



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:11 AM UTC

PDB ID : 5YB0 / pdb_00005yb0
Title : Crystal Structure of Wild Type Phosphoserine aminotransferase (PSAT) from *E. histolytica*
Authors : Singh, R.K.; Gourinath, S.
Deposited on : 2017-09-02
Resolution : 2.94 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

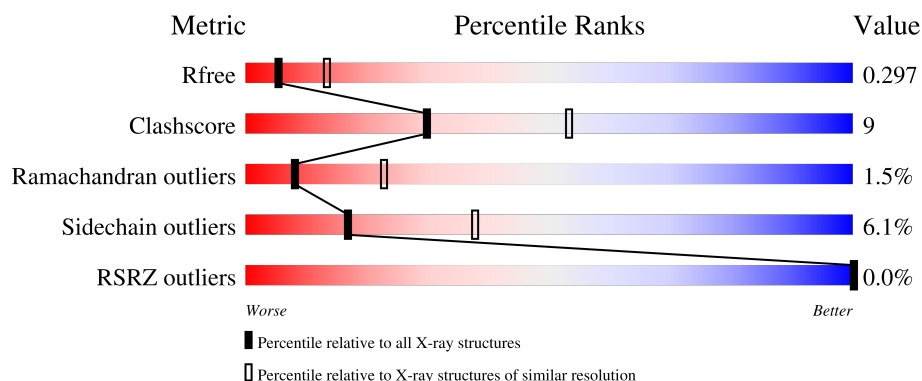
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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 $\leq 5\%$. 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	358	 73% 19% . . .
1	B	358	 72% 20% 6% . .
1	C	358	 73% 20% . . .
1	D	358	 75% 19% . .
1	E	358	 78% 15% . .

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Mol	Chain	Length	Quality of chain
1	F	358	 78%10% • 10%
1	G	358	 82%11% •• 5%
1	H	358	 86%9% •••
1	I	358	 83%10% • 6%
1	J	358	 65%5% • 29%
1	K	358	 82%6% • 12%
1	L	358	 55%•• 40%

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
2	PLP	A	401	-	-	X	-
2	PLP	F	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27402 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 Phosphoserine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2751	1765	458	513	15			
1	B	349	Total	C	N	O	S	0	0	0
			2759	1771	459	514	15			
1	C	349	Total	C	N	O	S	0	0	0
			2703	1734	450	504	15			
1	D	345	Total	C	N	O	S	0	0	0
			2603	1666	438	485	14			
1	E	342	Total	C	N	O	S	0	0	0
			2477	1579	419	464	15			
1	F	322	Total	C	N	O	S	0	0	0
			2300	1466	380	442	12			
1	G	341	Total	C	N	O	S	0	0	0
			2506	1600	425	466	15			
1	H	349	Total	C	N	O	S	0	0	0
			2225	1401	394	419	11			
1	I	336	Total	C	N	O	S	0	0	0
			2246	1407	395	431	13			
1	J	253	Total	C	N	O	S	0	0	0
			1491	926	265	291	9			
1	K	316	Total	C	N	O	S	0	0	0
			1752	1075	326	347	4			
1	L	216	Total	C	N	O	S	0	0	0
			1269	790	230	245	4			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	H	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	I	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	K	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

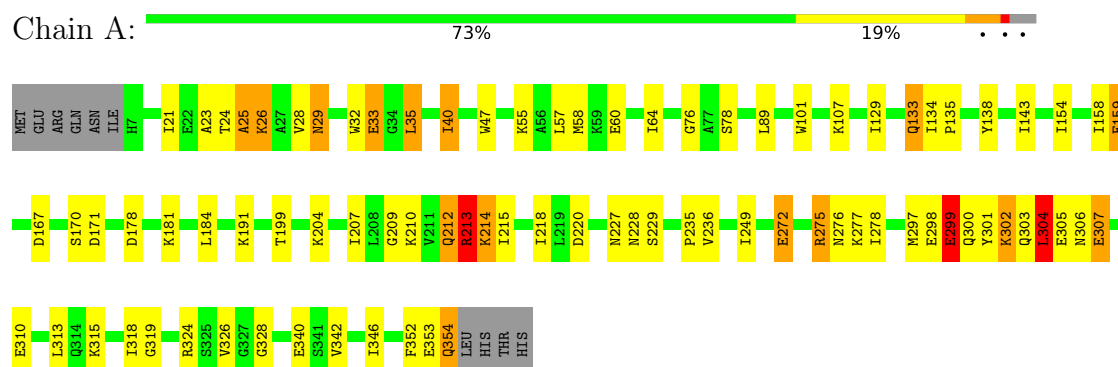
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	12	Total O 12 12	0	0
4	C	16	Total O 16 16	0	0
4	D	11	Total O 11 11	0	0
4	E	18	Total O 18 18	0	0
4	F	9	Total O 9 9	0	0
4	G	13	Total O 13 13	0	0
4	H	19	Total O 19 19	0	0
4	I	23	Total O 23 23	0	0
4	J	10	Total O 10 10	0	0
4	K	8	Total O 8 8	0	0
4	L	2	Total O 2 2	0	0

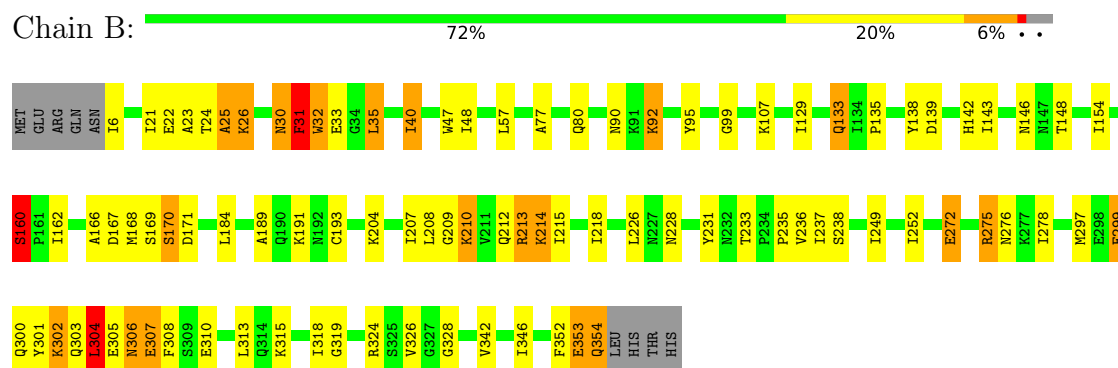
3 Residue-property plots

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.

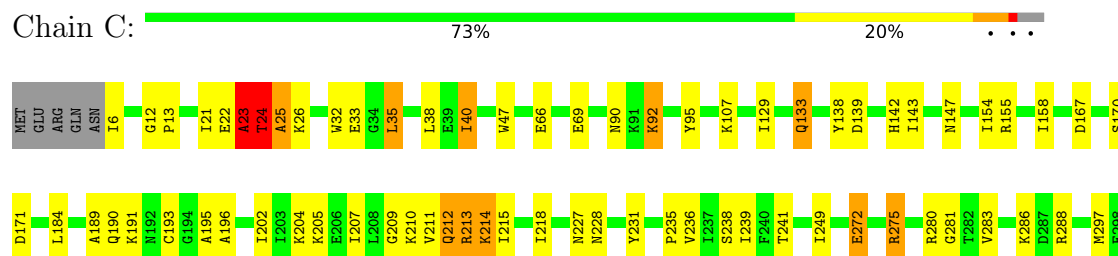
• Molecule 1: Phosphoserine aminotransferase



• Molecule 1: Phosphoserine aminotransferase



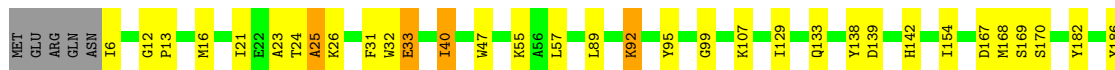
• Molecule 1: Phosphoserine aminotransferase





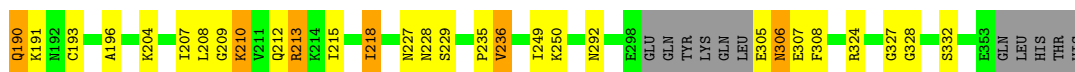
• Molecule 1: Phosphoserine aminotransferase

Chain D: 75% 19%



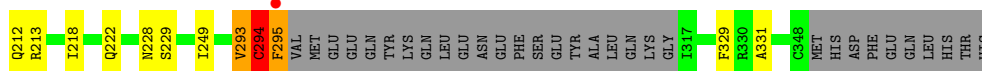
• Molecule 1: Phosphoserine aminotransferase

Chain E: 78% 15%



• Molecule 1: Phosphoserine aminotransferase

Chain F: 78% 10% 10%



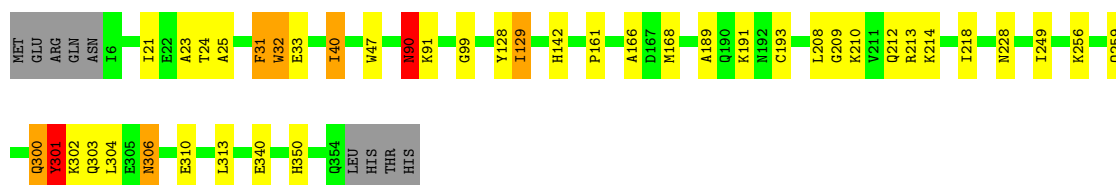
• Molecule 1: Phosphoserine aminotransferase

Chain G: 82% 11% 5%



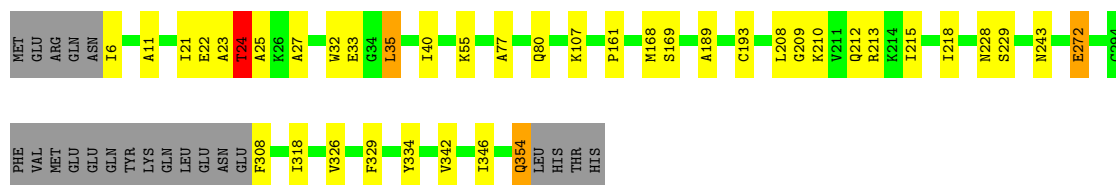
• Molecule 1: Phosphoserine aminotransferase

Chain H:  86% 9% . . .



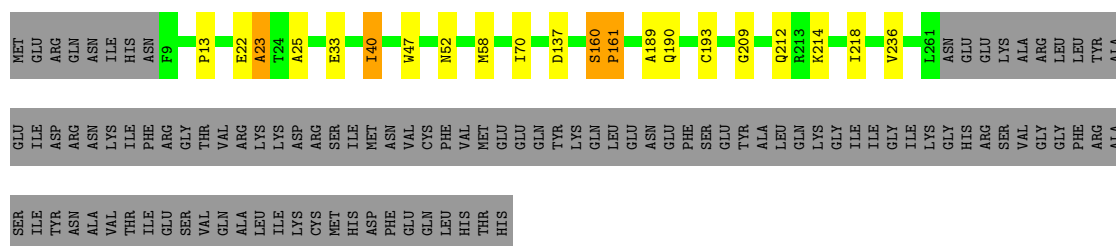
- Molecule 1: Phosphoserine aminotransferase

Chain I:  83% 10% • 6%



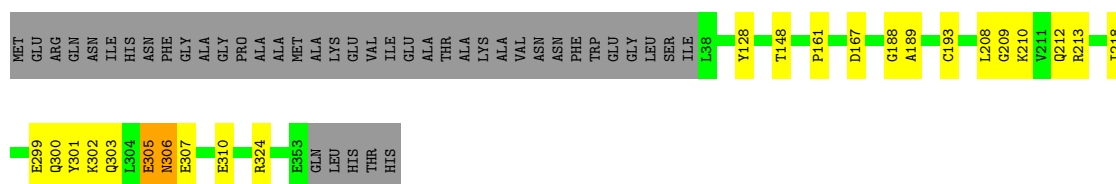
- Molecule 1: Phosphoserine aminotransferase

Chain J:  65% 5% • 29%



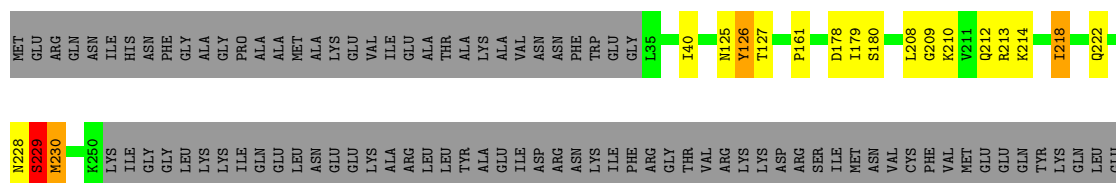
- Molecule 1: Phosphoserine aminotransferase

Chain K:  82% 6% • 12%



- Molecule 1: Phosphoserine aminotransferase

Chain L:  55% 40% . .



ASN	GLU	PHE	SER	GLU	TYR	ALA	LEU	GLN	LYS	GLY	ILE	ILE	GLY	ILE	LYS	GLY	HIS	ARG	SER	VAL	GLY	GLY	PHE	ARG	ALA	SER	ILE	TYR	ASN	ALA	VAL	THR	ILE	GLU	SER	VAL	GLN	ALA	LEU	ILE	LYS	CYS	MET	HIS	ASP	PHE	GLU	GLN	LEU	HIS	THR	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.45Å 134.07Å 139.06Å 62.85° 88.58° 74.92°	Depositor
Resolution (Å)	50.15 – 2.94 50.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.9 (50.15-2.94) 87.9 (50.15-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.265 , 0.301 0.258 , 0.297	Depositor DCC
R_{free} test set	3837 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 97.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,h-k,-l	Xtriage
Reported twinning fraction	0.888 for H, K, L 0.112 for H, H-K, -L	Depositor
Outliers	0 of 76766 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27402	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, PLP

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	0.91	2/2799 (0.1%)	1.12	12/3771 (0.3%)
1	B	0.84	3/2807 (0.1%)	1.16	18/3782 (0.5%)
1	C	0.79	0/2749	1.04	8/3710 (0.2%)
1	D	0.75	1/2644 (0.0%)	1.00	9/3571 (0.3%)
1	E	0.76	1/2515 (0.0%)	0.96	2/3410 (0.1%)
1	F	1.45	11/2336 (0.5%)	1.20	14/3178 (0.4%)
1	G	0.70	1/2547 (0.0%)	0.97	6/3448 (0.2%)
1	H	0.75	3/2255 (0.1%)	1.10	16/3096 (0.5%)
1	I	0.66	1/2275 (0.0%)	0.89	1/3100 (0.0%)
1	J	0.81	1/1508 (0.1%)	1.20	6/2082 (0.3%)
1	K	0.72	0/1769	1.02	3/2455 (0.1%)
1	L	0.71	1/1285 (0.1%)	1.02	3/1778 (0.2%)
All	All	0.85	25/27489 (0.1%)	1.06	98/37381 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	5
1	I	0	1
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	27

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	294	CYS	CA-C	33.73	1.94	1.52
1	F	295	PHE	CA-C	29.55	2.15	1.52
1	F	295	PHE	C-O	20.82	1.65	1.23
1	F	295	PHE	N-CA	18.74	1.81	1.46
1	F	294	CYS	C-N	17.86	1.58	1.33
1	F	294	CYS	N-CA	16.48	1.66	1.46
1	F	293	VAL	CA-C	10.17	1.65	1.52
1	F	295	PHE	CA-CB	9.45	1.72	1.53
1	H	128	TYR	C-O	-8.83	1.12	1.24
1	A	215	ILE	N-CA	8.42	1.52	1.45
1	F	294	CYS	CA-CB	7.73	1.65	1.53
1	E	215	ILE	N-CA	7.60	1.51	1.45
1	J	23	ALA	C-O	-7.42	1.14	1.24
1	H	32	TRP	C-O	-7.38	1.14	1.23
1	D	215	ILE	N-CA	7.28	1.51	1.45
1	B	160	SER	C-O	-7.18	1.15	1.24
1	B	31	PHE	C-O	-6.88	1.15	1.24
1	A	28	VAL	C-O	-6.81	1.14	1.23
1	H	301	TYR	CA-C	-6.51	1.44	1.52
1	F	293	VAL	N-CA	6.20	1.53	1.46
1	B	215	ILE	N-CA	6.05	1.50	1.45
1	F	32	TRP	C-O	-5.99	1.16	1.23
1	I	215	ILE	N-CA	5.54	1.50	1.45
1	L	229	SER	C-O	-5.39	1.17	1.24
1	G	297	MET	CA-C	-5.20	1.46	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	160	SER	CA-C-N	19.30	143.96	119.84
1	J	160	SER	C-N-CA	19.30	143.96	119.84
1	F	294	CYS	CA-C-O	-18.35	100.43	120.80
1	F	32	TRP	N-CA-C	-18.03	83.84	110.52
1	H	32	TRP	N-CA-C	-17.52	82.47	110.32
1	B	160	SER	C-N-CD	-17.05	83.08	120.60
1	B	160	SER	CA-C-N	16.53	166.68	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	SER	C-N-CA	16.53	166.68	127.00
1	L	127	THR	N-CA-C	13.51	129.09	112.87
1	F	294	CYS	N-CA-C	13.17	131.36	109.76
1	F	295	PHE	CA-C-O	-13.15	98.44	120.80
1	G	298	GLU	N-CA-C	-13.02	97.53	113.41
1	E	213	ARG	N-CA-C	12.07	124.43	111.28
1	L	213	ARG	N-CA-C	11.64	123.96	111.28
1	F	294	CYS	N-CA-CB	-11.63	91.33	110.52
1	H	91	LYS	N-CA-C	-11.29	99.21	113.43
1	F	294	CYS	CA-C-N	11.00	141.50	121.70
1	F	294	CYS	C-N-CA	11.00	141.50	121.70
1	K	213	ARG	N-CA-C	10.10	122.28	111.28
1	F	213	ARG	N-CA-C	9.81	123.00	111.71
1	H	301	TYR	N-CA-C	9.14	130.26	110.80
1	I	213	ARG	N-CA-C	8.67	121.68	111.71
1	H	304	LEU	N-CA-C	-8.23	102.31	111.28
1	A	28	VAL	N-CA-C	-8.20	101.11	110.05
1	D	304	LEU	N-CA-C	-8.12	102.37	111.71
1	D	32	TRP	CA-C-N	8.02	136.86	121.54
1	D	32	TRP	C-N-CA	8.02	136.86	121.54
1	C	23	ALA	N-CA-C	-7.59	94.62	110.80
1	H	128	TYR	N-CA-C	7.59	126.97	110.80
1	A	29	ASN	N-CA-C	7.51	126.80	110.80
1	J	161	PRO	N-CA-C	-7.33	97.38	112.47
1	A	304	LEU	N-CA-C	-7.32	102.32	111.11
1	H	32	TRP	CA-C-O	-7.22	112.70	121.36
1	F	294	CYS	CB-CA-C	7.17	121.53	109.48
1	J	23	ALA	N-CA-C	-7.17	95.53	110.80
1	H	90	ASN	N-CA-C	-7.17	95.53	110.80
1	B	214	LYS	N-CA-C	7.16	120.98	108.52
1	F	295	PHE	N-CA-CB	7.12	122.61	110.50
1	A	214	LYS	N-CA-C	6.72	120.81	108.58
1	J	25	ALA	N-CA-C	-6.68	105.12	113.20
1	G	214	LYS	N-CA-C	6.67	120.13	108.52
1	F	32	TRP	CA-C-O	-6.57	113.97	121.72
1	H	214	LYS	N-CA-C	6.51	119.85	108.52
1	A	215	ILE	CB-CA-C	-6.47	103.62	110.16
1	C	214	LYS	N-CA-C	6.46	119.77	108.52
1	C	25	ALA	N-CA-C	-6.42	105.20	113.16
1	B	30	ASN	N-CA-C	-6.37	102.32	110.53
1	D	214	LYS	N-CA-C	6.32	120.09	108.58
1	F	293	VAL	N-CA-C	6.32	117.87	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	214	LYS	N-CA-C	6.31	119.85	108.17
1	E	215	ILE	CB-CA-C	-6.30	103.80	110.16
1	C	214	LYS	N-CA-CB	-6.11	101.78	110.58
1	B	214	LYS	N-CA-CB	-6.02	101.91	110.58
1	B	148	THR	N-CA-C	5.94	119.36	111.75
1	B	304	LEU	N-CA-C	-5.93	104.00	111.11
1	A	64	ILE	CB-CA-C	-5.87	104.44	110.71
1	H	213	ARG	N-CA-C	5.85	119.67	112.54
1	A	213	ARG	N-CA-C	5.84	119.67	112.54
1	B	160	SER	CB-CA-C	5.83	121.66	110.17
1	H	129	ILE	CA-C-N	5.83	126.02	120.31
1	H	129	ILE	C-N-CA	5.83	126.02	120.31
1	C	213	ARG	N-CA-C	5.80	119.61	112.54
1	J	214	LYS	N-CA-C	5.80	118.89	108.17
1	F	32	TRP	CA-C-N	-5.74	112.71	121.66
1	F	32	TRP	C-N-CA	-5.74	112.71	121.66
1	H	32	TRP	CA-C-N	-5.71	112.75	121.66
1	H	32	TRP	C-N-CA	-5.71	112.75	121.66
1	D	99	GLY	N-CA-C	5.69	117.66	110.38
1	C	308	PHE	N-CA-CB	5.62	119.00	110.28
1	D	188	GLY	N-CA-C	-5.61	105.47	111.93
1	A	214	LYS	N-CA-CB	-5.58	101.15	110.42
1	A	302	LYS	N-CA-C	5.56	118.86	112.97
1	D	25	ALA	N-CA-C	-5.53	106.30	113.16
1	C	202	ILE	N-CA-C	-5.53	100.43	108.17
1	G	32	TRP	N-CA-C	5.49	116.95	110.97
1	B	231	TYR	N-CA-C	-5.48	104.54	111.11
1	D	302	LYS	N-CA-C	-5.45	99.07	108.56
1	B	308	PHE	N-CA-CB	5.43	118.69	110.28
1	A	25	ALA	N-CA-C	-5.38	106.75	113.15
1	B	160	SER	O-C-N	-5.38	115.14	121.32
1	K	148	THR	N-CA-C	5.37	118.62	111.75
1	G	297	MET	N-CA-C	-5.35	103.42	110.43
1	A	134	ILE	N-CA-C	5.34	112.42	107.56
1	B	252	ILE	N-CA-C	5.34	116.66	111.91
1	B	213	ARG	N-CA-C	-5.33	106.45	113.17
1	D	214	LYS	N-CA-CB	-5.28	101.65	110.42
1	B	160	SER	CA-C-O	-5.25	112.96	120.16
1	B	215	ILE	CB-CA-C	-5.25	104.86	110.16
1	A	159	GLU	CA-CB-CG	5.24	124.58	114.10
1	K	188	GLY	N-CA-C	-5.21	105.93	111.93
1	B	25	ALA	N-CA-C	-5.20	106.71	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	299	GLU	CA-C-N	5.16	130.98	121.70
1	G	299	GLU	C-N-CA	5.16	130.98	121.70
1	H	99	GLY	N-CA-C	5.14	116.96	110.38
1	H	300	GLN	CA-C-N	-5.07	111.86	121.54
1	H	300	GLN	C-N-CA	-5.07	111.86	121.54
1	C	231	TYR	N-CA-C	-5.04	105.06	111.11
1	B	99	GLY	N-CA-C	5.04	116.83	110.38

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	GLN	Peptide
1	A	299	GLU	Peptide
1	B	160	SER	Peptide
1	B	212	GLN	Peptide
1	B	299	GLU	Peptide
1	B	353	GLU	Peptide
1	C	212	GLN	Peptide
1	C	305	GLU	Peptide
1	D	212	GLN	Peptide
1	D	302	LYS	Peptide
1	E	212	GLN	Peptide
1	E	213	ARG	Peptide
1	F	212	GLN	Peptide
1	F	294	CYS	Peptide
1	G	212	GLN	Peptide
1	H	212	GLN	Peptide
1	H	300	GLN	Peptide
1	H	301	TYR	Peptide
1	H	302	LYS	Peptide
1	H	90	ASN	Peptide
1	I	212	GLN	Peptide
1	J	160	SER	Peptide
1	J	212	GLN	Peptide
1	K	212	GLN	Peptide
1	K	299	GLU	Peptide
1	L	126	TYR	Peptide
1	L	212	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2751	0	2813	74	0
1	B	2759	0	2823	89	1
1	C	2703	0	2726	70	0
1	D	2603	0	2592	42	0
1	E	2477	0	2358	45	0
1	F	2300	0	2138	37	0
1	G	2506	0	2407	29	1
1	H	2225	0	1837	22	0
1	I	2246	0	1931	27	0
1	J	1491	0	1103	12	0
1	K	1752	0	1108	10	0
1	L	1269	0	893	8	0
2	A	16	0	7	9	0
2	B	16	0	8	4	0
2	C	16	0	7	3	0
2	D	16	0	8	3	0
2	E	16	0	8	3	0
2	F	16	0	8	6	0
2	G	16	0	7	1	0
2	H	16	0	7	4	0
2	I	16	0	8	0	0
2	K	16	0	7	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	14	0	0	1	0
4	B	12	0	0	0	0
4	C	16	0	0	2	0
4	D	11	0	0	0	0
4	E	18	0	0	1	0
4	F	9	0	0	2	0
4	G	13	0	0	2	0
4	H	19	0	0	6	0
4	I	23	0	0	4	0
4	J	10	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	8	0	0	2	0
4	L	2	0	0	0	0
All	All	27402	0	24804	444	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (444) 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:F:295:PHE:N	1:F:295:PHE:CA	1.81	1.42
1:F:295:PHE:O	1:F:295:PHE:C	1.65	1.40
1:F:294:CYS:C	1:F:294:CYS:CA	1.94	1.40
1:B:354:GLN:O	1:B:354:GLN:NE2	1.62	1.33
1:F:295:PHE:CA	1:F:295:PHE:C	2.15	1.20
1:B:191:LYS:NZ	2:B:401:PLP:O3	1.79	1.13
1:A:301:TYR:C	1:A:303:GLN:HA	1.77	1.09
1:H:301:TYR:O	1:H:303:GLN:HA	1.52	1.08
1:A:278:ILE:HD11	1:A:353:GLU:HA	1.38	1.04
1:B:301:TYR:C	1:B:303:GLN:HA	1.83	1.04
1:F:191:LYS:NZ	2:F:401:PLP:O3	1.92	1.03
1:B:278:ILE:HD11	1:B:353:GLU:HA	1.38	1.02
1:B:305:GLU:O	1:B:307:GLU:N	1.94	1.01
1:B:301:TYR:O	1:B:303:GLN:HG2	1.60	1.01
1:B:354:GLN:O	1:B:354:GLN:CD	2.04	1.01
1:C:301:TYR:C	1:C:303:GLN:HA	1.85	1.00
1:B:354:GLN:CD	1:B:354:GLN:C	2.29	1.00
1:G:229:SER:O	1:G:230:MET:HG3	1.64	0.96
2:F:401:PLP:O3P	1:G:233:THR:OG1	1.83	0.96
1:C:22:GLU:O	1:C:23:ALA:O	1.86	0.93
1:C:22:GLU:C	1:C:23:ALA:O	2.12	0.92
1:C:353:GLU:OE2	4:C:501:HOH:O	1.86	0.91
1:D:272:GLU:HG2	1:D:346:ILE:HG23	1.50	0.91
1:H:166:ALA:HB3	4:H:502:HOH:O	1.71	0.91
1:F:294:CYS:C	1:F:294:CYS:HA	1.95	0.90
1:A:133:GLN:OE1	1:A:133:GLN:HA	1.70	0.89
1:E:191:LYS:NZ	2:E:401:PLP:O3	2.06	0.88
1:G:229:SER:O	1:G:230:MET:CG	2.22	0.87
1:A:191:LYS:HZ1	2:A:401:PLP:C4A	1.88	0.86
1:H:142:HIS:CB	4:H:517:HOH:O	2.22	0.86
1:F:293:VAL:O	1:F:331:ALA:N	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:O	1:A:307:GLU:N	2.09	0.85
1:B:272:GLU:HG2	1:B:346:ILE:HG23	1.57	0.84
1:A:301:TYR:O	1:A:303:GLN:HG2	1.77	0.83
1:A:302:LYS:N	1:A:303:GLN:HA	1.91	0.82
1:C:272:GLU:HG2	1:C:346:ILE:HG23	1.62	0.81
1:I:308:PHE:HB3	1:I:329:PHE:CZ	2.15	0.81
1:K:301:TYR:C	1:K:303:GLN:HA	2.05	0.81
1:C:23:ALA:O	1:C:25:ALA:N	2.15	0.80
1:I:272:GLU:HG2	1:I:346:ILE:HG23	1.63	0.79
1:C:212:GLN:NE2	4:C:502:HOH:O	2.14	0.79
1:B:302:LYS:N	1:B:303:GLN:HA	1.95	0.78
1:D:305:GLU:O	1:D:307:GLU:N	2.17	0.77
1:L:229:SER:O	1:L:230:MET:CB	2.33	0.77
1:A:272:GLU:HG2	1:A:346:ILE:HG23	1.65	0.76
1:E:32:TRP:CB	1:E:35:LEU:HB2	2.16	0.76
1:B:304:LEU:CD1	1:B:328:GLY:HA2	2.16	0.75
1:C:191:LYS:NZ	2:C:401:PLP:C3	2.45	0.75
1:E:228:ASN:CG	1:E:228:ASN:O	2.29	0.74
1:H:228:ASN:O	1:H:228:ASN:CG	2.30	0.74
1:B:278:ILE:CD1	1:B:353:GLU:HA	2.17	0.74
1:B:133:GLN:HA	1:B:133:GLN:OE1	1.85	0.74
1:A:32:TRP:CB	1:A:35:LEU:HB2	2.18	0.74
1:B:191:LYS:NZ	2:B:401:PLP:C3	2.50	0.74
1:B:30:ASN:C	1:B:31:PHE:O	2.30	0.73
1:C:297:MET:HG2	1:C:304:LEU:CB	2.18	0.73
1:F:228:ASN:O	1:F:228:ASN:CG	2.32	0.73
1:H:301:TYR:O	1:H:303:GLN:CA	2.36	0.73
1:B:228:ASN:CG	1:B:228:ASN:O	2.29	0.72
1:A:300:GLN:HB3	1:A:301:TYR:CD2	2.24	0.72
1:H:191:LYS:NZ	2:H:401:PLP:O4A	2.22	0.72
1:A:301:TYR:O	1:A:303:GLN:CG	2.37	0.72
1:G:133:GLN:HA	1:G:133:GLN:OE1	1.88	0.72
1:H:191:LYS:NZ	2:H:401:PLP:O3	2.24	0.71
1:C:32:TRP:CB	1:C:35:LEU:HB2	2.20	0.71
1:A:55:LYS:NZ	1:A:228:ASN:OD1	2.17	0.71
1:A:304:LEU:HD11	1:A:328:GLY:HA2	1.71	0.70
1:C:302:LYS:N	1:C:303:GLN:HA	2.06	0.70
1:C:23:ALA:O	1:C:24:THR:C	2.32	0.70
1:D:208:LEU:O	1:D:210:LYS:N	2.22	0.70
1:D:301:TYR:C	1:D:303:GLN:HA	2.16	0.70
1:C:191:LYS:NZ	2:C:401:PLP:O3	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:ALA:O	1:H:25:ALA:N	2.25	0.69
1:B:305:GLU:HG3	1:E:137:ASP:CG	2.16	0.69
1:E:305:GLU:O	1:E:307:GLU:N	2.25	0.69
1:A:301:TYR:O	1:A:303:GLN:HA	1.93	0.68
1:I:55:LYS:NZ	1:I:228:ASN:OD1	2.17	0.68
1:I:32:TRP:CB	1:I:35:LEU:HB2	2.24	0.68
1:D:191:LYS:NZ	2:D:401:PLP:C3	2.54	0.68
1:D:55:LYS:NZ	1:D:228:ASN:OD1	2.20	0.67
1:H:256:LYS:HA	4:H:501:HOH:O	1.95	0.67
1:F:133:GLN:OE1	1:F:133:GLN:HA	1.92	0.67
1:I:243:ASN:CB	4:I:512:HOH:O	2.42	0.67
1:B:191:LYS:HZ3	2:B:401:PLP:C3	2.08	0.67
1:A:304:LEU:CD1	1:A:328:GLY:HA2	2.24	0.66
1:A:191:LYS:NZ	2:A:401:PLP:C4A	2.58	0.66
1:A:133:GLN:NE2	1:C:283:VAL:C	2.53	0.66
1:C:228:ASN:CG	1:C:228:ASN:O	2.36	0.66
1:B:300:GLN:O	1:B:301:TYR:C	2.37	0.66
1:B:30:ASN:O	1:B:31:PHE:O	2.14	0.66
1:C:204:LYS:O	1:C:207:ILE:HG12	1.96	0.66
1:B:278:ILE:HG22	1:B:297:MET:HE1	1.77	0.65
1:C:66:GLU:HG2	1:J:52:ASN:ND2	2.11	0.65
1:C:133:GLN:OE1	1:C:133:GLN:HA	1.95	0.65
1:F:191:LYS:NZ	2:F:401:PLP:C3	2.60	0.65
1:E:189:ALA:HA	1:E:193:CYS:HB2	1.79	0.65
1:B:297:MET:HG3	1:B:304:LEU:N	2.12	0.64
1:G:228:ASN:O	1:G:229:SER:O	2.15	0.64
1:I:308:PHE:HB3	1:I:329:PHE:CE2	2.32	0.64
1:B:40:ILE:HD11	1:B:47:TRP:HB2	1.80	0.64
1:H:23:ALA:C	1:H:25:ALA:H	2.06	0.64
1:B:31:PHE:O	1:B:32:TRP:CB	2.46	0.63
1:I:272:GLU:CG	1:I:346:ILE:HG23	2.28	0.63
1:K:301:TYR:O	1:K:303:GLN:HA	1.98	0.63
1:C:297:MET:CG	1:C:304:LEU:CB	2.77	0.63
1:F:33:GLU:O	1:G:6:ILE:HD13	1.99	0.62
1:J:40:ILE:HD11	1:J:47:TRP:HB2	1.81	0.62
1:C:6:ILE:HD13	1:D:33:GLU:O	1.99	0.62
1:B:297:MET:HG2	1:B:304:LEU:HB2	1.82	0.62
1:J:22:GLU:C	1:J:23:ALA:O	2.36	0.62
1:E:250:LYS:HE2	1:I:354:GLN:NE2	2.15	0.61
1:E:23:ALA:C	1:E:25:ALA:H	2.08	0.61
1:A:278:ILE:CG2	1:A:297:MET:HE1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:ILE:HD11	1:H:47:TRP:HB2	1.83	0.61
1:A:278:ILE:HG22	1:A:297:MET:HE1	1.81	0.61
1:B:272:GLU:CG	1:B:346:ILE:HG23	2.31	0.60
1:F:295:PHE:H	1:F:329:PHE:CB	2.13	0.60
1:A:275:ARG:HH11	1:A:275:ARG:HB3	1.67	0.59
1:I:228:ASN:CG	1:I:228:ASN:O	2.44	0.59
1:A:278:ILE:HD13	1:A:352:PHE:HD1	1.67	0.59
1:F:184:LEU:HD23	1:F:184:LEU:C	2.28	0.59
1:B:307:GLU:HG3	1:B:352:PHE:HZ	1.67	0.59
1:C:40:ILE:HD11	1:C:47:TRP:HB2	1.85	0.59
1:K:306:ASN:O	1:K:310:GLU:N	2.35	0.58
1:A:228:ASN:O	1:A:228:ASN:CG	2.46	0.58
1:B:299:GLU:OE2	1:B:300:GLN:NE2	2.26	0.58
1:G:229:SER:O	1:G:230:MET:CB	2.51	0.58
1:I:308:PHE:CG	1:I:308:PHE:O	2.56	0.58
1:C:12:GLY:HA2	1:C:13:PRO:C	2.28	0.58
1:B:301:TYR:O	1:B:303:GLN:CG	2.46	0.58
1:B:23:ALA:C	1:B:25:ALA:H	2.11	0.58
1:C:147:ASN:HB3	3:C:402:CL:CL	2.41	0.58
1:F:204:LYS:O	1:F:207:ILE:HG12	2.04	0.58
1:L:228:ASN:C	1:L:229:SER:O	2.46	0.58
1:A:191:LYS:NZ	2:A:401:PLP:O3	2.37	0.57
1:A:299:GLU:HA	1:A:300:GLN:CB	2.32	0.57
1:B:275:ARG:HB3	1:B:275:ARG:HH11	1.69	0.57
1:G:280:ARG:HB2	1:G:298:GLU:OE2	2.05	0.57
1:A:307:GLU:HG3	1:A:352:PHE:HZ	1.70	0.57
1:C:297:MET:HG3	1:C:304:LEU:N	2.20	0.57
1:E:191:LYS:NZ	2:E:401:PLP:C3	2.66	0.57
1:A:191:LYS:NZ	2:A:401:PLP:C3	2.67	0.57
1:A:305:GLU:HA	1:F:137:ASP:CB	2.35	0.57
1:E:227:ASN:O	1:E:228:ASN:C	2.48	0.56
1:B:297:MET:HG3	1:B:304:LEU:CA	2.35	0.56
1:A:272:GLU:CG	1:A:346:ILE:HG23	2.33	0.56
1:E:40:ILE:HD11	1:E:47:TRP:HB2	1.87	0.56
1:A:297:MET:HG3	1:A:304:LEU:N	2.20	0.56
1:G:354:GLN:HA	1:G:354:GLN:NE2	2.20	0.56
1:D:191:LYS:NZ	2:D:401:PLP:O3	2.39	0.56
1:F:40:ILE:HD11	1:F:47:TRP:HB2	1.86	0.56
1:C:272:GLU:CG	1:C:346:ILE:HG23	2.34	0.56
1:A:60:GLU:HB2	4:A:506:HOH:O	2.05	0.56
1:B:304:LEU:HD11	1:B:328:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:LYS:O	1:F:210:LYS:HG2	2.06	0.56
1:G:333:ILE:O	1:G:333:ILE:HG13	2.06	0.55
1:A:278:ILE:HD11	1:A:353:GLU:CA	2.26	0.55
1:C:171:ASP:OD1	1:C:171:ASP:C	2.46	0.55
1:D:40:ILE:HD11	1:D:47:TRP:HB2	1.88	0.55
1:D:23:ALA:O	1:D:25:ALA:N	2.37	0.55
1:F:295:PHE:N	1:F:329:PHE:CB	2.70	0.55
1:F:18:LYS:HE3	4:F:509:HOH:O	2.07	0.55
1:A:32:TRP:N	1:A:33:GLU:HA	2.22	0.55
1:B:307:GLU:HA	1:B:307:GLU:OE1	2.06	0.55
1:A:297:MET:HG3	1:A:304:LEU:CA	2.38	0.54
1:B:354:GLN:NE2	1:B:354:GLN:C	2.50	0.54
1:C:301:TYR:O	1:C:303:GLN:HA	2.08	0.54
1:F:294:CYS:CA	1:F:294:CYS:O	2.50	0.54
1:A:23:ALA:C	1:A:25:ALA:H	2.15	0.54
1:B:204:LYS:O	1:B:207:ILE:HG12	2.07	0.54
1:E:32:TRP:CB	1:E:35:LEU:H	2.20	0.54
1:G:148:THR:OG1	2:G:401:PLP:O3	2.24	0.54
1:C:32:TRP:CB	1:C:35:LEU:H	2.21	0.54
1:G:6:ILE:HG23	1:G:318:ILE:HD12	1.90	0.54
1:A:129:ILE:HD13	1:A:154:ILE:HG13	1.88	0.53
1:C:95:TYR:CE2	1:C:142:HIS:CG	2.96	0.53
1:D:23:ALA:C	1:D:25:ALA:H	2.14	0.53
1:I:6:ILE:HD13	1:J:33:GLU:O	2.08	0.53
1:I:23:ALA:C	1:I:25:ALA:H	2.16	0.53
1:I:354:GLN:NE2	1:I:354:GLN:HA	2.24	0.53
1:B:160:SER:HB3	1:B:162:ILE:O	2.07	0.53
1:C:33:GLU:O	1:D:6:ILE:HD13	2.08	0.53
1:A:204:LYS:O	1:A:207:ILE:HG12	2.08	0.53
1:A:40:ILE:HD11	1:A:47:TRP:HB2	1.91	0.52
1:A:275:ARG:HG3	1:A:276:ASN:N	2.23	0.52
1:B:305:GLU:CG	1:E:137:ASP:CG	2.82	0.52
2:F:401:PLP:H4A	2:F:401:PLP:O4P	2.09	0.52
1:J:236:VAL:HG12	4:J:401:HOH:O	2.09	0.52
1:E:23:ALA:O	1:E:25:ALA:N	2.35	0.52
1:B:23:ALA:O	1:B:25:ALA:N	2.37	0.52
1:C:300:GLN:O	1:C:301:TYR:C	2.52	0.52
1:C:354:GLN:NE2	1:C:354:GLN:HA	2.25	0.52
1:H:191:LYS:HZ1	2:H:401:PLP:C4A	2.16	0.52
1:A:220:ASP:OD1	1:A:220:ASP:C	2.53	0.52
1:E:324:ARG:CB	4:E:504:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:GLN:HB3	4:H:501:HOH:O	2.09	0.52
1:A:23:ALA:O	1:A:26:LYS:HD3	2.09	0.52
1:A:101:TRP:CZ2	2:A:401:PLP:C4A	2.93	0.52
1:A:354:GLN:HA	1:A:354:GLN:NE2	2.25	0.51
1:B:324:ARG:NE	1:E:210:LYS:HA	2.25	0.51
1:E:305:GLU:O	1:E:306:ASN:C	2.53	0.51
1:A:300:GLN:O	1:A:301:TYR:C	2.52	0.51
1:E:305:GLU:C	1:E:307:GLU:N	2.68	0.51
1:B:305:GLU:HG3	1:E:137:ASP:OD1	2.11	0.51
1:F:125:ASN:HB2	4:F:503:HOH:O	2.10	0.51
1:H:208:LEU:O	1:H:210:LYS:N	2.40	0.51
1:I:189:ALA:HA	1:I:193:CYS:HB2	1.92	0.51
1:B:143:ILE:O	1:B:166:ALA:HA	2.11	0.51
1:B:278:ILE:CG2	1:B:297:MET:HE1	2.39	0.50
1:D:129:ILE:HD13	1:D:154:ILE:HG13	1.92	0.50
1:G:95:TYR:CE2	1:G:142:HIS:CG	2.99	0.50
1:K:189:ALA:HA	1:K:193:CYS:HB2	1.92	0.50
1:A:227:ASN:O	1:A:228:ASN:C	2.54	0.50
1:D:272:GLU:CG	1:D:346:ILE:HG23	2.34	0.50
1:A:301:TYR:O	1:A:303:GLN:CA	2.59	0.49
1:C:301:TYR:O	1:C:303:GLN:CB	2.60	0.49
1:I:23:ALA:O	1:I:25:ALA:N	2.38	0.49
1:C:69:GLU:HG3	1:C:205:LYS:HD3	1.94	0.49
1:C:184:LEU:C	1:C:184:LEU:HD23	2.37	0.49
1:H:168:MET:HG3	4:H:502:HOH:O	2.11	0.49
1:A:297:MET:HG2	1:A:304:LEU:HB2	1.94	0.49
1:C:275:ARG:HH11	1:C:275:ARG:CG	2.26	0.49
1:D:204:LYS:O	1:D:207:ILE:HG12	2.11	0.49
1:H:189:ALA:HA	1:H:193:CYS:HB2	1.94	0.49
1:E:204:LYS:O	1:E:207:ILE:HG12	2.12	0.49
1:L:208:LEU:O	1:L:210:LYS:N	2.41	0.49
1:A:300:GLN:HB3	1:A:301:TYR:HD2	1.73	0.49
1:B:184:LEU:C	1:B:184:LEU:HD23	2.38	0.49
1:E:218:ILE:HD12	1:E:218:ILE:O	2.13	0.49
1:B:92:LYS:HB3	1:B:138:TYR:CD1	2.47	0.49
2:F:401:PLP:O3P	1:G:233:THR:CB	2.59	0.49
1:D:303:GLN:O	1:D:307:GLU:CB	2.61	0.48
1:F:208:LEU:O	1:F:210:LYS:N	2.39	0.48
1:B:90:ASN:HB3	1:B:139:ASP:OD2	2.14	0.48
1:B:22:GLU:O	1:B:23:ALA:C	2.54	0.48
1:I:11:ALA:O	1:I:334:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:OD2	2:A:401:PLP:N1	2.47	0.48
1:B:342:VAL:O	1:B:346:ILE:HG13	2.13	0.48
1:L:125:ASN:O	1:L:126:TYR:C	2.56	0.48
1:A:191:LYS:NZ	2:A:401:PLP:C4	2.75	0.48
1:G:118:ILE:HG12	4:G:503:HOH:O	2.13	0.48
1:B:275:ARG:HG3	1:B:276:ASN:N	2.28	0.48
1:C:23:ALA:C	1:C:25:ALA:H	2.22	0.48
1:I:6:ILE:HG23	1:I:318:ILE:HD12	1.94	0.48
1:C:23:ALA:C	1:C:25:ALA:N	2.72	0.48
1:D:133:GLN:OE1	1:D:133:GLN:HA	2.12	0.48
1:K:302:LYS:N	1:K:303:GLN:HA	2.29	0.48
1:C:275:ARG:HH11	1:C:275:ARG:HB3	1.77	0.48
1:D:92:LYS:HB3	1:D:138:TYR:CD1	2.48	0.48
1:E:6:ILE:HD13	1:H:33:GLU:O	2.14	0.48
1:G:23:ALA:C	1:G:25:ALA:H	2.22	0.48
1:B:48:ILE:HD13	1:F:206:GLU:CD	2.38	0.47
1:A:354:GLN:HA	1:A:354:GLN:HE21	1.78	0.47
1:E:95:TYR:CE2	1:E:142:HIS:CG	3.02	0.47
1:G:6:ILE:N	4:G:502:HOH:O	2.47	0.47
1:J:58:MET:HE3	1:J:70:ILE:HG21	1.96	0.47
1:F:23:ALA:C	1:F:25:ALA:H	2.21	0.47
1:B:226:LEU:HD11	1:F:222:GLN:O	2.14	0.47
1:B:6:ILE:HG23	1:B:318:ILE:HD12	1.96	0.47
1:E:190:GLN:HB3	1:E:196:ALA:HA	1.97	0.47
1:G:204:LYS:O	1:G:207:ILE:HG12	2.14	0.47
1:A:301:TYR:O	1:A:303:GLN:CB	2.63	0.47
1:D:167:ASP:OD2	2:D:401:PLP:N1	2.48	0.47
1:I:77:ALA:O	1:I:80:GLN:N	2.47	0.47
1:E:208:LEU:O	1:E:210:LYS:N	2.38	0.47
1:H:23:ALA:C	1:H:25:ALA:N	2.72	0.47
1:C:12:GLY:CA	1:C:13:PRO:C	2.88	0.47
1:E:30:ASN:O	1:E:32:TRP:N	2.47	0.47
1:B:306:ASN:O	1:B:310:GLU:N	2.44	0.47
1:B:353:GLU:O	1:B:354:GLN:C	2.58	0.46
1:E:58:MET:HE3	1:E:70:ILE:HG21	1.97	0.46
1:C:143:ILE:HD13	1:C:158:ILE:HD12	1.97	0.46
1:K:305:GLU:O	1:K:306:ASN:CB	2.64	0.46
1:C:66:GLU:HG2	1:J:52:ASN:HD22	1.79	0.46
1:C:301:TYR:C	1:C:303:GLN:CA	2.75	0.46
1:G:13:PRO:HA	1:G:190:GLN:O	2.15	0.46
1:G:129:ILE:HD13	1:G:154:ILE:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:228:ASN:O	1:L:229:SER:O	2.34	0.46
1:D:92:LYS:O	1:D:139:ASP:HB2	2.15	0.46
1:I:168:MET:O	1:I:169:SER:C	2.59	0.46
1:C:155:ARG:NH1	1:C:286:LYS:O	2.49	0.46
1:I:354:GLN:HA	1:I:354:GLN:HE21	1.80	0.46
1:B:32:TRP:CB	1:B:35:LEU:H	2.28	0.46
1:G:167:ASP:OD1	1:G:167:ASP:C	2.59	0.46
1:E:184:LEU:C	1:E:184:LEU:HD23	2.41	0.46
1:A:297:MET:CG	1:A:304:LEU:HB2	2.46	0.46
1:B:32:TRP:CB	1:B:33:GLU:C	2.89	0.45
1:C:190:GLN:HB3	1:C:196:ALA:HA	1.98	0.45
1:E:133:GLN:HA	1:E:133:GLN:OE1	2.16	0.45
1:K:128:TYR:CB	4:K:505:HOH:O	2.63	0.45
1:C:13:PRO:HA	1:C:190:GLN:O	2.17	0.45
1:F:57:LEU:O	1:F:58:MET:C	2.60	0.45
1:J:236:VAL:O	4:J:401:HOH:O	2.21	0.45
1:L:218:ILE:HD12	1:L:218:ILE:O	2.16	0.45
1:A:275:ARG:HH11	1:A:275:ARG:CG	2.30	0.45
1:B:32:TRP:CB	1:B:35:LEU:HB2	2.47	0.45
1:A:342:VAL:O	1:A:346:ILE:HG13	2.17	0.45
1:B:189:ALA:HA	1:B:193:CYS:HB2	1.98	0.45
1:E:292:ASN:ND2	1:E:332:SER:OG	2.49	0.45
1:B:146:ASN:HB2	1:B:171:ASP:OD2	2.17	0.45
1:B:306:ASN:HD21	1:E:136:SER:H	1.64	0.45
1:D:168:MET:O	1:D:169:SER:C	2.60	0.45
1:E:235:PRO:O	1:E:236:VAL:C	2.60	0.45
1:B:302:LYS:N	1:B:303:GLN:CA	2.74	0.45
1:D:6:ILE:HG23	1:D:318:ILE:HD12	1.99	0.45
1:D:189:ALA:HA	1:D:193:CYS:HB2	1.99	0.45
1:I:27:ALA:N	4:I:501:HOH:O	2.45	0.45
1:A:302:LYS:N	1:A:303:GLN:CA	2.73	0.44
1:B:297:MET:CG	1:B:304:LEU:HB2	2.44	0.44
1:E:167:ASP:OD2	2:E:401:PLP:N1	2.50	0.44
1:B:30:ASN:O	1:B:31:PHE:C	2.60	0.44
1:B:32:TRP:CB	1:B:33:GLU:CA	2.94	0.44
1:C:167:ASP:OD1	1:C:167:ASP:C	2.60	0.44
1:C:167:ASP:OD2	2:C:401:PLP:N1	2.51	0.44
1:D:227:ASN:O	1:D:228:ASN:C	2.60	0.44
1:B:305:GLU:C	1:B:307:GLU:N	2.73	0.44
1:C:6:ILE:HG23	1:C:318:ILE:HD12	1.99	0.44
1:C:306:ASN:O	1:C:307:GLU:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:PHE:N	1:F:295:PHE:HA	2.11	0.44
1:J:58:MET:HE3	1:J:70:ILE:CG2	2.47	0.44
1:B:32:TRP:N	1:B:33:GLU:HA	2.32	0.44
1:B:275:ARG:HH11	1:B:275:ARG:CG	2.30	0.44
1:B:135:PRO:HG2	1:B:138:TYR:CD2	2.53	0.44
1:H:191:LYS:CE	2:H:401:PLP:O4A	2.65	0.44
1:A:78:SER:OG	2:A:401:PLP:O2P	2.27	0.44
1:B:208:LEU:O	1:B:210:LYS:N	2.45	0.44
1:D:218:ILE:O	1:D:218:ILE:HD12	2.17	0.44
1:F:32:TRP:CB	1:F:35:LEU:HB2	2.48	0.44
1:B:129:ILE:HD13	1:B:154:ILE:HG13	1.98	0.44
1:C:275:ARG:HH11	1:C:275:ARG:HG2	1.82	0.44
1:C:280:ARG:HD2	1:C:281:GLY:O	2.16	0.44
1:G:228:ASN:C	1:G:229:SER:O	2.60	0.44
1:L:178:ASP:O	1:L:180:SER:N	2.51	0.44
1:A:76:GLY:HA2	1:A:199:THR:OG1	2.17	0.44
1:A:304:LEU:O	1:A:305:GLU:C	2.60	0.44
1:F:294:CYS:HB3	1:F:329:PHE:O	2.18	0.44
1:B:26:LYS:HG3	1:B:30:ASN:HA	2.00	0.44
1:A:135:PRO:HG2	1:A:138:TYR:CD2	2.52	0.43
1:B:299:GLU:OE2	1:B:300:GLN:HB2	2.17	0.43
1:C:32:TRP:N	1:C:33:GLU:HA	2.33	0.43
1:F:167:ASP:OD2	2:F:401:PLP:N1	2.50	0.43
1:A:307:GLU:HG3	1:A:352:PHE:CZ	2.51	0.43
1:D:342:VAL:O	1:D:346:ILE:HG13	2.18	0.43
1:H:350:HIS:CB	4:H:516:HOH:O	2.66	0.43
1:I:342:VAL:O	1:I:346:ILE:HG13	2.18	0.43
1:F:129:ILE:HD13	1:F:154:ILE:HG13	2.01	0.43
1:G:23:ALA:O	1:G:26:LYS:HD3	2.18	0.43
1:A:212:GLN:HG3	1:A:213:ARG:HE	1.82	0.43
1:D:95:TYR:CE2	1:D:142:HIS:CG	3.07	0.43
1:A:178:ASP:OD2	1:A:181:LYS:HE2	2.17	0.43
1:A:306:ASN:OD1	1:A:310:GLU:CD	2.61	0.43
1:B:352:PHE:O	1:B:354:GLN:HA	2.19	0.43
1:C:283:VAL:HG23	1:C:288:ARG:HG2	1.99	0.43
1:B:354:GLN:O	1:B:354:GLN:CG	2.64	0.43
1:C:235:PRO:O	1:C:236:VAL:C	2.62	0.43
1:C:308:PHE:HB3	1:C:329:PHE:CZ	2.53	0.43
1:A:184:LEU:HD23	1:A:184:LEU:C	2.43	0.43
1:E:168:MET:O	1:E:169:SER:C	2.62	0.43
1:G:32:TRP:N	1:G:33:GLU:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ALA:O	1:B:80:GLN:N	2.52	0.43
1:C:301:TYR:O	1:C:303:GLN:CA	2.67	0.43
1:D:228:ASN:O	1:D:228:ASN:CG	2.62	0.43
1:D:354:GLN:NE2	1:D:354:GLN:HA	2.33	0.43
1:A:171:ASP:C	1:A:171:ASP:OD1	2.61	0.43
1:C:92:LYS:HB3	1:C:138:TYR:CD1	2.54	0.43
1:C:129:ILE:HD13	1:C:154:ILE:HG13	2.01	0.43
1:D:167:ASP:C	1:D:167:ASP:OD1	2.61	0.43
1:D:333:ILE:HG13	1:D:333:ILE:O	2.19	0.43
1:H:306:ASN:O	1:H:310:GLU:N	2.47	0.43
1:I:22:GLU:O	1:I:23:ALA:C	2.62	0.43
1:A:318:ILE:HG22	1:A:319:GLY:N	2.33	0.43
1:B:235:PRO:O	1:B:236:VAL:C	2.61	0.43
1:E:129:ILE:HD13	1:E:154:ILE:HG13	2.01	0.43
1:G:95:TYR:CD2	1:G:142:HIS:HB3	2.54	0.43
1:I:24:THR:HG22	4:I:501:HOH:O	2.18	0.43
1:I:208:LEU:O	1:I:210:LYS:N	2.46	0.43
1:A:235:PRO:O	1:A:236:VAL:C	2.61	0.42
1:J:189:ALA:HA	1:J:193:CYS:HB2	2.00	0.42
1:C:299:GLU:HA	1:C:300:GLN:HA	1.58	0.42
1:E:228:ASN:O	1:E:228:ASN:OD1	2.35	0.42
1:B:95:TYR:CE2	1:B:142:HIS:CG	3.07	0.42
1:B:297:MET:CG	1:B:304:LEU:CA	2.97	0.42
1:B:299:GLU:N	1:B:300:GLN:HA	2.30	0.42
1:E:327:GLY:O	1:E:328:GLY:C	2.63	0.42
1:K:167:ASP:OD2	2:K:401:PLP:N1	2.52	0.42
1:A:89:LEU:C	1:A:89:LEU:HD23	2.44	0.42
1:E:305:GLU:O	1:E:308:PHE:N	2.51	0.42
1:C:297:MET:HG3	1:C:304:LEU:CA	2.49	0.42
1:G:284:ARG:O	1:G:285:LYS:C	2.62	0.42
1:E:77:ALA:O	1:E:80:GLN:N	2.52	0.42
1:F:184:LEU:C	1:F:184:LEU:CD2	2.92	0.42
1:F:228:ASN:O	1:F:228:ASN:OD1	2.38	0.42
1:D:168:MET:CE	1:D:182:TYR:CE1	3.03	0.42
1:D:220:ASP:O	1:D:221:TYR:C	2.63	0.42
1:D:327:GLY:O	1:D:328:GLY:C	2.63	0.42
1:E:171:ASP:OD1	1:E:171:ASP:C	2.63	0.42
1:A:23:ALA:O	1:A:25:ALA:N	2.51	0.42
1:B:305:GLU:HG3	1:E:137:ASP:OD2	2.20	0.42
1:C:189:ALA:HA	1:C:193:CYS:HB2	2.00	0.42
1:G:12:GLY:HA2	1:G:13:PRO:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:ASP:OD2	1:G:124:LYS:HE3	2.19	0.42
1:J:13:PRO:HA	1:J:190:GLN:O	2.19	0.42
1:A:299:GLU:HA	1:A:300:GLN:HB2	2.02	0.41
1:D:320:ILE:HA	1:D:330:ARG:O	2.20	0.41
1:A:76:GLY:CA	1:A:199:THR:OG1	2.69	0.41
1:A:324:ARG:HD3	1:F:210:LYS:O	2.20	0.41
1:B:146:ASN:HD22	1:B:170:SER:HB3	1.84	0.41
1:C:211:VAL:HG11	1:C:215:ILE:HD11	2.02	0.41
1:C:297:MET:HG3	1:C:304:LEU:H	1.86	0.41
1:I:32:TRP:N	1:I:33:GLU:HA	2.35	0.41
1:C:238:SER:O	1:C:239:ILE:C	2.61	0.41
1:B:237:ILE:HG23	1:B:238:SER:N	2.36	0.41
1:H:31:PHE:C	1:H:32:TRP:O	2.39	0.41
1:J:137:ASP:CB	4:J:407:HOH:O	2.67	0.41
1:A:305:GLU:C	1:A:307:GLU:N	2.77	0.41
1:B:171:ASP:OD1	1:B:171:ASP:C	2.64	0.41
1:C:90:ASN:HB3	1:C:139:ASP:OD2	2.20	0.41
1:F:189:ALA:HA	1:F:193:CYS:HB2	2.01	0.41
1:C:69:GLU:CG	1:C:205:LYS:HD3	2.50	0.41
1:D:12:GLY:HA2	1:D:13:PRO:C	2.45	0.41
1:K:324:ARG:N	4:K:501:HOH:O	2.53	0.41
1:F:12:GLY:HA2	1:F:13:PRO:C	2.46	0.41
1:K:208:LEU:O	1:K:210:LYS:N	2.50	0.41
2:A:401:PLP:O1P	1:B:233:THR:OG1	2.36	0.41
1:I:24:THR:C	4:I:501:HOH:O	2.64	0.41
1:E:58:MET:HE3	1:E:70:ILE:CG2	2.51	0.41
1:C:227:ASN:O	1:C:228:ASN:C	2.63	0.41
1:D:23:ALA:C	1:D:25:ALA:N	2.79	0.41
1:E:108:GLU:OE2	1:E:108:GLU:HA	2.21	0.41
1:E:210:LYS:O	1:E:210:LYS:HG2	2.18	0.41
1:B:167:ASP:OD2	2:B:401:PLP:N1	2.54	0.40
1:B:168:MET:O	1:B:169:SER:C	2.64	0.40
1:A:143:ILE:HD13	1:A:158:ILE:HD12	2.03	0.40
1:B:306:ASN:HD21	1:E:136:SER:N	2.20	0.40
1:B:318:ILE:HG22	1:B:319:GLY:N	2.36	0.40
1:D:167:ASP:HB2	1:D:186:TYR:CZ	2.56	0.40
1:C:195:ALA:HB2	1:C:241:THR:HG21	2.04	0.40
1:D:235:PRO:O	1:D:236:VAL:C	2.63	0.40
1:C:38:LEU:HB2	1:D:16:MET:SD	2.61	0.40
1:D:226:LEU:HD21	1:L:222:GLN:CB	2.51	0.40
1:F:13:PRO:HA	1:F:190:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PRO:HG2	1:B:138:TYR:HD2	1.86	0.40
1:D:89:LEU:C	1:D:89:LEU:HD23	2.46	0.40
1:G:280:ARG:HB2	1:G:298:GLU:CD	2.46	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLU:OE1	1:G:128:TYR:OH[1_455]	2.17	0.03

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	346/358 (97%)	321 (93%)	21 (6%)	4 (1%)	10	27
1	B	347/358 (97%)	319 (92%)	22 (6%)	6 (2%)	7	20
1	C	347/358 (97%)	327 (94%)	15 (4%)	5 (1%)	9	24
1	D	341/358 (95%)	318 (93%)	17 (5%)	6 (2%)	6	19
1	E	338/358 (94%)	314 (93%)	17 (5%)	7 (2%)	5	15
1	F	318/358 (89%)	301 (95%)	15 (5%)	2 (1%)	21	45
1	G	337/358 (94%)	321 (95%)	11 (3%)	5 (2%)	8	23
1	H	347/358 (97%)	322 (93%)	18 (5%)	7 (2%)	6	17
1	I	332/358 (93%)	314 (95%)	15 (4%)	3 (1%)	14	34
1	J	251/358 (70%)	237 (94%)	12 (5%)	2 (1%)	16	36
1	K	314/358 (88%)	294 (94%)	14 (4%)	6 (2%)	6	17
1	L	214/358 (60%)	201 (94%)	8 (4%)	5 (2%)	5	14
All	All	3832/4296 (89%)	3589 (94%)	185 (5%)	58 (2%)	8	23

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLU
1	B	31	PHE
1	B	32	TRP
1	B	160	SER
1	B	306	ASN
1	C	23	ALA
1	C	24	THR
1	D	24	THR
1	D	33	GLU
1	D	306	ASN
1	E	24	THR
1	E	306	ASN
1	G	230	MET
1	H	24	THR
1	I	24	THR
1	J	161	PRO
1	K	300	GLN
1	L	229	SER
1	A	24	THR
1	A	29	ASN
1	B	24	THR
1	C	299	GLU
1	D	209	GLY
1	E	209	GLY
1	G	229	SER
1	G	299	GLU
1	K	306	ASN
1	L	179	ILE
1	L	230	MET
1	C	306	ASN
1	E	31	PHE
1	G	24	THR
1	H	90	ASN
1	I	209	GLY
1	J	209	GLY
1	L	209	GLY
1	A	209	GLY
1	B	209	GLY
1	D	31	PHE
1	E	190	GLN
1	E	236	VAL
1	F	24	THR

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Mol	Chain	Res	Type
1	H	31	PHE
1	I	161	PRO
1	K	305	GLU
1	K	307	GLU
1	H	306	ASN
1	K	209	GLY
1	H	129	ILE
1	H	161	PRO
1	H	209	GLY
1	C	209	GLY
1	D	236	VAL
1	F	209	GLY
1	G	209	GLY
1	K	161	PRO
1	L	161	PRO
1	E	161	PRO

5.3.2 Protein sidechains ⓘ

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	299/310 (96%)	271 (91%)	28 (9%)	8	21
1	B	300/310 (97%)	276 (92%)	24 (8%)	11	27
1	C	286/310 (92%)	266 (93%)	20 (7%)	14	32
1	D	267/310 (86%)	247 (92%)	20 (8%)	12	29
1	E	235/310 (76%)	225 (96%)	10 (4%)	26	51
1	F	214/310 (69%)	205 (96%)	9 (4%)	26	52
1	G	242/310 (78%)	228 (94%)	14 (6%)	18	40
1	H	159/310 (51%)	153 (96%)	6 (4%)	29	54
1	I	179/310 (58%)	169 (94%)	10 (6%)	19	41
1	J	86/310 (28%)	84 (98%)	2 (2%)	44	68
1	K	67/310 (22%)	66 (98%)	1 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	66/310 (21%)	63 (96%)	3 (4%)	24	49
All	All	2400/3720 (64%)	2253 (94%)	147 (6%)	17	38

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	26	LYS
1	A	33	GLU
1	A	35	LEU
1	A	40	ILE
1	A	57	LEU
1	A	58	MET
1	A	107	LYS
1	A	133	GLN
1	A	159	GLU
1	A	170	SER
1	A	210	LYS
1	A	213	ARG
1	A	214	LYS
1	A	218	ILE
1	A	229	SER
1	A	249	ILE
1	A	272	GLU
1	A	275	ARG
1	A	277	LYS
1	A	298	GLU
1	A	304	LEU
1	A	307	GLU
1	A	313	LEU
1	A	315	LYS
1	A	326	VAL
1	A	340	GLU
1	A	354	GLN
1	B	21	ILE
1	B	26	LYS
1	B	35	LEU
1	B	40	ILE
1	B	57	LEU
1	B	92	LYS
1	B	107	LYS
1	B	133	GLN

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Mol	Chain	Res	Type
1	B	160	SER
1	B	170	SER
1	B	210	LYS
1	B	213	ARG
1	B	214	LYS
1	B	218	ILE
1	B	249	ILE
1	B	272	GLU
1	B	275	ARG
1	B	302	LYS
1	B	304	LEU
1	B	307	GLU
1	B	313	LEU
1	B	315	LYS
1	B	326	VAL
1	B	354	GLN
1	C	21	ILE
1	C	24	THR
1	C	26	LYS
1	C	35	LEU
1	C	40	ILE
1	C	92	LYS
1	C	107	LYS
1	C	133	GLN
1	C	170	SER
1	C	210	LYS
1	C	213	ARG
1	C	214	LYS
1	C	218	ILE
1	C	249	ILE
1	C	272	GLU
1	C	275	ARG
1	C	313	LEU
1	C	315	LYS
1	C	326	VAL
1	C	354	GLN
1	D	21	ILE
1	D	26	LYS
1	D	40	ILE
1	D	57	LEU
1	D	92	LYS
1	D	107	LYS

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Mol	Chain	Res	Type
1	D	170	SER
1	D	210	LYS
1	D	213	ARG
1	D	214	LYS
1	D	218	ILE
1	D	233	THR
1	D	249	ILE
1	D	272	GLU
1	D	296	VAL
1	D	313	LEU
1	D	315	LYS
1	D	326	VAL
1	D	340	GLU
1	D	354	GLN
1	E	21	ILE
1	E	26	LYS
1	E	35	LEU
1	E	40	ILE
1	E	57	LEU
1	E	107	LYS
1	E	210	LYS
1	E	218	ILE
1	E	229	SER
1	E	249	ILE
1	F	21	ILE
1	F	35	LEU
1	F	40	ILE
1	F	107	LYS
1	F	133	GLN
1	F	210	LYS
1	F	218	ILE
1	F	229	SER
1	F	249	ILE
1	G	21	ILE
1	G	26	LYS
1	G	57	LEU
1	G	107	LYS
1	G	120	THR
1	G	133	GLN
1	G	170	SER
1	G	218	ILE
1	G	229	SER

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Mol	Chain	Res	Type
1	G	233	THR
1	G	249	ILE
1	G	298	GLU
1	G	326	VAL
1	G	354	GLN
1	H	21	ILE
1	H	40	ILE
1	H	218	ILE
1	H	249	ILE
1	H	313	LEU
1	H	340	GLU
1	I	21	ILE
1	I	24	THR
1	I	35	LEU
1	I	40	ILE
1	I	107	LYS
1	I	218	ILE
1	I	229	SER
1	I	272	GLU
1	I	326	VAL
1	I	354	GLN
1	J	40	ILE
1	J	218	ILE
1	K	218	ILE
1	L	40	ILE
1	L	218	ILE
1	L	229	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	52	ASN
1	A	111	ASN
1	A	243	ASN
1	A	303	GLN
1	A	314	GLN
1	A	350	HIS
1	A	354	GLN
1	B	243	ASN
1	B	303	GLN
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	350	HIS
1	B	354	GLN
1	C	52	ASN
1	C	259	GLN
1	C	343	GLN
1	C	354	GLN
1	D	52	ASN
1	D	243	ASN
1	D	314	GLN
1	D	354	GLN
1	E	52	ASN
1	E	292	ASN
1	F	52	ASN
1	F	243	ASN
1	F	259	GLN
1	G	52	ASN
1	G	354	GLN
1	H	52	ASN
1	H	80	GLN
1	I	52	ASN
1	I	111	ASN
1	I	354	GLN
1	J	52	ASN
1	K	350	HIS
1	L	52	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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
2	PLP	E	401	-	16,16,16	2.58	3 (18%)	20,23,23	2.37	8 (40%)
2	PLP	I	401	-	16,16,16	2.79	3 (18%)	20,23,23	2.02	5 (25%)
2	PLP	G	401	-	16,16,16	2.31	3 (18%)	20,23,23	1.92	5 (25%)
2	PLP	A	401	-	16,16,16	2.28	3 (18%)	20,23,23	1.78	7 (35%)
2	PLP	F	401	-	16,16,16	2.48	3 (18%)	20,23,23	2.06	6 (30%)
2	PLP	B	401	-	16,16,16	2.58	3 (18%)	20,23,23	2.22	5 (25%)
2	PLP	D	401	-	16,16,16	2.40	3 (18%)	20,23,23	1.98	5 (25%)
2	PLP	K	401	-	16,16,16	2.53	3 (18%)	20,23,23	1.86	5 (25%)
2	PLP	H	401	-	16,16,16	2.45	4 (25%)	20,23,23	2.41	7 (35%)
2	PLP	C	401	-	16,16,16	2.55	3 (18%)	20,23,23	1.61	6 (30%)

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
2	PLP	E	401	-	-	0/8/8/8	0/1/1/1
2	PLP	I	401	-	-	0/8/8/8	0/1/1/1
2	PLP	G	401	-	-	0/8/8/8	0/1/1/1
2	PLP	A	401	-	-	3/8/8/8	0/1/1/1
2	PLP	F	401	-	-	3/8/8/8	0/1/1/1
2	PLP	B	401	-	-	0/8/8/8	0/1/1/1
2	PLP	D	401	-	-	0/8/8/8	0/1/1/1
2	PLP	K	401	-	-	0/8/8/8	0/1/1/1
2	PLP	H	401	-	-	1/8/8/8	0/1/1/1
2	PLP	C	401	-	-	0/8/8/8	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	PLP	C3-C2	8.75	1.50	1.41
2	B	401	PLP	C3-C2	7.86	1.49	1.41
2	K	401	PLP	C3-C2	7.54	1.48	1.41
2	C	401	PLP	C3-C2	7.53	1.48	1.41
2	D	401	PLP	C3-C2	7.07	1.48	1.41
2	E	401	PLP	C3-C2	6.66	1.47	1.41
2	F	401	PLP	C3-C2	6.43	1.47	1.41
2	G	401	PLP	C3-C2	6.23	1.47	1.41
2	E	401	PLP	C4-C3	6.08	1.51	1.41
2	F	401	PLP	C4-C3	5.90	1.50	1.41
2	A	401	PLP	C3-C2	5.86	1.47	1.41
2	H	401	PLP	C3-C2	5.85	1.47	1.41
2	H	401	PLP	C4-C3	5.56	1.50	1.41
2	C	401	PLP	C4-C3	5.34	1.49	1.41
2	A	401	PLP	C4-C3	5.16	1.49	1.41
2	B	401	PLP	C4-C3	4.98	1.49	1.41
2	H	401	PLP	C4-C5	4.87	1.48	1.42
2	I	401	PLP	C4-C5	4.61	1.48	1.42
2	E	401	PLP	C4-C5	4.48	1.48	1.42
2	G	401	PLP	C4-C3	4.47	1.48	1.41
2	K	401	PLP	C4-C3	4.46	1.48	1.41
2	G	401	PLP	C4-C5	4.43	1.48	1.42
2	D	401	PLP	C4-C3	4.40	1.48	1.41
2	K	401	PLP	C4-C5	4.37	1.48	1.42
2	D	401	PLP	C4-C5	4.28	1.47	1.42
2	F	401	PLP	C4-C5	4.22	1.47	1.42
2	I	401	PLP	C4-C3	4.17	1.48	1.41
2	B	401	PLP	C4-C5	3.99	1.47	1.42
2	A	401	PLP	C4-C5	3.90	1.47	1.42
2	C	401	PLP	C4-C5	3.74	1.47	1.42
2	H	401	PLP	C4-C4A	2.07	1.51	1.46

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	PLP	C3-C4-C4A	6.67	129.01	119.84
2	E	401	PLP	C4-C3-C2	-6.51	116.48	120.14
2	B	401	PLP	C4-C3-C2	-6.47	116.50	120.14
2	D	401	PLP	C4-C3-C2	-6.25	116.62	120.14
2	I	401	PLP	C4-C3-C2	-5.39	117.11	120.14
2	F	401	PLP	C4-C3-C2	-4.92	117.38	120.14
2	H	401	PLP	C3-C4-C5	-4.74	114.47	118.28
2	G	401	PLP	C4-C3-C2	-4.59	117.56	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	PLP	O4P-C5A-C5	4.25	117.31	109.36
2	E	401	PLP	O4P-C5A-C5	4.23	117.29	109.36
2	I	401	PLP	O3-C3-C2	3.60	125.05	117.58
2	C	401	PLP	C4-C3-C2	-3.58	118.12	120.14
2	K	401	PLP	C4-C3-C2	-3.58	118.13	120.14
2	B	401	PLP	O3P-P-O4P	-3.51	97.52	106.67
2	E	401	PLP	C3-C4-C4A	3.47	124.61	119.84
2	G	401	PLP	O3P-P-O4P	-3.43	97.72	106.67
2	A	401	PLP	C6-N1-C2	3.38	125.34	119.20
2	F	401	PLP	O4P-C5A-C5	3.37	115.68	109.36
2	H	401	PLP	C4-C3-C2	-3.22	118.33	120.14
2	C	401	PLP	C3-C4-C4A	3.17	124.19	119.84
2	I	401	PLP	O3P-P-O2P	3.08	119.33	107.80
2	I	401	PLP	O4A-C4A-C4	-3.05	117.57	124.80
2	A	401	PLP	C4-C3-C2	-3.03	118.44	120.14
2	B	401	PLP	C3-C4-C4A	2.99	123.96	119.84
2	E	401	PLP	C6-N1-C2	2.99	124.62	119.20
2	D	401	PLP	O4A-C4A-C4	-2.93	117.86	124.80
2	F	401	PLP	O4A-C4A-C4	-2.86	118.02	124.80
2	F	401	PLP	C6-N1-C2	2.84	124.36	119.20
2	D	401	PLP	C6-N1-C2	2.83	124.33	119.20
2	G	401	PLP	O3P-P-O2P	2.82	118.37	107.80
2	E	401	PLP	O3P-P-O4P	-2.81	99.35	106.67
2	H	401	PLP	O3-C3-C4	2.79	126.96	119.44
2	B	401	PLP	C6-N1-C2	2.73	124.14	119.20
2	K	401	PLP	C3-C4-C5	-2.64	116.16	118.28
2	K	401	PLP	C6-N1-C2	2.57	123.86	119.20
2	C	401	PLP	O3P-P-O4P	-2.51	100.13	106.67
2	G	401	PLP	C6-N1-C2	2.44	123.62	119.20
2	D	401	PLP	O3P-P-O1P	2.37	120.09	110.83
2	F	401	PLP	O2P-P-O4P	-2.37	100.48	106.67
2	A	401	PLP	C2A-C2-N1	2.36	122.08	117.64
2	H	401	PLP	O3P-P-O2P	2.35	116.62	107.80
2	C	401	PLP	C3-C4-C5	-2.35	116.39	118.28
2	G	401	PLP	O4A-C4A-C4	-2.35	119.23	124.80
2	B	401	PLP	O4A-C4A-C4	-2.33	119.27	124.80
2	E	401	PLP	O3-C3-C4	2.33	125.71	119.44
2	A	401	PLP	O4A-C4A-C4	-2.33	119.29	124.80
2	I	401	PLP	C6-N1-C2	2.25	123.28	119.20
2	H	401	PLP	C6-N1-C2	2.24	123.26	119.20
2	K	401	PLP	O3P-P-O2P	2.24	116.19	107.80
2	E	401	PLP	O4A-C4A-C4	-2.24	119.50	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C3-C2-N1	-2.21	118.17	120.96
2	A	401	PLP	C3-C4-C4A	2.18	122.84	119.84
2	F	401	PLP	C3-C4-C4A	2.15	122.81	119.84
2	A	401	PLP	O3P-P-O2P	2.15	115.87	107.80
2	E	401	PLP	O3P-P-O2P	2.06	115.53	107.80
2	C	401	PLP	O3P-P-O2P	2.05	115.47	107.80
2	C	401	PLP	C6-N1-C2	2.02	122.87	119.20
2	D	401	PLP	O3-C3-C2	2.02	121.77	117.58
2	H	401	PLP	O4P-C5A-C5	2.00	113.11	109.36

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PLP	C5A-O4P-P-O2P
2	A	401	PLP	C5A-O4P-P-O3P
2	F	401	PLP	C4-C5-C5A-O4P
2	F	401	PLP	C6-C5-C5A-O4P
2	A	401	PLP	C5A-O4P-P-O1P
2	F	401	PLP	C5A-O4P-P-O3P
2	H	401	PLP	C5A-O4P-P-O1P

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	PLP	3	0
2	G	401	PLP	1	0
2	A	401	PLP	9	0
2	F	401	PLP	6	0
2	B	401	PLP	4	0
2	D	401	PLP	3	0
2	K	401	PLP	1	0
2	H	401	PLP	4	0
2	C	401	PLP	3	0

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 [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, 95th 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	A	348/358 (97%)	-1.18	0	100	100	36, 60, 97, 137	0
1	B	349/358 (97%)	-1.11	0	100	100	37, 66, 111, 163	0
1	C	349/358 (97%)	-1.14	0	100	100	35, 68, 102, 127	0
1	D	345/358 (96%)	-0.97	0	100	100	42, 86, 125, 153	0
1	E	342/358 (95%)	-1.05	0	100	100	45, 75, 115, 131	0
1	F	322/358 (89%)	-1.09	1 (0%)	90	88	43, 78, 121, 146	0
1	G	341/358 (95%)	-0.91	0	100	100	48, 90, 125, 155	0
1	H	349/358 (97%)	-0.88	0	100	100	62, 100, 136, 160	0
1	I	336/358 (93%)	-0.84	0	100	100	55, 94, 137, 156	0
1	J	253/358 (70%)	-0.72	0	100	100	61, 100, 158, 199	0
1	K	316/358 (88%)	-0.84	0	100	100	68, 104, 143, 163	0
1	L	216/358 (60%)	-0.82	0	100	100	58, 107, 146, 165	0
All	All	3866/4296 (89%)	-0.97	1 (0%)	100	100	35, 85, 133, 199	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	295	PHE	2.2

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 oligosaccharides in this entry.

6.4 Ligands

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, 95th 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
3	CL	A	402	1/1	0.98	0.05	74,74,74,74	0
2	PLP	B	401	16/16	0.99	0.05	49,64,70,75	0
2	PLP	C	401	16/16	0.99	0.04	61,69,76,79	0
2	PLP	D	401	16/16	0.99	0.05	57,86,93,95	0
2	PLP	E	401	16/16	0.99	0.05	64,71,78,79	0
2	PLP	F	401	16/16	0.99	0.05	64,71,74,75	0
2	PLP	G	401	16/16	0.99	0.05	69,86,89,91	0
2	PLP	H	401	16/16	0.99	0.06	75,85,94,97	0
2	PLP	I	401	16/16	0.99	0.04	75,89,94,97	0
2	PLP	K	401	16/16	0.99	0.04	62,70,73,74	0
2	PLP	A	401	16/16	0.99	0.04	56,75,92,101	0
3	CL	B	402	1/1	0.99	0.03	67,67,67,67	0
3	CL	C	402	1/1	0.99	0.09	81,81,81,81	0
3	CL	D	402	1/1	0.99	0.05	78,78,78,78	0
3	CL	E	402	1/1	0.99	0.03	92,92,92,92	0

6.5 Other polymers

There are no such residues in this entry.