



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:59 am BST

PDB ID : 1M32  
Title : Crystal Structure of 2-aminoethylphosphonate Transaminase  
Authors : Chen, C.C.H.; Zhang, H.; Kim, A.D.; Howard, A.; Sheldrick, G.M.; Mariano-Dunnaway, D.; Herzberg, O.  
Deposited on : 2002-06-26  
Resolution : 2.20 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

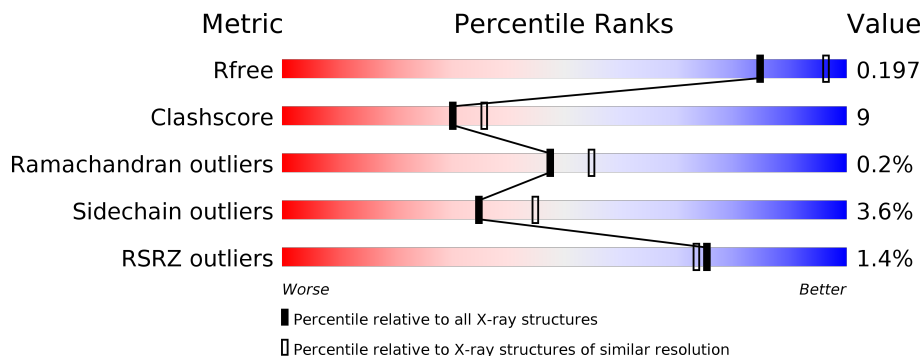
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	366	 81% 16% ..
1	B	366	 81% 17% ..
1	C	366	 84% 13% ..
1	D	366	 80% 17% ..
1	E	366	 76% 20% ..
1	F	366	 83% 14% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19906 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 2-aminoethylphosphonate-pyruvate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	361	2783	1762	479	525	6	11	24	1	0
1	B	362	2800	1777	480	526	6	11	31	4	0
1	C	361	2799	1776	479	526	7	11	39	4	0
1	D	362	2798	1775	480	526	6	11	11	3	0
1	E	361	2782	1763	478	524	6	11	15	1	0
1	F	362	2786	1763	480	526	6	11	20	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
A	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	146	MSE	MET	MODIFIED RESIDUE	UNP P96060

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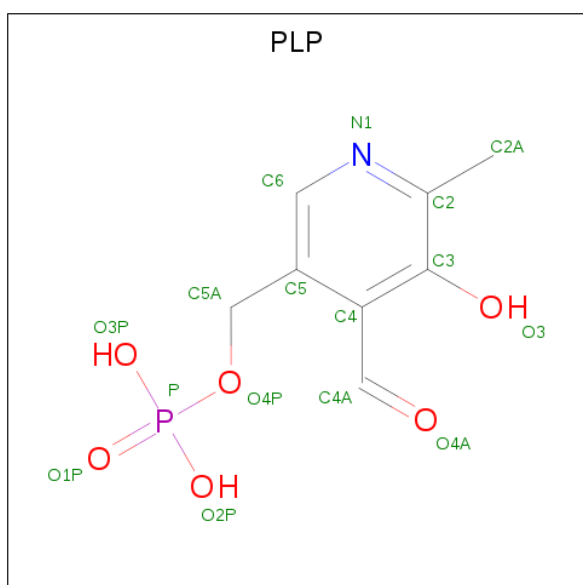
Chain	Residue	Modelled	Actual	Comment	Reference
B	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
B	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
C	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
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D	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
D	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	102	MSE	MET	MODIFIED RESIDUE	UNP P96060
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E	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
E	362	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	23	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	95	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	98	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	102	MSE	MET	MODIFIED RESIDUE	UNP P96060

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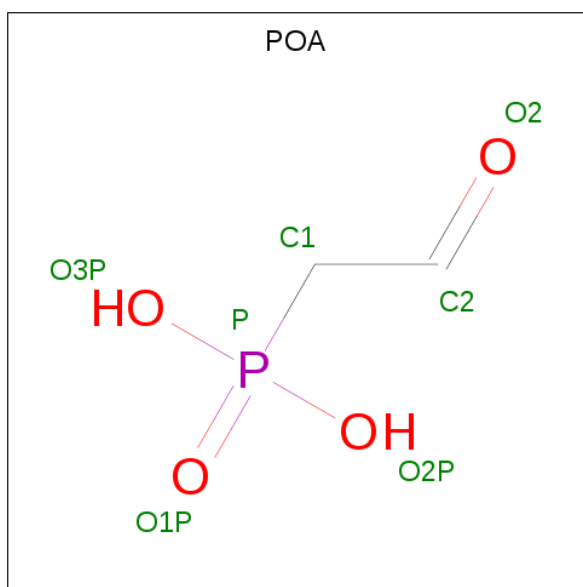
Chain	Residue	Modelled	Actual	Comment	Reference
F	137	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	146	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	169	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	177	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	232	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	282	MSE	MET	MODIFIED RESIDUE	UNP P96060
F	362	MSE	MET	MODIFIED RESIDUE	UNP P96060

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



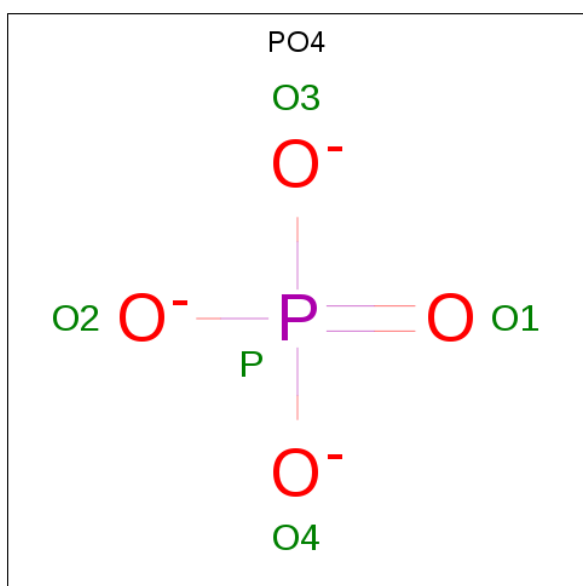
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			14	7	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			14	7	1	5	1		

- Molecule 3 is PHOSPHONOACETALDEHYDE (three-letter code: POA) (formula: C<sub>2</sub>H<sub>5</sub>O<sub>4</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			7	2	4	1		
3	C	1	Total	C	O	P	0	0
			7	2	4	1		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

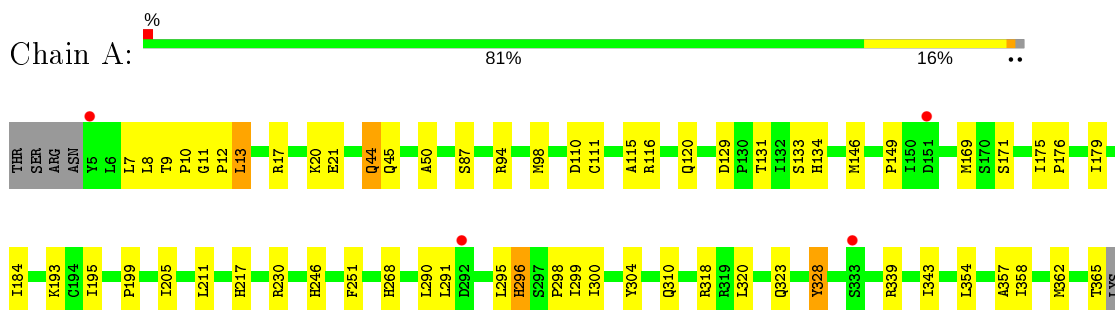
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	500	Total	O	0	1
			501	501		
5	B	506	Total	O	0	1
			507	507		
5	C	481	Total	O	0	1
			482	482		
5	D	499	Total	O	0	1
			500	500		
5	E	518	Total	O	0	1
			519	519		
5	F	530	Total	O	0	1
			531	531		

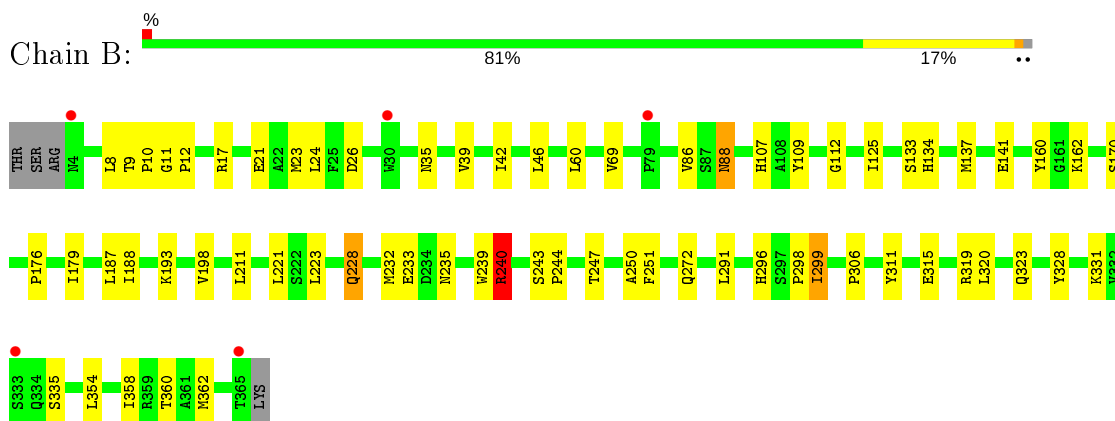
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

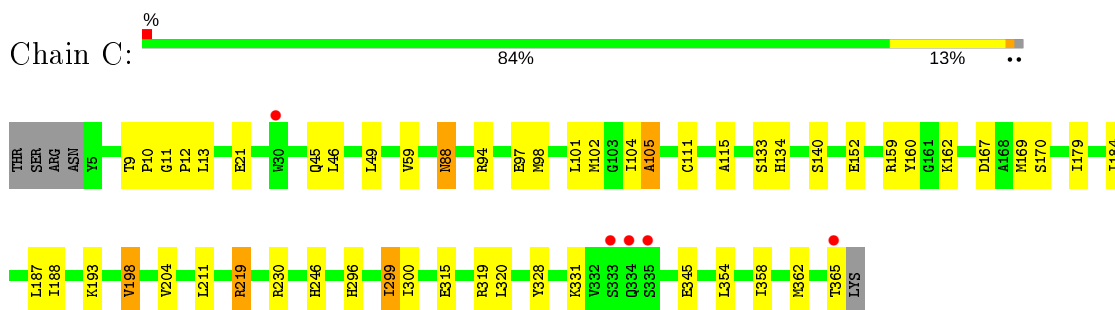
- Molecule 1: 2-aminoethylphosphonate-pyruvate aminotransferase



- Molecule 1: 2-aminoethylphosphonate-pyruvate aminotransferase

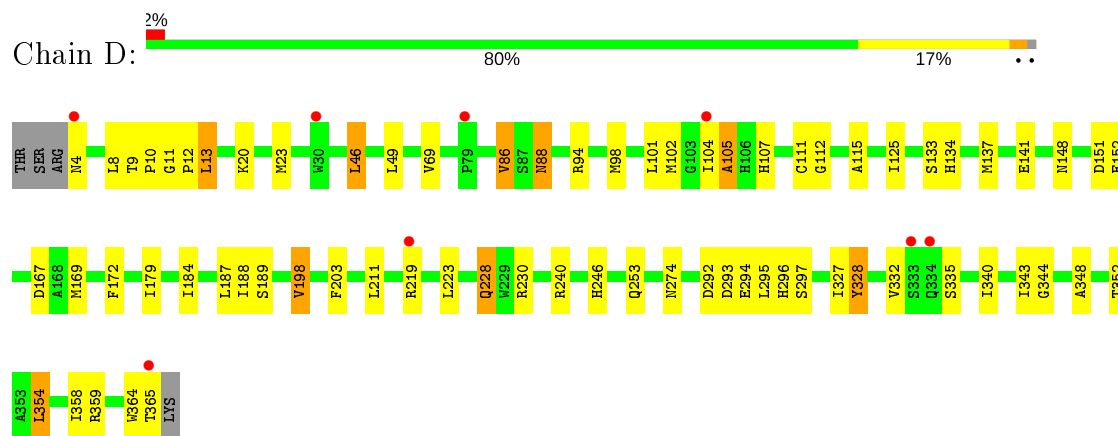


- Molecule 1: 2-aminoethylphosphonate-pyruvate aminotransferase

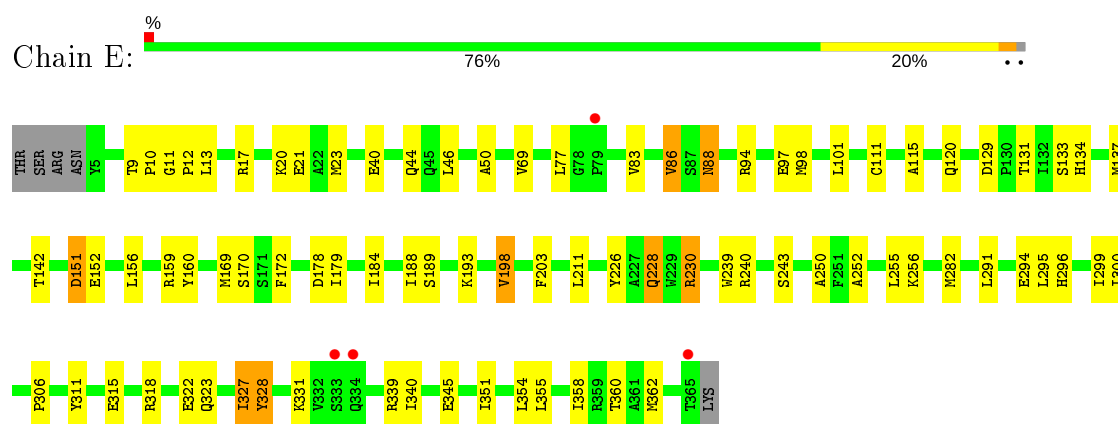


- Molecule 1: 2-aminoethylphosphonate-pyruvate aminotransferase

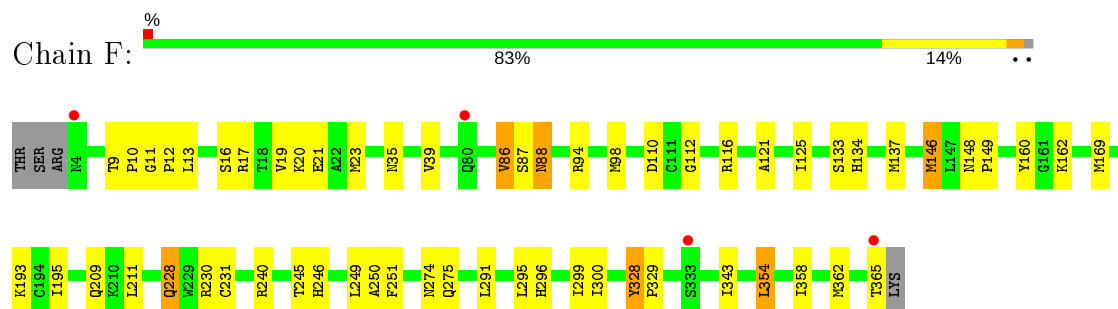




- Molecule 1: 2-aminoethylphosphonate-pyruvate aminotransferase



- Molecule 1: 2-aminoethylphosphonate-pyruvate aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.60Å 155.30Å 168.60Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.92 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.20) 99.2 (19.92-2.15)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.15Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.166 , 0.200 0.164 , 0.197	Depositor DCC
$R_{free}$ test set	12785 reflections (9.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PLP, POA

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	0.39	0/2836	0.57	0/3832
1	B	0.46	1/2865 (0.0%)	0.62	3/3874 (0.1%)
1	C	0.40	0/2866	0.57	0/3874
1	D	0.39	0/2859	0.57	1/3864 (0.0%)
1	E	0.40	0/2835	0.56	0/3831
1	F	0.40	0/2835	0.57	0/3831
All	All	0.41	1/17096 (0.0%)	0.58	4/23106 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	ASN	C-N	-7.07	1.17	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	240	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	B	240	ARG	NH1-CZ-NH2	-5.85	112.97	119.40
1	D	297	SER	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	A	2783	0	2735	46	0
1	B	2800	0	2760	57	0
1	C	2799	0	2747	43	0
1	D	2798	0	2758	64	0
1	E	2782	0	2738	64	0
1	F	2786	0	2737	44	0
2	A	14	0	6	1	0
2	B	14	0	6	1	0
2	C	14	0	6	1	0
2	D	14	0	6	1	0
2	E	14	0	6	1	0
2	F	14	0	6	1	0
3	A	7	0	3	3	0
3	C	7	0	3	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	501	0	0	4	0
5	B	507	0	0	8	0
5	C	482	0	0	9	0
5	D	500	0	0	10	0
5	E	519	0	0	8	0
5	F	531	0	0	6	0
All	All	19906	0	16517	307	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 9.

All (307) 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:E:282:MSE:HE1	1:E:358:ILE:HG13	1.25	1.14
1:B:228:GLN:NE2	1:B:240:ARG:HG3	1.84	0.91
2:E:4405:PLP:C4	5:E:5123[A]:HOH:O	2.26	0.82
1:B:221:LEU:O	1:B:240:ARG:NH2	2.12	0.81
1:B:240:ARG:HG3	1:B:240:ARG:HH11	1.42	0.80
2:B:4402:PLP:C4	5:B:5108[A]:HOH:O	2.32	0.77
1:B:179:ILE:HG21	1:B:187[B]:LEU:HD22	1.68	0.75
1:F:146:MSE:HE3	1:F:295:LEU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:O	1:A:21:GLU:HG3	1.88	0.74
1:D:102:MSE:HB2	1:D:104:ILE:HD13	1.70	0.73
1:D:228:GLN:HE21	1:D:240:ARG:HE	1.36	0.72
1:B:170:SER:HB2	1:B:299:ILE:CD1	2.19	0.71
1:C:97:GLU:O	1:C:101:LEU:HD23	1.91	0.70
1:D:86:VAL:HG21	1:D:137:MSE:HG3	1.73	0.70
1:C:331:LYS:HB3	5:C:4766:HOH:O	1.91	0.69
1:A:146:MSE:HE2	1:A:295:LEU:HD13	1.76	0.68
1:F:228:GLN:NE2	1:F:240:ARG:HE	1.93	0.67
1:B:228:GLN:HE22	1:B:240:ARG:HG3	1.57	0.67
1:E:86:VAL:CG2	1:E:137:MSE:HG3	2.25	0.67
1:F:228:GLN:HE21	1:F:240:ARG:HE	1.41	0.66
1:E:97:GLU:O	1:E:101:LEU:HD23	1.95	0.66
1:B:46:LEU:HD21	1:B:251:PHE:HE2	1.61	0.65
1:D:327:ILE:HG23	1:D:328:TYR:H	1.62	0.65
1:D:327:ILE:CG2	1:D:328:TYR:N	2.60	0.64
1:C:11:GLY:HA2	1:C:12:PRO:C	2.16	0.64
1:E:327:ILE:HG23	1:E:328:TYR:N	2.12	0.64
1:E:327:ILE:HG13	1:E:340:ILE:HG12	1.79	0.64
1:D:11:GLY:HA2	1:D:12:PRO:C	2.18	0.64
1:D:49[B]:LEU:HD22	5:D:4433:HOH:O	1.97	0.64
1:A:20:LYS:HE3	5:A:4714:HOH:O	1.96	0.64
1:E:294:GLU:HG3	1:E:295:LEU:HD13	1.80	0.63
1:F:362:MSE:O	1:F:365:THR:HG22	1.99	0.63
1:C:320:LEU:HD21	1:C:358:ILE:HD13	1.81	0.63
1:E:11:GLY:HA2	1:E:12:PRO:C	2.18	0.63
1:D:228:GLN:NE2	1:D:240:ARG:HE	1.97	0.63
1:C:9:THR:HB	1:C:10:PRO:HD2	1.82	0.62
1:C:169:MSE:HE2	1:C:188:ILE:HG22	1.81	0.62
1:C:104:ILE:O	1:C:105:ALA:HB3	2.00	0.62
1:E:86:VAL:HG21	1:E:137:MSE:HG3	1.81	0.62
1:D:86:VAL:CG2	1:D:137:MSE:HG3	2.29	0.62
1:F:11:GLY:HA2	1:F:12:PRO:C	2.21	0.62
1:B:42:ILE:O	1:B:46:LEU:HD23	2.00	0.61
1:E:131:THR:HG21	5:E:5052:HOH:O	1.99	0.61
1:A:116:ARG:NH1	1:A:149:PRO:HB3	2.16	0.61
1:E:228:GLN:NE2	1:E:240:ARG:HE	1.98	0.61
1:E:318:ARG:NH1	1:E:322:GLU:OE1	2.34	0.60
1:B:228:GLN:HE21	1:B:240:ARG:HG3	1.66	0.60
1:D:104:ILE:O	1:D:105:ALA:HB3	2.00	0.60
1:A:13:LEU:H	1:A:13:LEU:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:SER:OG	1:C:299[A]:ILE:HD11	2.02	0.60
1:E:226:TYR:CZ	1:E:230:ARG:HD2	2.36	0.59
1:D:293:ASP:HA	1:D:296:HIS:CD2	2.37	0.59
1:B:320:LEU:HD21	1:B:358:ILE:HD13	1.83	0.59
1:B:170:SER:HB2	1:B:299:ILE:HD13	1.83	0.59
1:E:9:THR:HB	1:E:10:PRO:HD2	1.85	0.59
1:F:86:VAL:CG2	1:F:137:MSE:HG3	2.33	0.59
1:B:11:GLY:HA2	1:B:12:PRO:C	2.23	0.58
1:D:111:CYS:O	1:D:115:ALA:HB3	2.02	0.58
1:E:327:ILE:CG2	1:E:328:TYR:N	2.66	0.58
1:D:104:ILE:O	1:D:105:ALA:CB	2.51	0.58
1:D:365:THR:O	1:D:365:THR:HG23	2.02	0.58
1:D:327:ILE:HG13	1:D:340:ILE:HG12	1.84	0.58
1:A:111:CYS:O	1:A:115:ALA:HB3	2.03	0.58
1:E:315:GLU:HG3	5:E:4859:HOH:O	2.03	0.58
1:C:133:SER:OG	1:C:134:HIS:HD2	1.87	0.58
1:C:152:GLU:HG3	5:C:4830:HOH:O	2.03	0.58
1:E:327:ILE:HG23	1:E:328:TYR:H	1.69	0.58
1:F:94:ARG:O	1:F:98:MSE:HG3	2.04	0.58
1:E:86:VAL:HG21	1:E:137:MSE:SE	2.54	0.57
1:C:104:ILE:O	1:C:105:ALA:CB	2.52	0.57
1:B:9:THR:HB	1:B:10:PRO:HD2	1.87	0.57
1:C:88:ASN:H	1:C:88:ASN:HD22	1.52	0.57
5:C:4699:HOH:O	1:E:21:GLU:HG2	2.04	0.57
5:B:4904:HOH:O	1:D:335:SER:HB3	2.04	0.57
1:F:209:GLN:HG2	5:F:4826:HOH:O	2.04	0.57
1:E:228:GLN:HE21	1:E:240:ARG:HE	1.52	0.57
1:F:146:MSE:CE	1:F:295:LEU:HB3	2.34	0.56
1:F:86:VAL:HG22	1:F:137:MSE:HG3	1.87	0.56
1:C:219:ARG:HD2	1:D:102:MSE:HA	1.86	0.56
1:D:20:LYS:HA	1:D:23:MSE:HE2	1.87	0.56
2:F:4406:PLP:C4	5:F:5136[A]:HOH:O	2.53	0.56
1:C:246:HIS:NE2	1:D:198:VAL:HG22	2.21	0.56
1:D:327:ILE:HG23	1:D:328:TYR:N	2.20	0.56
1:E:151:ASP:OD1	1:E:152:GLU:HG3	2.06	0.56
1:E:282:MSE:HE2	1:E:355:LEU:HD23	1.88	0.55
1:C:88:ASN:HD22	1:C:88:ASN:N	2.04	0.55
1:B:228:GLN:NE2	1:B:240:ARG:HH11	2.05	0.55
1:F:9:THR:HB	1:F:10:PRO:HD2	1.88	0.55
1:E:111:CYS:O	1:E:115:ALA:HB3	2.06	0.55
1:F:133:SER:OG	1:F:134:HIS:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:ILE:HD12	1:F:300:ILE:HB	1.89	0.55
1:E:331:LYS:HB2	5:E:4947:HOH:O	2.06	0.55
2:A:4401:PLP:C4	5:A:5101[A]:HOH:O	2.56	0.54
1:C:179:ILE:HG21	1:C:187:LEU:HD22	1.88	0.54
1:A:133:SER:OG	1:A:134:HIS:HD2	1.90	0.54
1:E:354:LEU:C	1:E:354:LEU:HD13	2.28	0.54
1:B:244:PRO:HB2	1:B:247:THR:OG1	2.08	0.54
1:E:282:MSE:HE2	1:E:355:LEU:CD2	2.38	0.54
1:B:179:ILE:CG2	1:B:187[B]:LEU:HD22	2.38	0.54
1:E:323:GLN:HE22	1:E:360:THR:HB	1.73	0.54
1:C:111:CYS:O	1:C:115:ALA:HB3	2.07	0.53
1:D:88:ASN:HD22	1:D:88:ASN:H	1.53	0.53
1:E:86:VAL:HG21	1:E:137:MSE:CG	2.38	0.53
1:C:21:GLU:HG2	5:E:4694:HOH:O	2.07	0.53
1:D:133:SER:OG	1:D:134:HIS:HD2	1.91	0.53
1:A:11:GLY:HA2	1:A:12:PRO:C	2.28	0.53
1:B:160:TYR:HB3	1:B:162:LYS:HE2	1.90	0.53
1:C:299[B]:ILE:HD12	1:C:300:ILE:HB	1.90	0.53
1:B:315:GLU:O	1:B:319:ARG:HG3	2.07	0.53
1:C:198:VAL:HG22	1:D:246:HIS:NE2	2.23	0.53
1:C:102:MSE:HA	1:D:219:ARG:HD2	1.90	0.52
1:D:179:ILE:HG21	1:D:187:LEU:HD22	1.92	0.52
1:F:116:ARG:NH1	1:F:149:PRO:HB3	2.24	0.52
1:A:320:LEU:HD21	1:A:358:ILE:HD13	1.92	0.52
1:B:306:PRO:HG2	1:B:311:TYR:CG	2.45	0.52
1:D:274:ASN:ND2	5:D:4646:HOH:O	2.41	0.52
1:E:230:ARG:HB3	1:E:230:ARG:NH1	2.24	0.52
1:B:170:SER:HA	1:B:193:LYS:HD3	1.92	0.51
1:E:129:ASP:OD1	1:E:131:THR:HB	2.11	0.51
1:B:306:PRO:HG2	1:B:311:TYR:CD1	2.45	0.51
2:D:4404:PLP:C4	5:D:4903[A]:HOH:O	2.57	0.51
1:F:275:GLN:HE22	1:F:296:HIS:CD2	2.28	0.51
1:A:13:LEU:HD12	1:A:343:ILE:HG13	1.91	0.51
1:B:331:LYS:HB2	5:B:5055:HOH:O	2.10	0.51
1:D:86:VAL:HG21	1:D:137:MSE:CG	2.41	0.51
1:A:362:MSE:HE2	1:A:365:THR:HG21	1.93	0.51
1:A:9:THR:HB	1:A:10:PRO:HD2	1.92	0.51
1:E:40:GLU:O	1:E:44:GLN:HG3	2.11	0.51
1:B:17:ARG:O	1:B:21:GLU:HG3	2.11	0.50
1:B:86[B]:VAL:HG13	1:B:109:TYR:CD1	2.47	0.50
1:C:101:LEU:O	1:D:219:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:TRP:CD1	1:D:365:THR:HG22	2.47	0.50
1:E:294:GLU:HG3	1:E:295:LEU:CD1	2.41	0.50
1:A:299:ILE:HD12	1:A:300:ILE:HB	1.94	0.49
1:B:133:SER:OG	1:B:134:HIS:HD2	1.96	0.49
1:D:359:ARG:HB3	1:D:359:ARG:NH2	2.27	0.49
1:B:88:ASN:HD22	1:B:88:ASN:H	1.59	0.49
1:D:9:THR:HB	1:D:10:PRO:HD2	1.94	0.49
1:A:169:MSE:O	1:A:193:LYS:HD2	2.13	0.49
1:B:176:PRO:HG2	5:B:4772:HOH:O	2.12	0.49
1:C:179:ILE:HB	1:C:184:ILE:HB	1.95	0.49
1:A:129:ASP:OD1	1:A:131:THR:HB	2.12	0.49
1:B:23:MSE:HG2	1:B:250:ALA:HB2	1.94	0.49
1:B:170:SER:O	1:B:299:ILE:HD13	2.12	0.49
1:F:17:ARG:O	1:F:21:GLU:HG3	2.12	0.49
2:C:4403:PLP:C4	5:C:5085[B]:HOH:O	2.61	0.49
1:D:88:ASN:N	1:D:88:ASN:HD22	2.09	0.49
1:F:88:ASN:N	1:F:88:ASN:HD22	2.11	0.48
1:C:219:ARG:HG3	5:D:4805:HOH:O	2.13	0.48
1:B:239:TRP:CD2	1:B:243:SER:HB3	2.49	0.48
1:C:219:ARG:HG2	1:D:101:LEU:O	2.14	0.48
1:E:282:MSE:CE	1:E:355:LEU:HD23	2.43	0.48
1:F:20:LYS:HA	1:F:23:MSE:HE2	1.95	0.48
1:E:133:SER:OG	1:E:134:HIS:HD2	1.96	0.48
1:E:198:VAL:HG22	1:F:246:HIS:NE2	2.29	0.48
1:D:354:LEU:O	1:D:358:ILE:HG12	2.14	0.48
1:B:86[A]:VAL:HG11	1:B:137:MSE:SE	2.64	0.47
1:D:179:ILE:HB	1:D:184:ILE:HB	1.95	0.47
1:A:318:ARG:NH2	1:D:295[B]:LEU:HD11	2.28	0.47
1:F:146:MSE:HE1	1:F:295:LEU:HD22	1.95	0.47
1:B:69:VAL:HA	1:B:188:ILE:HD13	1.97	0.47
1:C:362:MSE:O	1:C:365:THR:HG22	2.15	0.47
1:E:88:ASN:HD22	1:E:88:ASN:N	2.12	0.47
1:F:328:TYR:CG	1:F:329:PRO:HD2	2.50	0.47
1:A:291:LEU:O	1:A:296:HIS:HE1	1.97	0.47
1:B:291:LEU:O	1:B:296:HIS:HE1	1.98	0.47
1:D:359:ARG:HB3	1:D:359:ARG:HH21	1.80	0.47
1:D:13:LEU:HD22	1:D:13:LEU:H	1.79	0.47
1:B:244:PRO:HG3	5:B:4692:HOH:O	2.15	0.47
1:E:23:MSE:HG2	1:E:250:ALA:HB2	1.97	0.47
1:C:102:MSE:HA	1:D:219:ARG:CD	2.45	0.47
1:A:44[A]:GLN:NE2	1:A:45:GLN:N	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198[B]:VAL:HG22	1:B:250:ALA:HB3	1.96	0.46
1:D:253:GLN:CD	5:D:4640:HOH:O	2.53	0.46
1:E:300:ILE:HD11	1:E:339:ARG:HB3	1.97	0.46
1:A:120:GLN:HG3	5:A:4906:HOH:O	2.15	0.46
1:C:219:ARG:NH2	5:C:5003:HOH:O	2.48	0.46
1:F:274:ASN:ND2	5:F:4713:HOH:O	2.46	0.46
1:F:299:ILE:C	1:F:299:ILE:HD12	2.36	0.46
1:B:60:LEU:HB2	1:B:232:MSE:HE1	1.98	0.46
1:B:228:GLN:NE2	1:B:240:ARG:NH1	2.63	0.46
1:D:112:GLY:HA3	5:D:4525:HOH:O	2.14	0.46
1:F:88:ASN:H	1:F:88:ASN:HD22	1.62	0.46
1:C:345:GLU:HG2	5:C:4863:HOH:O	2.15	0.46
1:B:88:ASN:N	1:B:88:ASN:HD22	2.13	0.46
1:C:21:GLU:OE1	1:E:21:GLU:OE1	2.34	0.46
1:F:88:ASN:HD21	1:F:148:ASN:HD21	1.64	0.46
1:E:170:SER:O	1:E:299:ILE:HG13	2.16	0.45
1:B:46:LEU:HD21	1:B:251:PHE:CE2	2.48	0.45
1:E:179:ILE:HB	1:E:184:ILE:HB	1.99	0.45
1:E:230:ARG:HB3	1:E:230:ARG:HH11	1.81	0.45
1:A:217:HIS:HE1	5:A:4816:HOH:O	1.98	0.45
1:C:94:ARG:O	1:C:98:MSE:HG3	2.17	0.45
1:D:352:THR:HG21	5:D:4549:HOH:O	2.16	0.45
1:D:94:ARG:O	1:D:98:MSE:HG3	2.17	0.45
1:A:50:ALA:HB2	1:A:205:ILE:HD13	1.98	0.45
1:A:246:HIS:NE2	1:B:198[A]:VAL:HG22	2.31	0.45
1:A:323:GLN:OE1	1:A:357:ALA:HA	2.17	0.45
1:D:296:HIS:HD2	5:D:4494:HOH:O	2.00	0.45
1:F:162:LYS:NZ	5:F:4699:HOH:O	2.46	0.45
1:E:169:MSE:O	1:E:193:LYS:HD2	2.17	0.44
1:A:199:PRO:HB2	1:B:244:PRO:HA	1.99	0.44
1:B:240:ARG:CG	1:B:240:ARG:HH11	2.23	0.44
1:C:354:LEU:HD13	1:C:354:LEU:C	2.37	0.44
1:F:231:CYS:HB3	5:F:4637:HOH:O	2.17	0.44
1:F:195:ILE:HG21	1:F:251:PHE:CE1	2.52	0.44
1:A:12:PRO:HG3	1:A:199:PRO:HG3	1.98	0.44
1:F:88:ASN:HB2	1:F:112:GLY:O	2.17	0.44
1:D:69:VAL:HA	1:D:188:ILE:HD13	1.99	0.44
1:F:23:MSE:HG2	1:F:250:ALA:HB2	1.98	0.44
1:B:354:LEU:HD13	1:B:354:LEU:C	2.38	0.44
1:E:345:GLU:HG2	5:E:4860:HOH:O	2.16	0.44
1:B:198[B]:VAL:CG2	1:B:250:ALA:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:GLN:HE21	1:E:228:GLN:HA	1.82	0.43
1:B:112:GLY:HA3	5:B:4779:HOH:O	2.18	0.43
1:E:226:TYR:CE1	1:E:230:ARG:HG3	2.53	0.43
1:A:328:TYR:HE1	3:A:4601:POA:H12	1.83	0.43
1:B:272:GLN:HB3	1:B:298:PRO:HB3	2.00	0.43
1:E:252:ALA:O	1:E:256:LYS:HG3	2.18	0.43
1:E:291:LEU:O	1:E:296:HIS:HE1	2.01	0.43
1:F:86:VAL:HG21	1:F:137:MSE:HG3	2.00	0.43
1:F:112:GLY:HA3	5:F:4763:HOH:O	2.19	0.43
1:A:44[A]:GLN:HE21	1:A:45:GLN:N	2.17	0.43
1:B:228:GLN:HE21	1:B:228:GLN:HA	1.83	0.43
1:C:170:SER:HA	1:C:193:LYS:HD3	2.01	0.43
1:D:172:PHE:HB3	1:D:189:SER:OG	2.18	0.43
1:E:358:ILE:O	1:E:362:MSE:HG3	2.19	0.43
1:E:94:ARG:O	1:E:98:MSE:HG3	2.19	0.43
1:A:87:SER:O	1:A:110:ASP:HA	2.18	0.43
1:F:87:SER:O	1:F:110:ASP:HA	2.18	0.43
1:F:86:VAL:HG21	1:F:137:MSE:SE	2.69	0.43
1:E:69:VAL:HA	1:E:188:ILE:HD13	2.01	0.43
1:E:88:ASN:HD22	1:E:88:ASN:H	1.66	0.43
1:F:121:ALA:O	1:F:125:ILE:HG12	2.19	0.43
1:B:228:GLN:NE2	1:B:240:ARG:CG	2.70	0.42
1:C:167:ASP:OD1	1:C:169:MSE:HG2	2.18	0.42
1:D:167:ASP:OD1	1:D:169:MSE:HB2	2.18	0.42
1:D:348:ALA:O	1:D:352:THR:HG23	2.19	0.42
1:A:94:ARG:O	1:A:98:MSE:HG3	2.19	0.42
1:B:323:GLN:HE22	1:B:360:THR:HB	1.84	0.42
1:E:172:PHE:HB3	1:E:189:SER:OG	2.19	0.42
1:D:253:GLN:NE2	5:D:4453:HOH:O	2.51	0.42
1:E:331:LYS:HB3	5:E:4844:HOH:O	2.19	0.42
1:E:77:LEU:HD21	1:E:83:VAL:HB	2.02	0.42
1:A:20:LYS:HZ1	1:B:26:ASP:CG	2.21	0.42
1:A:320:LEU:HD21	1:A:358:ILE:HA	2.02	0.42
1:A:8:LEU:HD22	1:A:8:LEU:N	2.34	0.42
1:C:159:ARG:HD3	5:C:4901:HOH:O	2.20	0.42
1:E:189:SER:HB3	1:E:203:PHE:CE1	2.54	0.42
1:E:50:ALA:O	1:E:178:ASP:HA	2.19	0.42
1:B:319:ARG:HD3	5:B:4848:HOH:O	2.19	0.42
1:A:116:ARG:HG2	1:A:116:ARG:HH21	1.85	0.42
1:A:328:TYR:CE1	3:A:4601:POA:H12	2.54	0.42
1:E:159:ARG:HD2	1:E:160:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HG21	1:A:251:PHE:CE1	2.55	0.42
1:C:315[A]:GLU:OE2	1:C:319:ARG:NE	2.53	0.42
1:C:21:GLU:HG2	1:E:17:ARG:HD2	2.02	0.42
1:F:35:ASN:O	1:F:39:VAL:HB	2.20	0.42
1:A:175:ILE:HD11	1:A:298:PRO:HD2	2.02	0.41
1:D:332:VAL:HG23	5:D:4901:HOH:O	2.19	0.41
1:F:16:SER:OG	1:F:19:VAL:HG23	2.19	0.41
1:A:176:PRO:HD3	1:A:268:HIS:CG	2.55	0.41
1:C:59:VAL:CG1	1:C:204:VAL:HB	2.51	0.41
1:D:13:LEU:HD12	1:D:343:ILE:HG13	2.01	0.41
1:A:44[A]:GLN:NE2	1:A:45:GLN:HG3	2.35	0.41
1:D:151:ASP:OD1	1:D:152:GLU:N	2.50	0.41
1:D:189:SER:HB3	1:D:203:PHE:CE1	2.55	0.41
1:C:160:TYR:HB3	1:C:162:LYS:HE2	2.02	0.41
1:C:21:GLU:OE2	1:E:21:GLU:OE2	2.38	0.41
1:C:45:GLN:O	1:C:49:LEU:HB2	2.21	0.41
1:C:88:ASN:ND2	5:C:4617:HOH:O	2.53	0.41
1:E:239:TRP:CD2	1:E:243:SER:HB3	2.54	0.41
1:F:160:TYR:O	1:F:162:LYS:HE3	2.21	0.41
1:F:169:MSE:O	1:F:193:LYS:HD2	2.20	0.41
1:A:171:SER:HB2	1:A:175:ILE:HD12	2.03	0.41
1:B:107:HIS:CE1	1:B:125:ILE:HG23	2.55	0.41
1:A:318:ARG:NH1	1:D:292:ASP:OD2	2.46	0.41
1:F:245:THR:O	1:F:249:LEU:HD13	2.20	0.41
1:B:323:GLN:NE2	5:B:4979:HOH:O	2.54	0.41
1:F:354:LEU:HD22	1:F:358:ILE:HG12	2.02	0.41
1:A:310:GLN:HG2	1:A:310:GLN:O	2.21	0.41
1:A:358:ILE:O	1:A:362:MSE:HG3	2.21	0.41
1:A:318:ARG:NH2	1:D:294:GLU:OE1	2.54	0.41
1:E:20:LYS:HA	1:E:23:MSE:HE2	2.03	0.41
1:F:362:MSE:HB3	1:F:365:THR:HG22	2.03	0.41
1:B:35:ASN:O	1:B:39:VAL:HB	2.20	0.41
1:E:120:GLN:HG2	5:E:5099:HOH:O	2.20	0.41
1:C:101:LEU:HD21	5:C:5045:HOH:O	2.22	0.40
1:D:13:LEU:HD23	1:D:13:LEU:C	2.41	0.40
1:D:88:ASN:HD21	1:D:148:ASN:HD21	1.68	0.40
1:F:291:LEU:O	1:F:296:HIS:HE1	2.04	0.40
1:B:358:ILE:O	1:B:362:MSE:HG3	2.22	0.40
1:F:299:ILE:HB	1:F:343:ILE:HG21	2.04	0.40
1:A:339:ARG:HH22	3:A:4601:POA:C2	2.34	0.40
1:D:107:HIS:CD2	1:D:125:ILE:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HG	1:D:344:GLY:HA3	2.04	0.40
1:E:306:PRO:HD2	1:E:311:TYR:CZ	2.57	0.40
1:A:179:ILE:HB	1:A:184:ILE:HB	2.04	0.40
1:A:290:LEU:HA	1:A:304:TYR:CE1	2.57	0.40
1:D:8:LEU:N	1:D:8:LEU:HD22	2.37	0.40
1:E:351:ILE:O	1:E:355:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/366 (98%)	350 (97%)	10 (3%)	0	100	100
1	B	364/366 (100%)	352 (97%)	10 (3%)	2 (0%)	29	31
1	C	363/366 (99%)	348 (96%)	14 (4%)	1 (0%)	41	46
1	D	363/366 (99%)	350 (96%)	12 (3%)	1 (0%)	41	46
1	E	360/366 (98%)	346 (96%)	14 (4%)	0	100	100
1	F	360/366 (98%)	347 (96%)	13 (4%)	0	100	100
All	All	2170/2196 (99%)	2093 (96%)	73 (3%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	105	ALA
1	D	105	ALA
1	B	335	SER
1	B	24	LEU

### 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	291/284 (102%)	282 (97%)	9 (3%)	40	51
1	B	295/284 (104%)	286 (97%)	9 (3%)	40	51
1	C	294/284 (104%)	283 (96%)	11 (4%)	34	43
1	D	294/284 (104%)	280 (95%)	14 (5%)	25	32
1	E	291/284 (102%)	277 (95%)	14 (5%)	25	32
1	F	291/284 (102%)	282 (97%)	9 (3%)	40	51
All	All	1756/1704 (103%)	1690 (96%)	66 (4%)	35	42

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	13	LEU
1	A	44[A]	GLN
1	A	44[B]	GLN
1	A	211	LEU
1	A	230	ARG
1	A	296	HIS
1	A	328	TYR
1	A	354	LEU
1	B	88	ASN
1	B	141	GLU
1	B	211	LEU
1	B	223	LEU
1	B	228	GLN
1	B	233	GLU
1	B	240	ARG
1	B	299	ILE
1	B	328	TYR
1	C	13	LEU
1	C	46	LEU
1	C	88	ASN
1	C	198	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	211	LEU
1	C	219	ARG
1	C	230	ARG
1	C	296	HIS
1	C	299[A]	ILE
1	C	299[B]	ILE
1	C	328	TYR
1	D	4	ASN
1	D	13	LEU
1	D	46[A]	LEU
1	D	46[B]	LEU
1	D	86	VAL
1	D	88	ASN
1	D	141	GLU
1	D	198	VAL
1	D	211	LEU
1	D	223	LEU
1	D	228	GLN
1	D	230	ARG
1	D	328	TYR
1	D	354	LEU
1	E	13	LEU
1	E	46	LEU
1	E	86	VAL
1	E	88	ASN
1	E	142	THR
1	E	151	ASP
1	E	156	LEU
1	E	198	VAL
1	E	211	LEU
1	E	228	GLN
1	E	230	ARG
1	E	255	LEU
1	E	327	ILE
1	E	328	TYR
1	F	13	LEU
1	F	86	VAL
1	F	88	ASN
1	F	146	MSE
1	F	211	LEU
1	F	228	GLN
1	F	230	ARG

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Mol	Chain	Res	Type
1	F	328	TYR
1	F	354	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	272	GLN
1	A	296	HIS
1	A	310	GLN
1	B	44	GLN
1	B	88	ASN
1	B	134	HIS
1	B	228	GLN
1	B	246	HIS
1	B	296	HIS
1	B	310	GLN
1	B	323	GLN
1	C	41	GLN
1	C	88	ASN
1	C	127	ASN
1	C	134	HIS
1	C	192	ASN
1	C	253	GLN
1	C	296	HIS
1	C	323	GLN
1	D	4	ASN
1	D	44	GLN
1	D	88	ASN
1	D	127	ASN
1	D	134	HIS
1	D	217	HIS
1	D	228	GLN
1	D	246	HIS
1	D	274	ASN
1	D	296	HIS
1	D	323	GLN
1	E	88	ASN
1	E	127	ASN
1	E	134	HIS
1	E	183	HIS
1	E	228	GLN

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Mol	Chain	Res	Type
1	E	246	HIS
1	E	253	GLN
1	E	296	HIS
1	E	323	GLN
1	F	4	ASN
1	F	80	GLN
1	F	88	ASN
1	F	120	GLN
1	F	134	HIS
1	F	217	HIS
1	F	228	GLN
1	F	253	GLN
1	F	274	ASN
1	F	296	HIS
1	F	323	GLN
1	F	342	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	F	4606	-	4,4,4	1.67	0	6,6,6	0.42	0
3	POA	A	4601	-	6,6,6	2.06	1 (16%)	8,8,8	0.93	0
2	PLP	D	4404	-	13,14,16	1.54	3 (23%)	17,20,23	1.79	4 (23%)
4	PO4	E	4605	-	4,4,4	1.68	0	6,6,6	0.43	0
2	PLP	B	4402	-	13,14,16	1.47	2 (15%)	17,20,23	1.85	5 (29%)
2	PLP	C	4403	-	13,14,16	1.45	2 (15%)	17,20,23	1.84	5 (29%)
4	PO4	B	4602	-	4,4,4	1.66	0	6,6,6	0.43	0
3	POA	C	4603	-	6,6,6	2.25	2 (33%)	8,8,8	1.05	0
2	PLP	F	4406	-	13,14,16	1.47	3 (23%)	17,20,23	1.83	4 (23%)
4	PO4	C	4604	-	4,4,4	1.66	0	6,6,6	0.43	0
2	PLP	A	4401	-	13,14,16	1.52	3 (23%)	17,20,23	1.84	4 (23%)
2	PLP	E	4405	-	13,14,16	1.46	2 (15%)	17,20,23	1.81	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POA	A	4601	-	-	3/3/4/4	-
2	PLP	D	4404	-	-	0/6/6/8	0/1/1/1
2	PLP	B	4402	-	-	0/6/6/8	0/1/1/1
2	PLP	C	4403	-	-	0/6/6/8	0/1/1/1
3	POA	C	4603	-	-	0/3/4/4	-
2	PLP	F	4406	-	-	0/6/6/8	0/1/1/1
2	PLP	A	4401	-	-	0/6/6/8	0/1/1/1
2	PLP	E	4405	-	-	0/6/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4603	POA	P-C1	4.42	1.86	1.79
3	A	4601	POA	P-C1	4.07	1.86	1.79
2	D	4404	PLP	C2-N1	3.15	1.39	1.33
2	A	4401	PLP	C2-N1	3.10	1.39	1.33
2	B	4402	PLP	C2-N1	3.04	1.39	1.33
2	F	4406	PLP	C2-N1	2.93	1.39	1.33
2	E	4405	PLP	C2-N1	2.88	1.39	1.33
2	C	4403	PLP	C2-N1	2.83	1.39	1.33
2	A	4401	PLP	C4-C5	2.29	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4603	POA	P-O1P	2.28	1.55	1.50
2	D	4404	PLP	C4-C5	2.19	1.43	1.39
2	F	4406	PLP	C4-C5	2.14	1.42	1.39
2	C	4403	PLP	C4-C5	2.08	1.42	1.39
2	E	4405	PLP	C4-C5	2.06	1.42	1.39
2	A	4401	PLP	C2A-C2	2.06	1.53	1.50
2	D	4404	PLP	P-O3P	-2.05	1.47	1.54
2	B	4402	PLP	P-O3P	-2.04	1.47	1.54
2	F	4406	PLP	P-O3P	-2.01	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4406	PLP	O4P-C5A-C5	4.47	120.68	109.35
2	B	4402	PLP	O4P-C5A-C5	4.43	120.57	109.35
2	E	4405	PLP	O4P-C5A-C5	4.36	120.40	109.35
2	D	4404	PLP	O4P-C5A-C5	4.23	120.06	109.35
2	A	4401	PLP	O4P-C5A-C5	4.22	120.03	109.35
2	C	4403	PLP	O4P-C5A-C5	4.19	119.95	109.35
2	D	4404	PLP	C5-C6-N1	-3.17	118.96	123.95
2	B	4402	PLP	C5-C6-N1	-3.16	118.98	123.95
2	A	4401	PLP	C5-C6-N1	-3.05	119.15	123.95
2	E	4405	PLP	C5-C6-N1	-3.03	119.18	123.95
2	C	4403	PLP	C5-C6-N1	-2.96	119.30	123.95
2	F	4406	PLP	C5-C6-N1	-2.92	119.36	123.95
2	A	4401	PLP	C4-C5-C6	2.80	119.41	116.71
2	A	4401	PLP	O2P-P-O4P	-2.71	99.51	106.73
2	F	4406	PLP	C4-C5-C6	2.67	119.29	116.71
2	C	4403	PLP	O2P-P-O4P	-2.66	99.67	106.73
2	D	4404	PLP	C4-C5-C6	2.65	119.27	116.71
2	C	4403	PLP	C4-C5-C6	2.61	119.23	116.71
2	B	4402	PLP	O2P-P-O4P	-2.54	99.96	106.73
2	E	4405	PLP	C4-C5-C6	2.52	119.14	116.71
2	B	4402	PLP	C4-C5-C6	2.51	119.14	116.71
2	F	4406	PLP	O2P-P-O4P	-2.51	100.06	106.73
2	E	4405	PLP	O2P-P-O4P	-2.49	100.12	106.73
2	D	4404	PLP	O2P-P-O4P	-2.41	100.32	106.73
2	C	4403	PLP	C6-N1-C2	2.01	122.90	119.17
2	B	4402	PLP	C6-N1-C2	2.01	122.89	119.17

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4601	POA	C2-C1-P-O1P
3	A	4601	POA	C2-C1-P-O2P
3	A	4601	POA	C2-C1-P-O3P

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4601	POA	3	0
2	D	4404	PLP	1	0
2	B	4402	PLP	1	0
2	C	4403	PLP	1	0
2	F	4406	PLP	1	0
2	A	4401	PLP	1	0
2	E	4405	PLP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	235:ASN	C	236:HIS	N	1.17

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	350/366 (95%)	-0.51	4 (1%) 80 79	9, 15, 30, 40	7 (2%)
1	B	351/366 (95%)	-0.42	5 (1%) 75 73	11, 19, 29, 37	9 (2%)
1	C	350/366 (95%)	-0.44	5 (1%) 75 73	10, 19, 30, 40	11 (3%)
1	D	351/366 (95%)	-0.34	8 (2%) 60 58	12, 19, 31, 38	3 (0%)
1	E	350/366 (95%)	-0.41	4 (1%) 80 79	11, 19, 29, 39	4 (1%)
1	F	351/366 (95%)	-0.49	4 (1%) 80 79	10, 18, 29, 37	5 (1%)
All	All	2103/2196 (95%)	-0.44	30 (1%) 75 73	9, 18, 30, 40	39 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	333	SER	4.4
1	D	334	GLN	3.9
1	F	4	ASN	3.8
1	D	365	THR	3.8
1	B	4	ASN	3.6
1	D	79	PRO	3.4
1	A	5	TYR	3.3
1	C	333	SER	3.3
1	C	365	THR	3.1
1	B	333	SER	3.0
1	A	333	SER	3.0
1	D	333	SER	3.0
1	F	365	THR	2.9
1	F	333	SER	2.8
1	F	80	GLN	2.7
1	B	30	TRP	2.7
1	C	335	SER	2.6
1	C	334	GLN	2.5
1	D	4	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	30[A]	TRP	2.4
1	B	365	THR	2.3
1	B	79	PRO	2.3
1	E	79	PRO	2.3
1	D	104	ILE	2.3
1	D	30	TRP	2.2
1	A	292	ASP	2.1
1	A	151	ASP	2.1
1	E	365	THR	2.1
1	E	334	GLN	2.0
1	D	219	ARG	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 carbohydrates 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
3	POA	A	4601	7/7	0.57	0.31	63,65,65,65	0
3	POA	C	4603	7/7	0.78	0.26	57,58,59,59	0
4	PO4	C	4604	5/5	0.83	0.28	64,64,65,65	0
4	PO4	F	4606	5/5	0.85	0.20	69,69,69,69	0
4	PO4	B	4602	5/5	0.85	0.27	91,91,91,91	0
4	PO4	E	4605	5/5	0.89	0.21	72,72,72,72	0
2	PLP	F	4406	14/16	0.94	0.12	19,22,23,23	0
2	PLP	B	4402	14/16	0.94	0.12	20,25,26,26	0
2	PLP	A	4401	14/16	0.94	0.12	17,21,22,22	0
2	PLP	E	4405	14/16	0.94	0.12	21,23,24,24	0
2	PLP	C	4403	14/16	0.95	0.10	20,22,23,23	0
2	PLP	D	4404	14/16	0.96	0.11	20,22,23,24	0

## 6.5 Other polymers

There are no such residues in this entry.