA1
JJJ	477	HIS	-	expression tag	UNP A0A7Y3RUA1
JJJ	478	HIS	-	expression tag	UNP A0A7Y3RUA1
KKK	465	LEU	-	expression tag	UNP A0A7Y3RUA1
KKK	466	VAL	-	expression tag	UNP A0A7Y3RUA1
KKK	467	PRO	-	expression tag	UNP A0A7Y3RUA1
KKK	468	ARG	-	expression tag	UNP A0A7Y3RUA1
KKK	469	GLY	-	expression tag	UNP A0A7Y3RUA1
KKK	470	SER	-	expression tag	UNP A0A7Y3RUA1
KKK	471	LEU	-	expression tag	UNP A0A7Y3RUA1
KKK	472	GLU	-	expression tag	UNP A0A7Y3RUA1
KKK	473	HIS	-	expression tag	UNP A0A7Y3RUA1
KKK	474	HIS	-	expression tag	UNP A0A7Y3RUA1
KKK	475	HIS	-	expression tag	UNP A0A7Y3RUA1
KKK	476	HIS	-	expression tag	UNP A0A7Y3RUA1
KKK	477	HIS	-	expression tag	UNP A0A7Y3RUA1
KKK	478	HIS	-	expression tag	UNP A0A7Y3RUA1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	2	Total Ca 2 2	0	0
2	BBB	2	Total Ca 2 2	0	0
2	CCC	3	Total Ca 3 3	0	0
2	DDD	3	Total Ca 3 3	0	0
2	EEE	2	Total Ca 2 2	0	0
2	FFF	1	Total Ca 1 1	0	0
2	GGG	3	Total Ca 3 3	0	0
2	HHH	3	Total Ca 3 3	0	0
2	III	3	Total Ca 3 3	0	0

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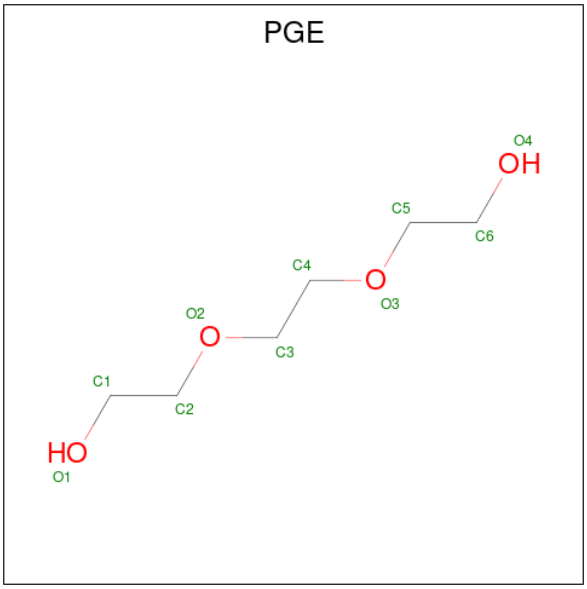
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	JJJ	2	Total Ca 2 2	0	0
2	KKK	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

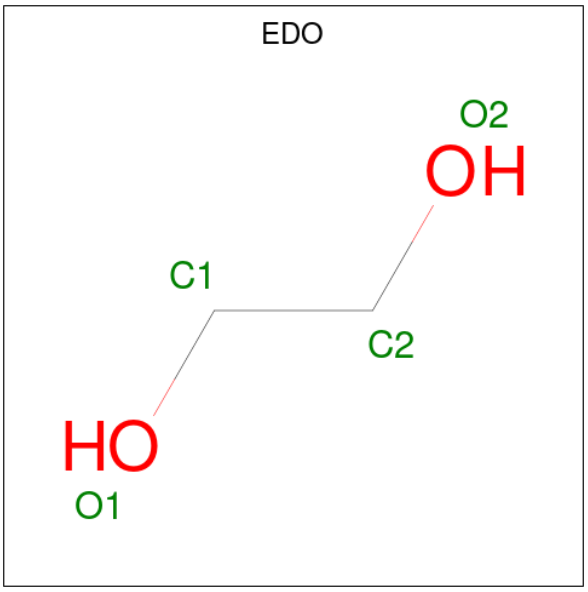
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	2	Total Cl 2 2	0	0
3	JJJ	1	Total Cl 1 1	0	0

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



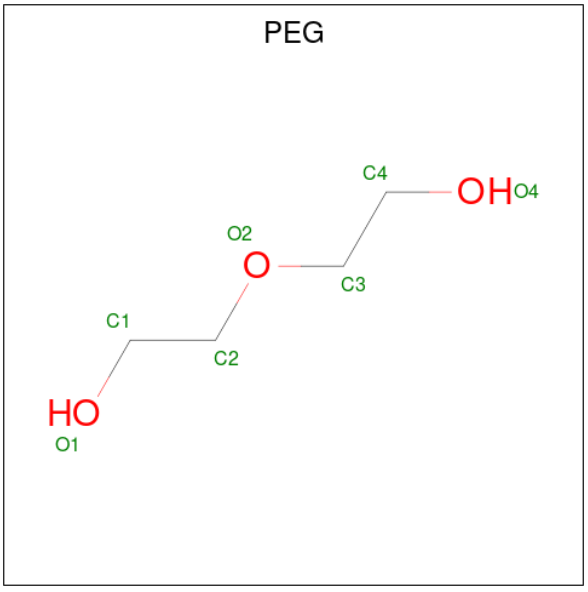
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	EEE	1	Total C O 10 6 4	0	0

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



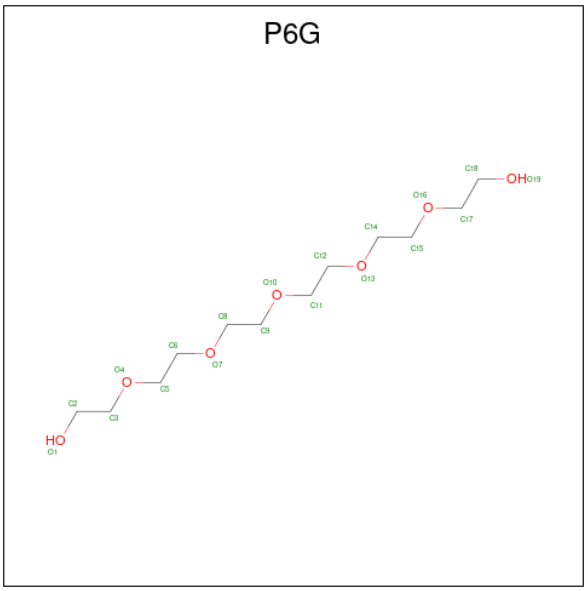
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	GGG	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	GGG	1	Total C O 7 4 3	0	0

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	HHH	1	Total C O 19 12 7	0	0

- Molecule 8 is water.

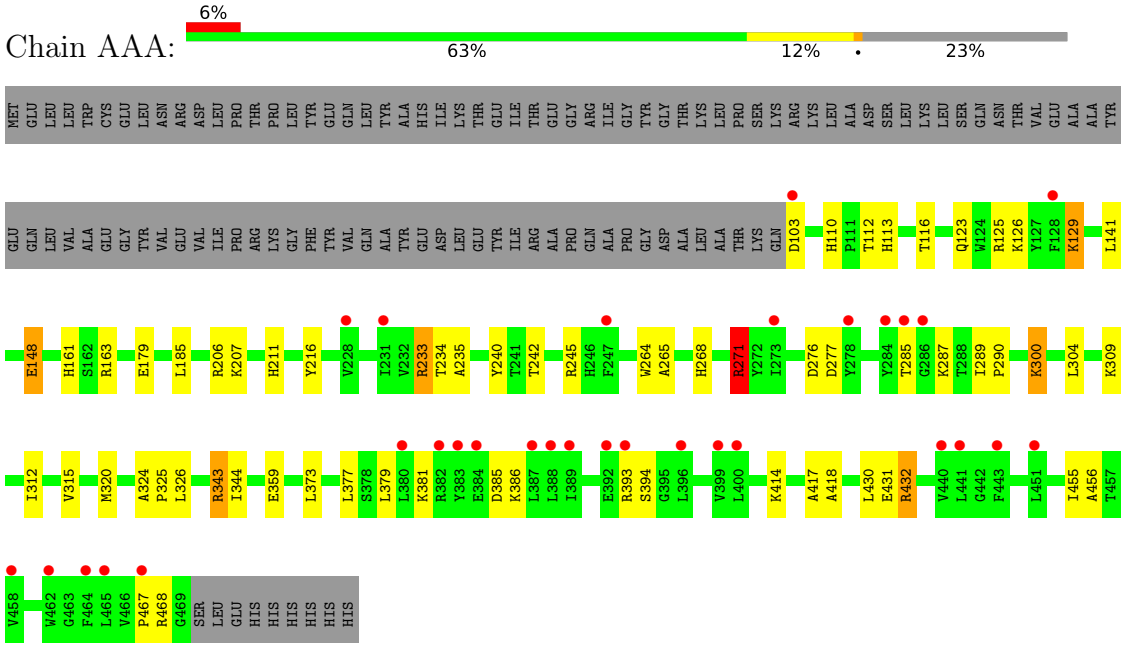
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	6	Total O 6 6	0	0
8	BBB	7	Total O 7 7	0	0
8	CCC	15	Total O 15 15	0	0
8	DDD	11	Total O 11 11	0	0
8	EEE	6	Total O 6 6	0	0
8	FFF	8	Total O 8 8	0	0
8	GGG	12	Total O 12 12	0	0
8	HHH	15	Total O 15 15	0	0
8	III	6	Total O 6 6	0	0
8	JJJ	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

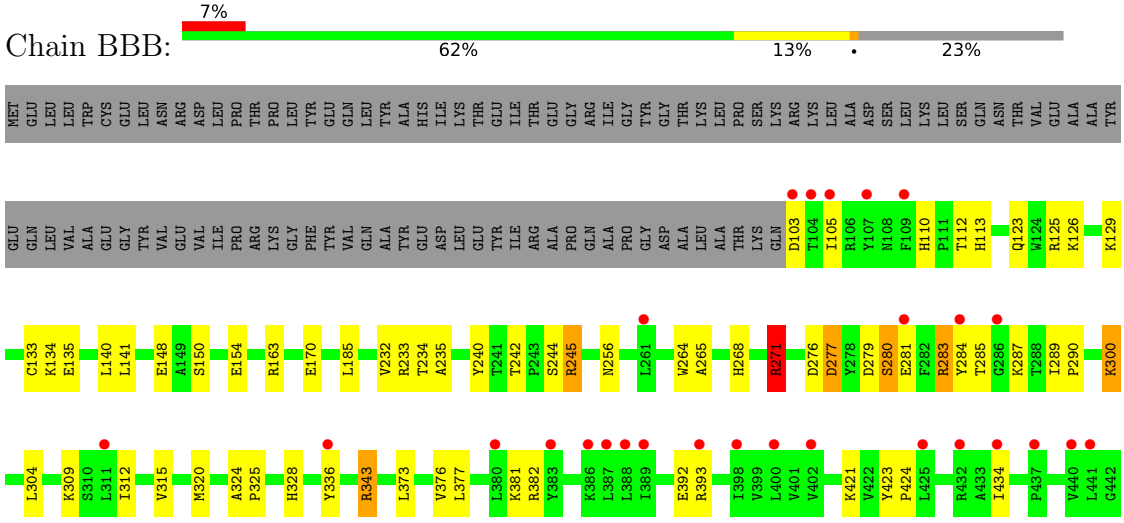
• Molecule 1: PLP-dependent aminotransferase family protein

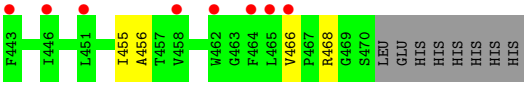
Chain AAA:



• Molecule 1: PLP-dependent aminotransferase family protein

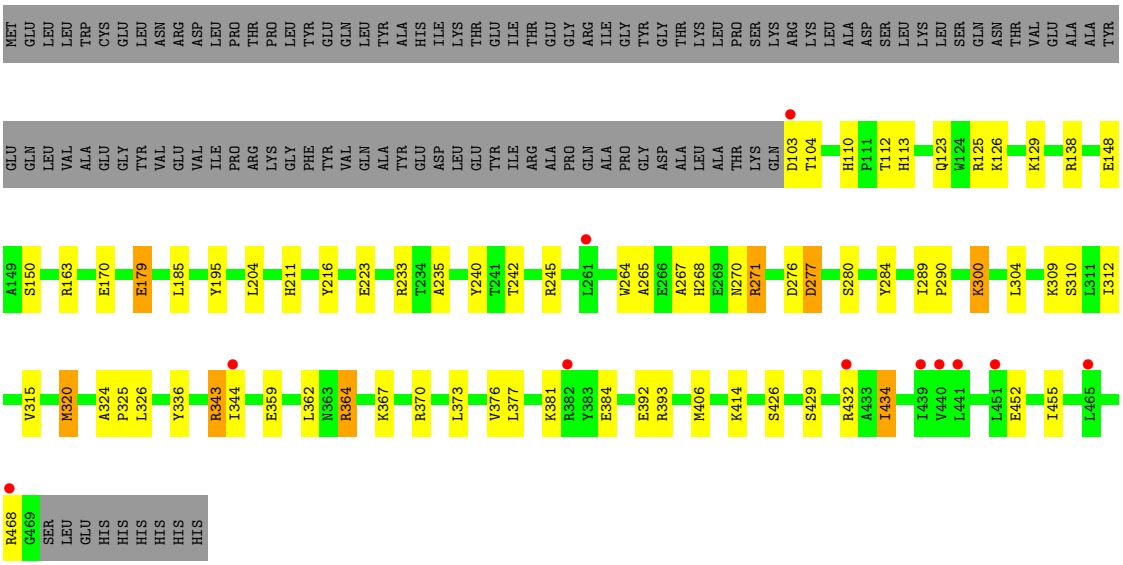
Chain BBB:





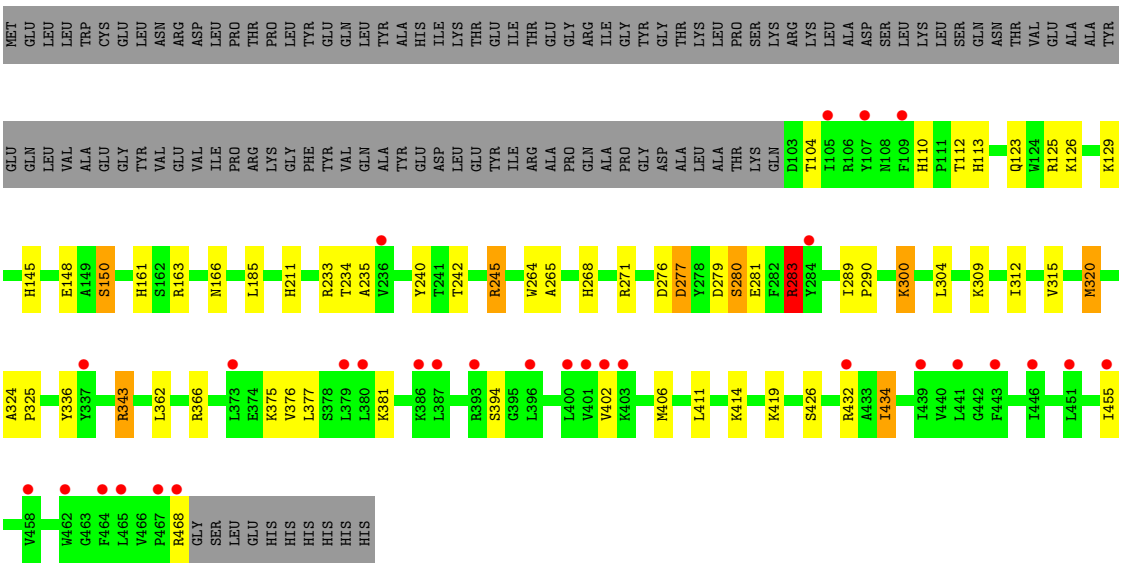
• Molecule 1: PLP-dependent aminotransferase family protein

Chain CCC:



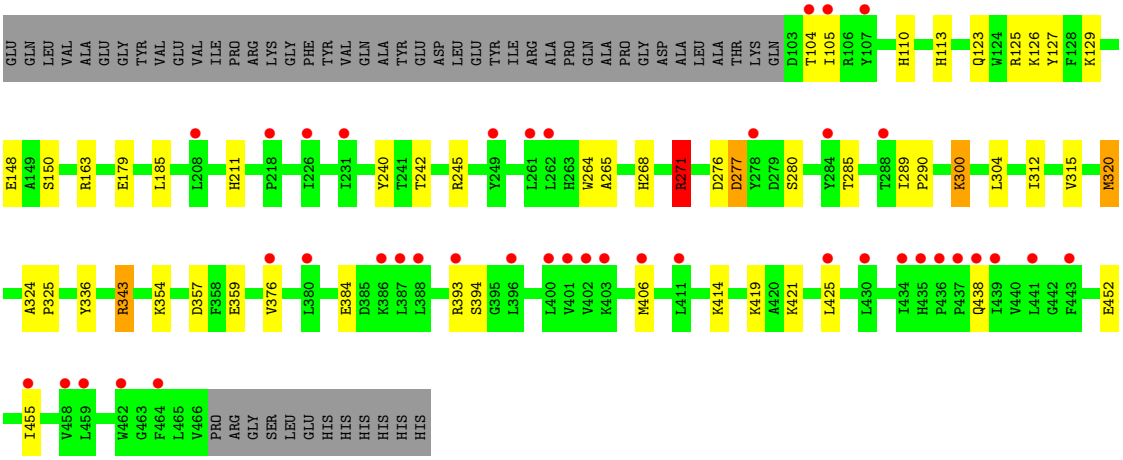
• Molecule 1: PLP-dependent aminotransferase family protein

Chain DDD:



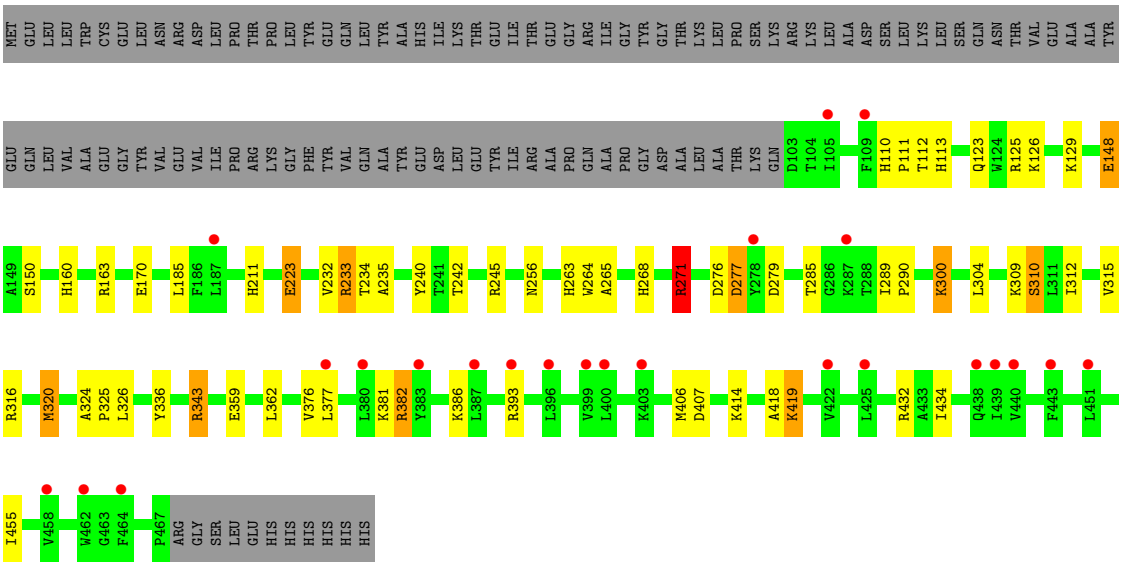
• Molecule 1: PLP-dependent aminotransferase family protein

Chain EEE:



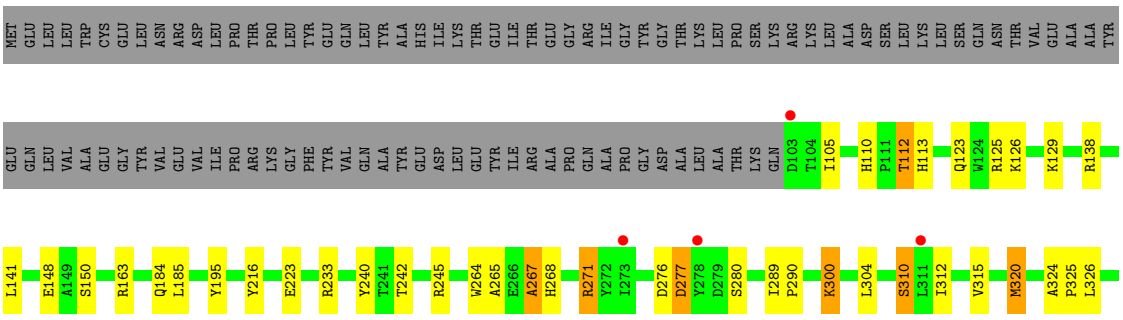
• Molecule 1: PLP-dependent aminotransferase family protein

Chain FFF:



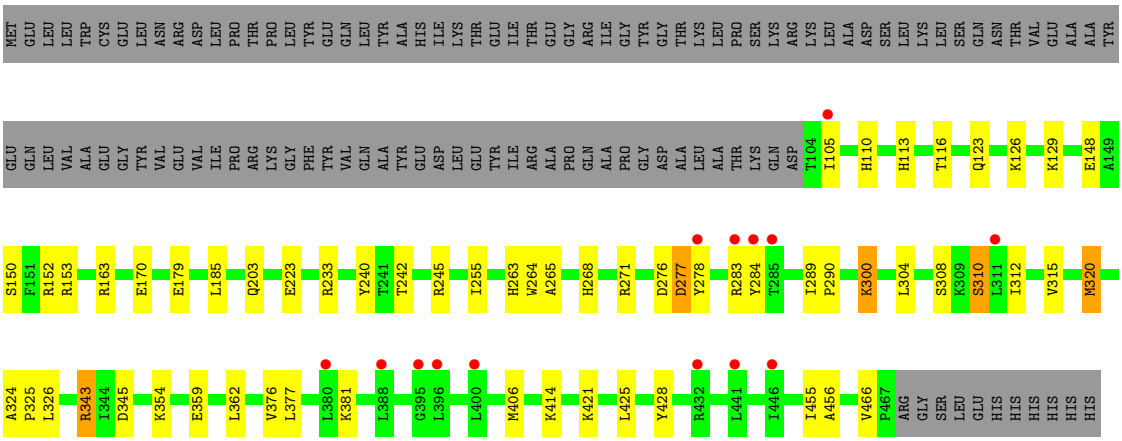
• Molecule 1: PLP-dependent aminotransferase family protein

Chain GGG:



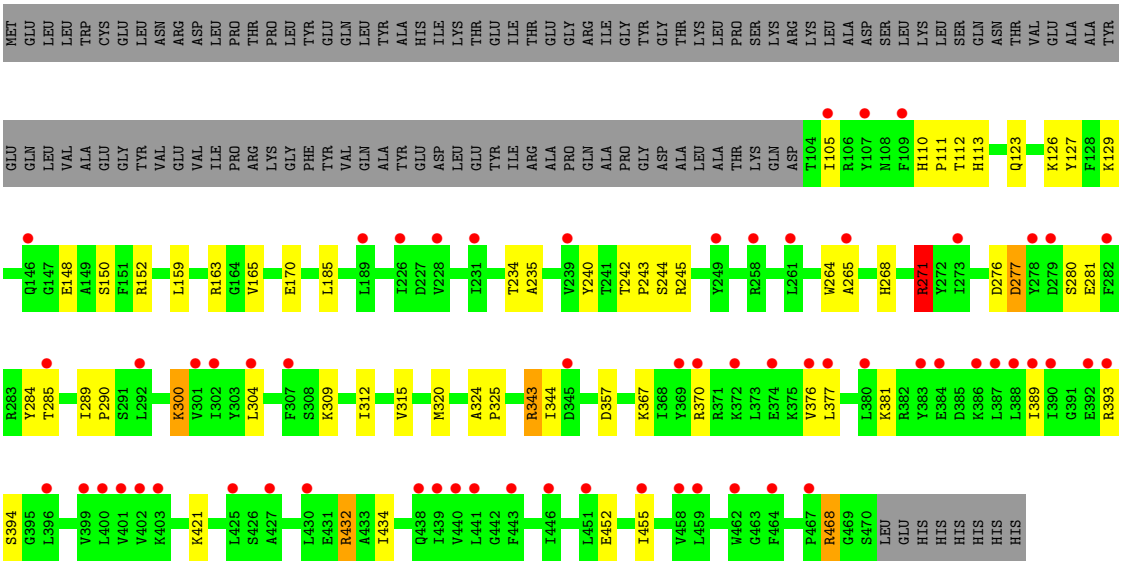
• Molecule 1: PLP-dependent aminotransferase family protein

Chain HHH:



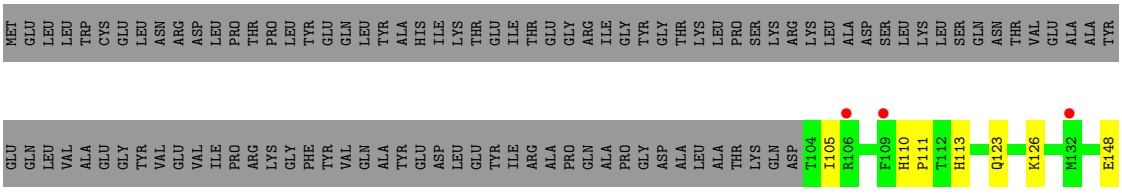
• Molecule 1: PLP-dependent aminotransferase family protein

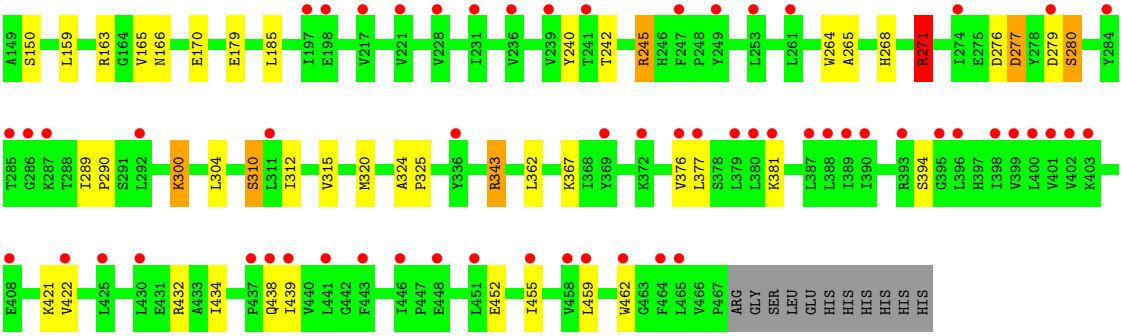
Chain III:



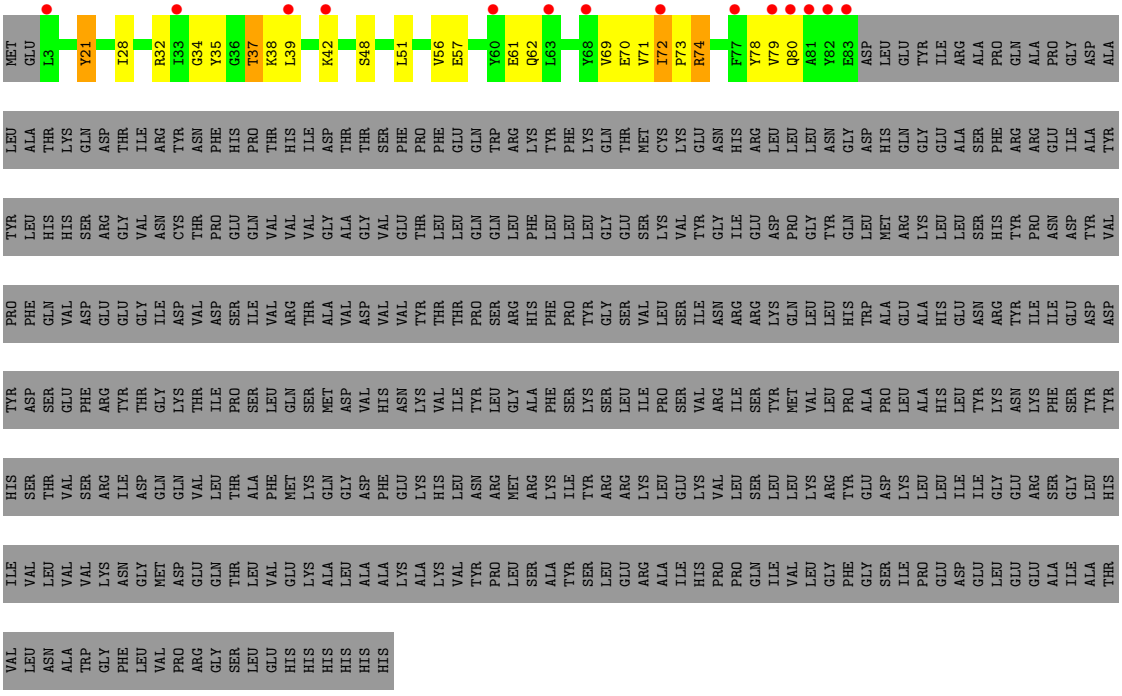
• Molecule 1: PLP-dependent aminotransferase family protein

Chain JJJ:





• Molecule 1: PLP-dependent aminotransferase family protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	250.84Å 250.84Å 370.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	125.73 – 2.80 125.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (125.73-2.80) 98.2 (125.42-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.254 0.209 , 0.254	Depositor DCC
R_{free} test set	8331 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	89.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 82.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30729	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: P6G, CA, CL, PGE, EDO, 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	AAA	0.49	1/3074 (0.0%)	0.94	4/4163 (0.1%)
1	BBB	0.49	1/3080 (0.0%)	0.91	3/4171 (0.1%)
1	CCC	0.54	1/3074 (0.0%)	0.92	3/4163 (0.1%)
1	DDD	0.51	0/3070	0.91	2/4158 (0.0%)
1	EEE	0.42	0/3051	0.83	1/4132 (0.0%)
1	FFF	0.45	1/3059 (0.0%)	0.88	4/4144 (0.1%)
1	GGG	0.48	0/3080	0.93	6/4171 (0.1%)
1	HHH	0.51	0/3051	0.91	2/4133 (0.0%)
1	III	0.42	0/3072	0.86	3/4160 (0.1%)
1	JJJ	0.41	0/3051	0.83	1/4133 (0.0%)
1	KKK	0.42	0/672	1.00	1/911 (0.1%)
All	All	0.47	4/31334 (0.0%)	0.90	30/42439 (0.1%)

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	AAA	0	1
1	BBB	0	3
1	CCC	0	3
1	DDD	0	1
1	EEE	0	1
1	GGG	0	2
1	III	0	1
1	JJJ	0	1
1	KKK	0	1
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	154	GLU	CD-OE2	6.42	1.32	1.25
1	AAA	148	GLU	CD-OE1	6.25	1.32	1.25
1	FFF	148	GLU	CD-OE1	5.46	1.31	1.25
1	CCC	359	GLU	CD-OE1	5.15	1.31	1.25

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	163	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	GGG	271	ARG	CG-CD-NE	8.71	130.08	111.80
1	CCC	271	ARG	CG-CD-NE	8.09	128.78	111.80
1	KKK	74	ARG	CG-CD-NE	7.77	128.13	111.80
1	HHH	245	ARG	CG-CD-NE	6.79	126.06	111.80

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	103	ASP	Peptide
1	BBB	103	ASP	Peptide
1	BBB	280	SER	Peptide
1	BBB	281	GLU	Mainchain
1	CCC	104	THR	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	AAA	2999	0	2995	55	0
1	BBB	3005	0	3000	68	0
1	CCC	2999	0	2995	74	0
1	DDD	2995	0	2992	55	0
1	EEE	2977	0	2972	46	0
1	FFF	2984	0	2979	68	0
1	GGG	3005	0	3000	49	0
1	HHH	2976	0	2975	42	0
1	III	2997	0	2996	43	1
1	JJJ	2976	0	2975	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	KKK	658	0	662	19	0
2	AAA	2	0	0	0	0
2	BBB	2	0	0	0	0
2	CCC	3	0	0	0	0
2	DDD	3	0	0	0	0
2	EEE	2	0	0	0	0
2	FFF	1	0	0	0	0
2	GGG	3	0	0	0	0
2	HHH	3	0	0	0	0
2	III	3	0	0	0	0
2	JJJ	2	0	0	0	0
2	KKK	1	0	0	0	0
3	AAA	2	0	0	0	0
3	JJJ	1	0	0	0	0
4	EEE	10	0	14	4	1
5	GGG	4	0	6	0	0
6	GGG	7	0	10	0	0
7	HHH	19	0	26	1	0
8	AAA	6	0	0	0	0
8	BBB	7	0	0	1	0
8	CCC	15	0	0	1	0
8	DDD	11	0	0	2	0
8	EEE	6	0	0	3	0
8	FFF	8	0	0	2	0
8	GGG	12	0	0	1	0
8	HHH	15	0	0	3	0
8	III	6	0	0	0	0
8	JJJ	4	0	0	1	0
All	All	30729	0	30597	492	2

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.

The worst 5 of 492 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:BBB:232:VAL:CG1	1:GGG:268:HIS:CD2	2.33	1.12
1:AAA:379:LEU:HD23	1:AAA:455:ILE:HD11	1.37	1.06
1:CCC:268:HIS:CD2	1:FFF:232:VAL:CG1	2.38	1.06
1:BBB:328:HIS:HB3	1:KKK:74:ARG:NH1	1.76	0.98
1:CCC:267:ALA:HB3	1:FFF:233:ARG:HH21	1.24	0.98

All (2) 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)
1:III:129:LYS:NZ	1:III:129:LYS:NZ[8_675]	2.06	0.14
4:EEE:501:PGE:O4	4:EEE:501:PGE:O4[12_565]	2.19	0.01

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	AAA	365/478 (76%)	353 (97%)	12 (3%)	0	100	100
1	BBB	366/478 (77%)	357 (98%)	9 (2%)	0	100	100
1	CCC	365/478 (76%)	355 (97%)	10 (3%)	0	100	100
1	DDD	364/478 (76%)	357 (98%)	7 (2%)	0	100	100
1	EEE	362/478 (76%)	354 (98%)	8 (2%)	0	100	100
1	FFF	363/478 (76%)	355 (98%)	8 (2%)	0	100	100
1	GGG	366/478 (77%)	356 (97%)	10 (3%)	0	100	100
1	HHH	362/478 (76%)	353 (98%)	9 (2%)	0	100	100
1	III	365/478 (76%)	356 (98%)	9 (2%)	0	100	100
1	JJJ	362/478 (76%)	350 (97%)	12 (3%)	0	100	100
1	KKK	79/478 (16%)	76 (96%)	3 (4%)	0	100	100
All	All	3719/5258 (71%)	3622 (97%)	97 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	328/423 (78%)	317 (97%)	11 (3%)	37	71
1	BBB	329/423 (78%)	318 (97%)	11 (3%)	38	72
1	CCC	328/423 (78%)	312 (95%)	16 (5%)	25	57
1	DDD	328/423 (78%)	315 (96%)	13 (4%)	31	65
1	EEE	326/423 (77%)	318 (98%)	8 (2%)	47	80
1	FFF	327/423 (77%)	314 (96%)	13 (4%)	31	65
1	GGG	329/423 (78%)	318 (97%)	11 (3%)	38	72
1	HHH	326/423 (77%)	314 (96%)	12 (4%)	34	68
1	III	328/423 (78%)	317 (97%)	11 (3%)	37	71
1	JJJ	326/423 (77%)	314 (96%)	12 (4%)	34	68
1	KKK	70/423 (16%)	66 (94%)	4 (6%)	20	50
All	All	3345/4653 (72%)	3223 (96%)	122 (4%)	35	69

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	384	GLU
1	JJJ	300	LYS
1	FFF	432	ARG
1	JJJ	277	ASP
1	KKK	21	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 28 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
7	P6G	HHH	504	-	18,18,18	0.94	0	17,17,17	0.90	0
5	EDO	GGG	501	-	3,3,3	0.15	0	2,2,2	0.50	0
6	PEG	GGG	502	-	6,6,6	0.35	0	5,5,5	0.23	0
4	PGE	EEE	501	-	9,9,9	0.16	0	8,8,8	0.46	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
7	P6G	HHH	504	-	-	7/16/16/16	-
5	EDO	GGG	501	-	-	1/1/1/1	-
6	PEG	GGG	502	-	-	1/4/4/4	-
4	PGE	EEE	501	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	EEE	501	PGE	O2-C3-C4-O3
7	HHH	504	P6G	O7-C8-C9-O10
7	HHH	504	P6G	O13-C14-C15-O16

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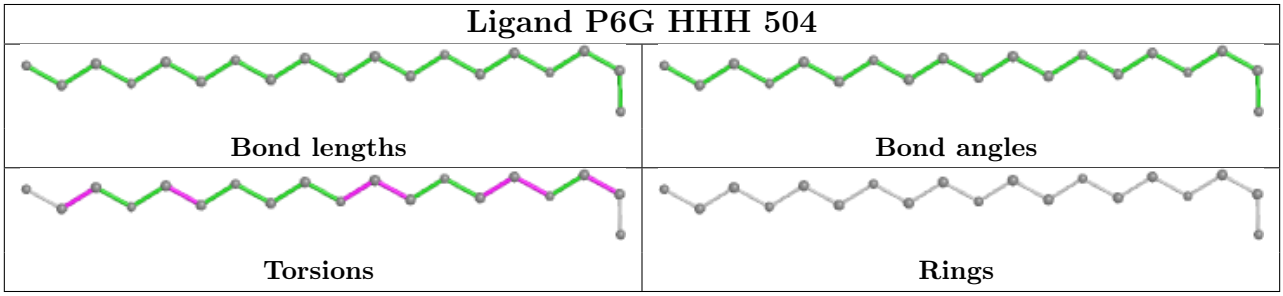
Mol	Chain	Res	Type	Atoms
7	HHH	504	P6G	O16-C17-C18-O19
4	EEE	501	PGE	O3-C5-C6-O4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	HHH	504	P6G	1	0
4	EEE	501	PGE	4	1

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.



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^{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	AAA	367/478 (76%)	0.69	31 (8%) 11 5	54, 97, 172, 229	0
1	BBB	368/478 (76%)	0.71	35 (9%) 8 4	51, 90, 175, 207	0
1	CCC	367/478 (76%)	0.57	11 (2%) 50 40	50, 83, 155, 245	0
1	DDD	366/478 (76%)	0.75	30 (8%) 11 6	52, 93, 176, 223	0
1	EEE	364/478 (76%)	0.77	41 (11%) 5 3	64, 128, 196, 239	0
1	FFF	365/478 (76%)	0.64	24 (6%) 18 11	59, 100, 181, 236	0
1	GGG	368/478 (76%)	0.57	12 (3%) 46 36	61, 97, 147, 201	0
1	HHH	364/478 (76%)	0.57	14 (3%) 40 30	58, 90, 150, 238	0
1	III	367/478 (76%)	0.98	62 (16%) 1 1	72, 133, 192, 222	0
1	JJJ	364/478 (76%)	1.03	63 (17%) 1 1	73, 134, 198, 241	0
1	KKK	81/478 (16%)	0.83	14 (17%) 1 1	85, 124, 183, 217	0
All	All	3741/5258 (71%)	0.73	337 (9%) 9 5	50, 102, 183, 245	0

The worst 5 of 337 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	284	TYR	7.4
1	JJJ	388	LEU	7.4
1	JJJ	376	VAL	7.0
1	EEE	402	VAL	7.0
1	HHH	284	TYR	6.4

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)

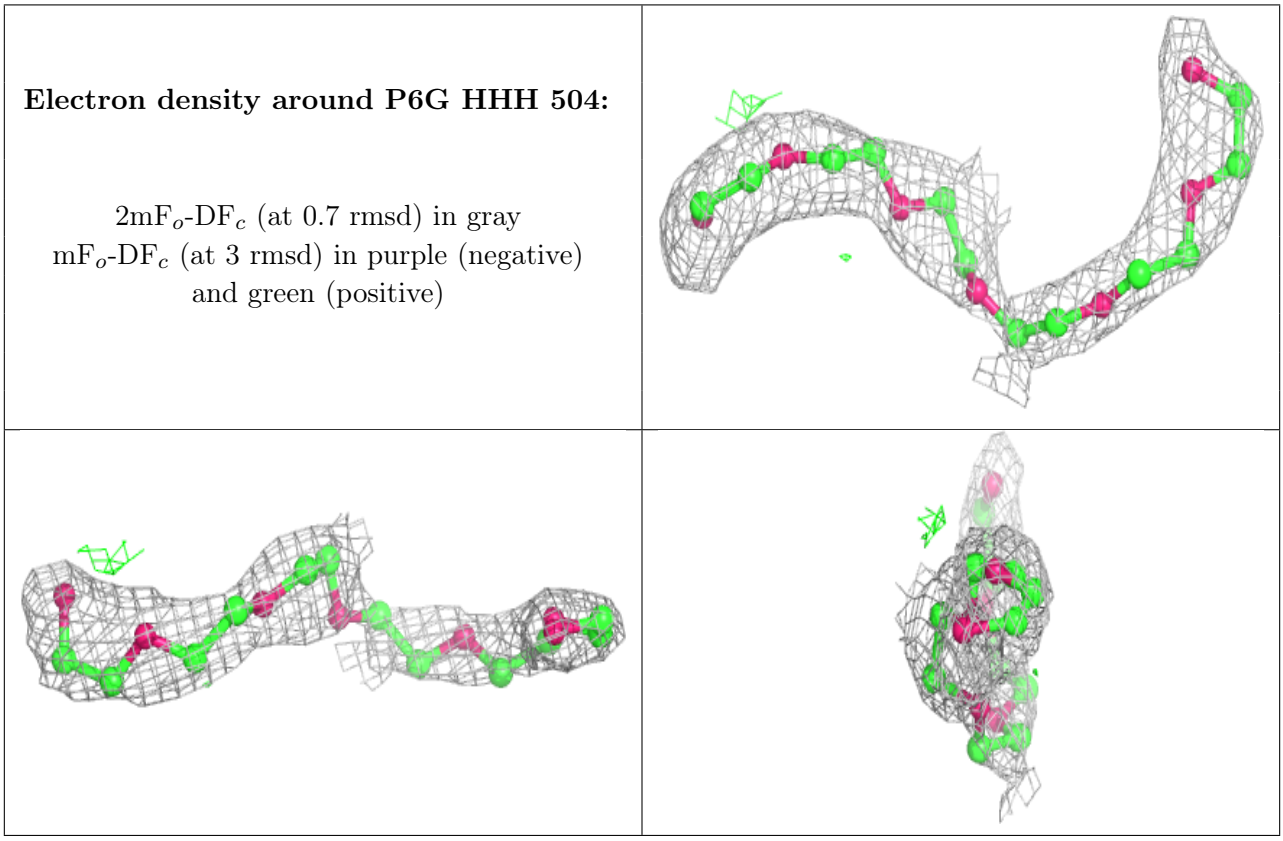
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	CA	KKK	501	1/1	0.51	0.11	159,159,159,159	0
5	EDO	GGG	501	4/4	0.60	0.45	118,135,143,143	0
6	PEG	GGG	502	7/7	0.63	0.24	91,142,171,197	0
3	CL	AAA	504	1/1	0.65	0.47	113,113,113,113	0
2	CA	HHH	503	1/1	0.75	0.13	165,165,165,165	0
3	CL	AAA	503	1/1	0.77	0.59	137,137,137,137	0
2	CA	EEE	502	1/1	0.83	0.20	120,120,120,120	0
2	CA	DDD	503	1/1	0.84	0.06	147,147,147,147	0
3	CL	JJJ	503	1/1	0.84	0.15	125,125,125,125	0
2	CA	CCC	502	1/1	0.85	0.13	107,107,107,107	0
7	P6G	HHH	504	19/19	0.85	0.36	86,103,123,146	0
2	CA	AAA	502	1/1	0.87	0.06	132,132,132,132	0
2	CA	EEE	503	1/1	0.87	0.14	135,135,135,135	0
2	CA	III	501	1/1	0.89	0.13	152,152,152,152	0
2	CA	HHH	501	1/1	0.90	0.07	117,117,117,117	0
2	CA	DDD	501	1/1	0.91	0.13	108,108,108,108	0
2	CA	AAA	501	1/1	0.92	0.10	123,123,123,123	0
2	CA	BBB	501	1/1	0.92	0.15	117,117,117,117	0
2	CA	CCC	501	1/1	0.92	0.16	107,107,107,107	0
4	PGE	EEE	501	10/10	0.93	0.19	77,82,106,107	0
2	CA	DDD	502	1/1	0.93	0.23	163,163,163,163	0
2	CA	GGG	504	1/1	0.94	0.17	104,104,104,104	0
2	CA	GGG	505	1/1	0.94	0.09	159,159,159,159	0
2	CA	III	502	1/1	0.94	0.21	203,203,203,203	0
2	CA	III	503	1/1	0.94	0.23	96,96,96,96	1
2	CA	BBB	502	1/1	0.94	0.20	158,158,158,158	0
2	CA	HHH	502	1/1	0.94	0.30	166,166,166,166	0
2	CA	CCC	503	1/1	0.95	0.14	148,148,148,148	0
2	CA	JJJ	502	1/1	0.96	0.07	165,165,165,165	0
2	CA	FFF	501	1/1	0.96	0.09	136,136,136,136	0
2	CA	GGG	503	1/1	0.96	0.11	102,102,102,102	0
2	CA	JJJ	501	1/1	0.97	0.20	114,114,114,114	1

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 P6G HHH 504:

$2mF_o$-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

There are no such residues in this entry.