



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:09 AM GMT

PDB ID : 2ZP7  
Title : Crystal structure of LysN, alpha-aminoadipate aminotransferase (Leucine complex), from *Thermus thermophilus* HB27  
Authors : Tomita, T.; Miyazaki, T.; Miyagawa, T.; Fushinobu, S.; Kuzuyama, T.; Nishiyama, M.  
Deposited on : 2008-06-30  
Resolution : 2.26 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

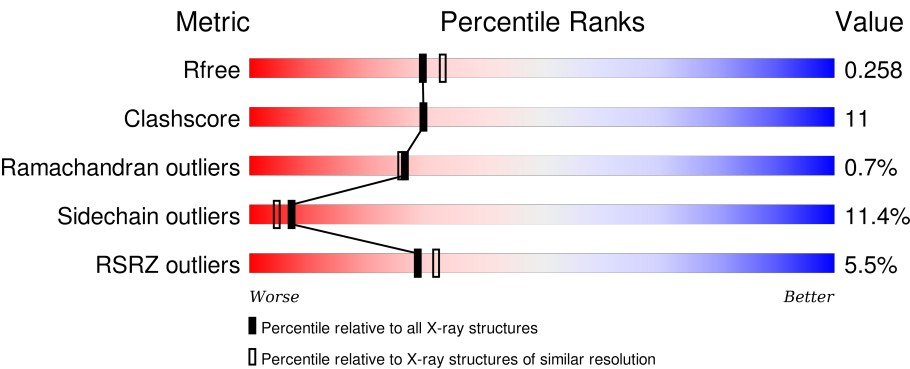
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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 <sub>free</sub>	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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	397	<div><div>4%</div><div>71%24%</div><div></div></div>
1	B	397	<div><div>4%</div><div>74%20%</div><div></div></div>
1	C	397	<div><div>6%</div><div>71%24%</div><div></div></div>
1	D	397	<div><div>6%</div><div>73%22%</div><div></div></div>
1	E	397	<div><div>8%</div><div>72%23%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	397	

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	D	600	-	-	X	-
3	LEU	B	700	-	-	-	X

## 2 Entry composition [i](#)

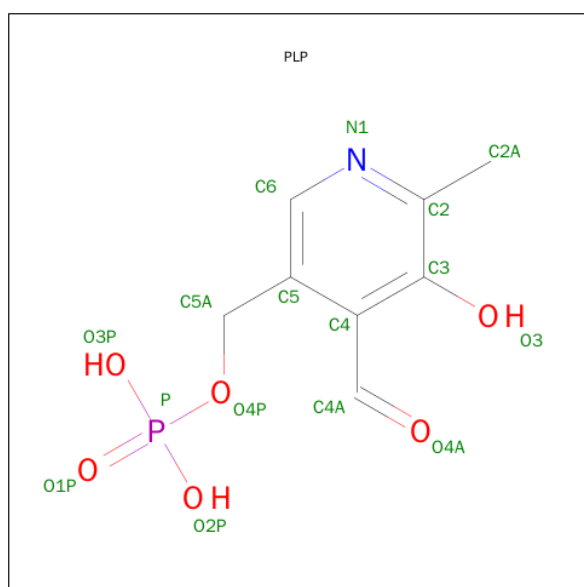
There are 4 unique types of molecules in this entry. The entry contains 18870 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-aminodipate aminotransferase.

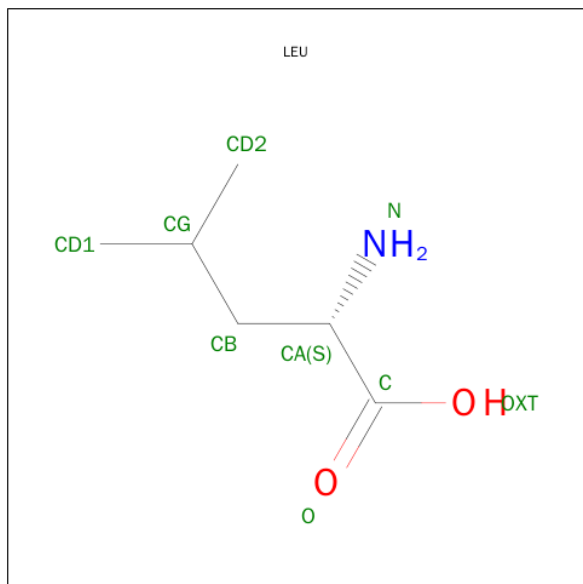
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3033	1946	535	544	8			
1	B	391	Total	C	N	O	S	0	0	0
			3033	1946	535	544	8			
1	C	391	Total	C	N	O	S	0	0	0
			3033	1946	535	544	8			
1	D	391	Total	C	N	O	S	0	0	0
			3033	1946	535	544	8			
1	E	391	Total	C	N	O	S	0	0	0
			3033	1946	535	544	8			
1	F	391	Total	C	N	O	S	0	0	0
			3033	1946	535	544	8			

- 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
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	E	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		

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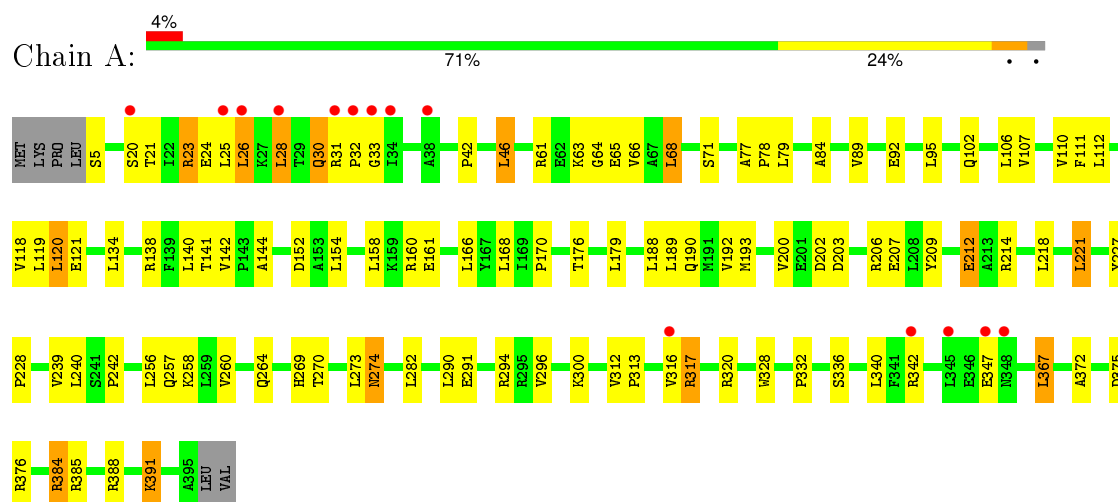
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	95	Total 95	O 95	0	0
4	C	97	Total 97	O 97	0	0
4	D	112	Total 112	O 112	0	0
4	E	76	Total 76	O 76	0	0
4	F	78	Total 78	O 78	0	0

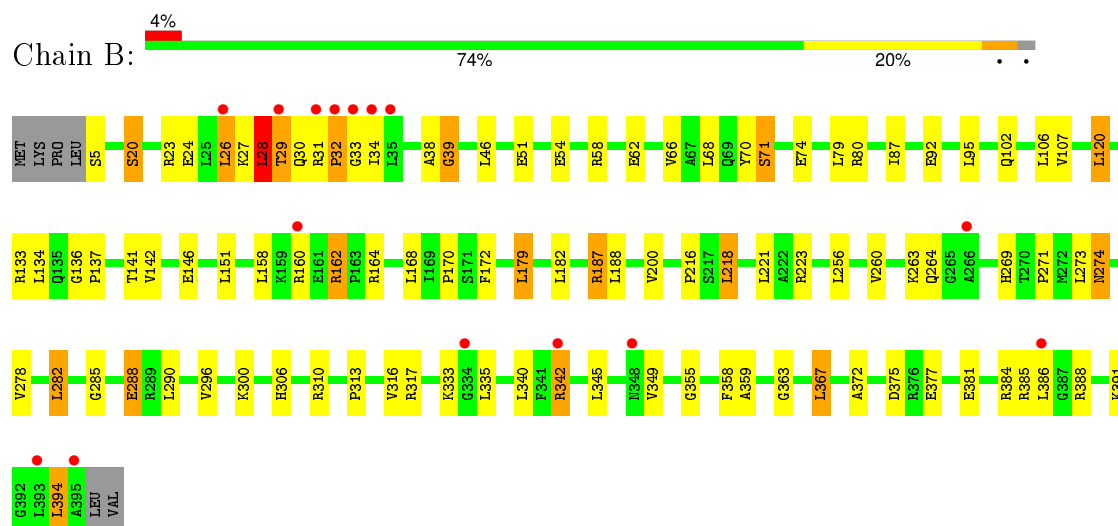
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Alpha-aminodipate aminotransferase

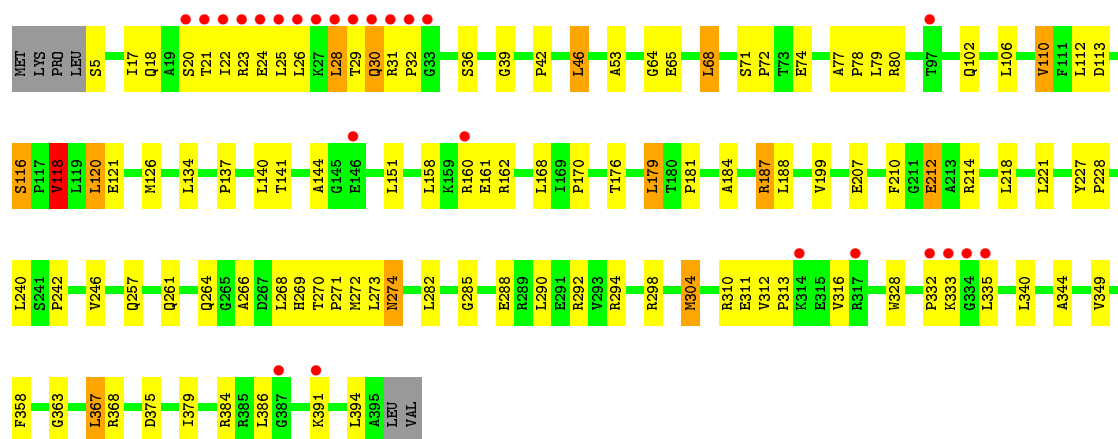


#### • Molecule 1: Alpha-aminodipate aminotransferase

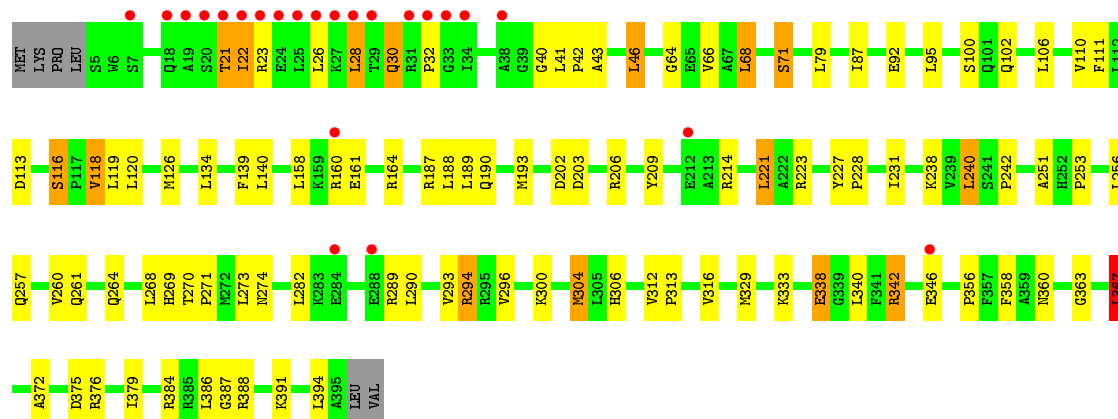


#### • Molecule 1: Alpha-aminodipate aminotransferase

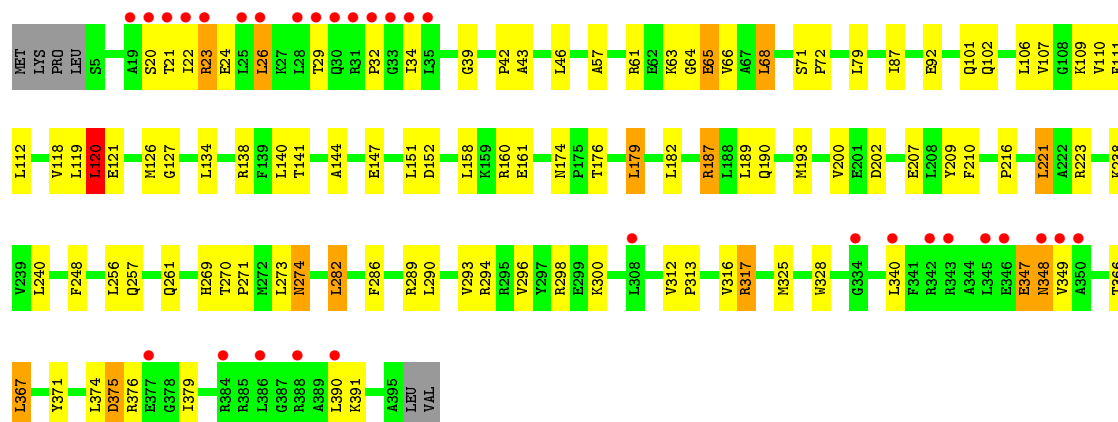




• Molecule 1: Alpha-aminodipate aminotransferase



• Molecule 1: Alpha-aminodipate aminotransferase



• Molecule 1: Alpha-aminodipate aminotransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.95Å 167.64Å 119.36Å 90.00° 97.87° 90.00°	Depositor
Resolution (Å)	41.92 – 2.26 41.91 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.1 (41.92-2.26) 99.1 (41.91-2.26)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.205 , 0.263 0.202 , 0.258	Depositor DCC
$R_{free}$ test set	5030 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 100703 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.57 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5456e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	0/3099	0.76	3/4191 (0.1%)
1	B	0.60	0/3099	0.72	1/4191 (0.0%)
1	C	0.60	0/3099	0.75	4/4191 (0.1%)
1	D	0.58	0/3099	0.72	2/4191 (0.0%)
1	E	0.59	0/3099	0.73	2/4191 (0.0%)
1	F	0.58	0/3099	0.73	2/4191 (0.0%)
All	All	0.59	0/18594	0.73	14/25146 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	367	LEU	CA-CB-CG	6.80	130.93	115.30
1	A	367	LEU	CA-CB-CG	5.81	128.67	115.30
1	E	367	LEU	CA-CB-CG	5.59	128.16	115.30
1	F	367	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	46	LEU	CA-CB-CG	5.41	127.74	115.30
1	F	118	VAL	CB-CA-C	-5.38	101.18	111.40
1	D	367	LEU	CA-CB-CG	5.37	127.65	115.30
1	E	120	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	160	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	221	LEU	CB-CG-CD1	5.16	119.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	VAL	CB-CA-C	-5.07	101.78	111.40
1	C	179	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	367	LEU	CA-CB-CG	5.01	126.83	115.30
1	D	118	VAL	CB-CA-C	-5.00	101.89	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	31	ARG	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	3033	0	3081	78	0
1	B	3033	0	3082	72	0
1	C	3033	0	3081	76	0
1	D	3033	0	3084	80	0
1	E	3033	0	3082	76	0
1	F	3033	0	3082	60	0
2	A	15	0	7	1	0
2	B	15	0	6	1	0
2	C	15	0	7	0	0
2	D	15	0	7	7	0
2	E	15	0	7	3	0
2	F	15	0	6	0	0
3	A	9	0	10	2	0
3	B	9	0	10	2	0
3	E	9	0	10	1	0
4	A	97	0	0	10	0
4	B	95	0	0	11	0
4	C	97	0	0	9	0
4	D	112	0	0	13	0
4	E	76	0	0	8	0
4	F	78	0	0	10	0
All	All	18870	0	18562	410	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 11.

All (410) 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:D:110:VAL:HB	4:D:698:HOH:O	1.12	1.27
1:E:118:VAL:HB	4:E:786:HOH:O	1.19	1.26
1:C:375:ASP:HB3	4:C:864:HOH:O	1.36	1.25
1:A:118:VAL:HB	4:A:789:HOH:O	1.45	1.11
1:A:257:GLN:HE22	1:C:23:ARG:NH1	1.51	1.08
1:B:162:ARG:HG2	1:B:162:ARG:HH21	1.15	1.06
1:D:92:GLU:HG2	4:D:674:HOH:O	1.55	1.06
1:E:66:VAL:HB	4:E:791:HOH:O	1.56	1.04
1:D:238:LYS:HZ1	2:D:600:PLP:C4A	1.44	1.03
1:E:140:LEU:HD11	1:E:161:GLU:HG2	1.45	0.98
1:F:140:LEU:HD11	1:F:161:GLU:HG2	1.44	0.97
1:A:140:LEU:HD11	1:A:161:GLU:HG2	1.48	0.95
1:D:238:LYS:HZ2	2:D:600:PLP:C4A	1.55	0.95
1:A:5:SER:CB	4:A:765:HOH:O	2.15	0.94
1:A:257:GLN:HE22	1:C:23:ARG:HH12	1.10	0.94
1:F:87:ILE:HG12	4:F:637:HOH:O	1.65	0.93
1:E:140:LEU:CD1	1:E:161:GLU:HG2	1.98	0.93
1:E:238:LYS:HZ2	2:E:600:PLP:C4A	1.76	0.92
1:A:140:LEU:CD1	1:A:161:GLU:HG2	2.00	0.92
1:B:162:ARG:CG	1:B:162:ARG:HH21	1.86	0.88
1:E:57:ALA:HB1	1:E:61:ARG:HH11	1.37	0.88
1:C:140:LEU:CD1	1:C:161:GLU:HG2	2.05	0.87
1:A:257:GLN:NE2	1:C:23:ARG:HH12	1.72	0.86
1:B:264:GLN:OE1	1:D:23:ARG:HB3	1.75	0.86
1:C:140:LEU:HD11	1:C:161:GLU:HG2	1.57	0.84
1:F:384:ARG:HH22	1:F:388:ARG:HH11	1.23	0.84
1:C:112:LEU:HD21	1:C:118:VAL:HG13	1.61	0.83
1:C:272:MET:HB2	4:C:827:HOH:O	1.80	0.82
1:E:22:ILE:HB	1:F:264:GLN:HE21	1.43	0.82
1:B:46:LEU:HD11	1:B:296:VAL:HG21	1.62	0.82
1:D:140:LEU:HD11	1:D:161:GLU:HG2	1.60	0.81
1:B:375:ASP:HB3	4:B:741:HOH:O	1.78	0.81
1:C:168:LEU:CD1	1:C:188:LEU:HD21	2.12	0.80
1:F:151:LEU:HD13	1:F:187:ARG:HG2	1.64	0.80
1:C:168:LEU:HD13	1:C:188:LEU:HD21	1.62	0.79
1:C:162:ARG:CZ	4:C:814:HOH:O	2.29	0.79
1:B:23:ARG:H	1:D:264:GLN:HE21	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:HH11	1:A:342:ARG:HG3	1.48	0.78
1:B:28:LEU:HA	1:B:30:GLN:OE1	1.83	0.78
1:A:26:LEU:HG	1:C:71:SER:O	1.83	0.78
1:D:110:VAL:HG13	1:D:111:PHE:CD2	2.20	0.77
1:D:40:GLY:HA3	4:D:711:HOH:O	1.85	0.76
2:D:600:PLP:H5A1	4:D:643:HOH:O	1.85	0.75
1:B:164:ARG:NE	4:B:783:HOH:O	2.13	0.75
1:C:23:ARG:HG3	1:C:24:GLU:H	1.52	0.75
1:F:59:ILE:HD11	1:F:280:GLU:HG3	1.67	0.75
1:A:317:ARG:HH12	1:A:332:PRO:HA	1.52	0.74
1:B:384:ARG:HH22	1:B:388:ARG:HH11	1.36	0.73
1:C:23:ARG:HG3	1:C:24:GLU:N	2.04	0.73
1:A:257:GLN:NE2	1:C:23:ARG:NH1	2.29	0.72
1:B:164:ARG:NH2	4:B:783:HOH:O	2.23	0.72
1:C:274:ASN:HD22	1:C:274:ASN:H	1.36	0.72
1:F:126:MET:SD	1:F:356:PRO:O	2.48	0.72
1:E:112:LEU:HD21	1:E:118:VAL:HG22	1.72	0.72
1:D:346:GLU:OE2	4:D:710:HOH:O	2.08	0.71
1:D:306:HIS:HD2	4:D:709:HOH:O	1.73	0.71
1:A:23:ARG:HH22	1:C:257:GLN:HE22	1.39	0.71
1:E:92:GLU:OE2	4:E:794:HOH:O	2.08	0.71
1:E:46:LEU:HD11	1:E:296:VAL:HG11	1.73	0.70
1:B:168:LEU:HD13	1:B:188:LEU:HD21	1.72	0.70
1:E:110:VAL:HG13	1:E:111:PHE:CD2	2.26	0.70
1:F:87:ILE:O	1:F:223:ARG:NH1	2.25	0.70
1:A:23:ARG:H	1:C:264:GLN:HE21	1.40	0.69
1:E:138:ARG:HH22	1:E:161:GLU:CD	1.96	0.69
1:F:384:ARG:NH2	1:F:388:ARG:HH11	1.90	0.69
1:E:112:LEU:CD2	1:E:118:VAL:HG22	2.21	0.69
1:F:87:ILE:HD11	1:F:248:PHE:CE1	2.27	0.69
1:D:253:PRO:O	1:D:257:GLN:HG2	1.93	0.69
1:E:274:ASN:H	1:E:274:ASN:HD22	1.41	0.68
1:B:28:LEU:C	1:B:30:GLN:H	1.95	0.68
1:B:274:ASN:H	1:B:274:ASN:HD22	1.42	0.68
1:D:238:LYS:HZ3	2:D:600:PLP:C4A	2.05	0.68
1:C:292:ARG:HH21	1:C:292:ARG:HG3	1.59	0.68
1:A:5:SER:HB3	4:A:765:HOH:O	1.85	0.67
1:A:274:ASN:HD22	1:A:274:ASN:H	1.42	0.67
1:E:300:LYS:HD3	1:E:371:TYR:O	1.94	0.67
1:E:190:GLN:HB3	4:E:813:HOH:O	1.93	0.67
1:E:120:LEU:O	1:E:141:THR:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ARG:NE	4:C:814:HOH:O	2.28	0.67
1:D:306:HIS:CD2	4:D:709:HOH:O	2.48	0.67
2:B:600:PLP:C4A	3:B:700:LEU:N	2.58	0.67
1:A:121:GLU:HB3	1:A:144:ALA:HB2	1.77	0.66
1:C:162:ARG:NH1	4:C:814:HOH:O	2.28	0.66
1:B:71:SER:O	1:D:26:LEU:HD12	1.96	0.66
1:F:274:ASN:HD22	1:F:274:ASN:H	1.43	0.66
1:E:300:LYS:HE3	1:E:374:LEU:O	1.96	0.65
1:E:207:GLU:O	1:E:294:ARG:HD2	1.97	0.65
1:F:28:LEU:HD21	1:F:41:LEU:HD21	1.77	0.65
1:F:172:PHE:CE1	1:F:179:LEU:HG	2.31	0.65
1:B:162:ARG:HG2	1:B:162:ARG:NH2	1.98	0.65
1:A:23:ARG:HH12	1:C:257:GLN:NE2	1.93	0.65
1:A:189:LEU:O	1:A:193:MET:HG3	1.96	0.65
1:C:188:LEU:HB2	4:C:841:HOH:O	1.97	0.65
1:D:304:MET:CE	1:D:379:ILE:HG23	2.27	0.64
1:B:146:GLU:OE2	4:B:757:HOH:O	2.14	0.64
1:F:207:GLU:O	1:F:294:ARG:HD3	1.97	0.64
1:D:113:ASP:O	1:D:116:SER:HB2	1.98	0.64
1:F:384:ARG:HH22	1:F:388:ARG:NH1	1.96	0.64
1:B:26:LEU:HG	1:D:71:SER:O	1.97	0.64
1:E:271:PRO:HB2	1:E:274:ASN:ND2	2.13	0.64
1:B:264:GLN:HE21	1:D:22:ILE:HD13	1.62	0.63
1:B:384:ARG:NH2	1:B:388:ARG:HH11	1.97	0.62
1:F:346:GLU:HG2	4:F:630:HOH:O	1.98	0.62
1:D:338:GLU:HG3	4:D:668:HOH:O	2.00	0.62
1:A:106:LEU:O	1:A:110:VAL:HG12	2.00	0.62
1:C:140:LEU:HD13	1:C:161:GLU:HG2	1.81	0.62
1:F:187:ARG:O	1:F:190:GLN:HB2	1.99	0.62
1:D:164:ARG:NE	4:D:667:HOH:O	2.22	0.62
1:E:257:GLN:HG2	4:E:785:HOH:O	1.99	0.62
1:D:274:ASN:H	1:D:274:ASN:HD22	1.47	0.62
1:B:27:LYS:C	1:B:29:THR:H	2.04	0.61
1:B:23:ARG:HH22	1:D:257:GLN:HE22	1.47	0.61
1:D:46:LEU:HD11	1:D:296:VAL:HG21	1.81	0.61
1:B:92:GLU:HG2	4:B:735:HOH:O	1.99	0.61
1:F:140:LEU:CD1	1:F:161:GLU:HG2	2.24	0.60
1:A:25:LEU:O	1:A:28:LEU:HB3	2.01	0.60
1:D:187:ARG:HH11	1:D:187:ARG:HG3	1.67	0.60
1:F:24:GLU:HG2	4:F:638:HOH:O	2.01	0.60
1:B:172:PHE:CE1	1:B:179:LEU:HG	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ASP:O	1:C:116:SER:HB2	2.02	0.60
1:F:112:LEU:HD21	1:F:118:VAL:HG13	1.82	0.60
1:B:162:ARG:CG	1:B:162:ARG:NH2	2.54	0.60
1:A:152:ASP:HB3	1:B:306:HIS:HE1	1.65	0.60
1:A:375:ASP:CG	1:A:376:ARG:H	2.04	0.60
1:E:57:ALA:HB1	1:E:61:ARG:NH1	2.13	0.60
1:A:138:ARG:NH2	1:A:161:GLU:OE2	2.34	0.60
1:D:384:ARG:HH22	1:D:388:ARG:HD3	1.67	0.60
1:E:121:GLU:HB3	1:E:144:ALA:HB2	1.84	0.59
1:C:304:MET:HE3	1:C:379:ILE:HG23	1.83	0.59
1:A:257:GLN:HG2	4:A:781:HOH:O	2.03	0.59
1:B:23:ARG:HH22	1:D:257:GLN:NE2	2.00	0.59
1:F:17:ILE:O	1:F:19:ALA:N	2.35	0.59
1:F:21:THR:HG21	1:F:126:MET:HG2	1.84	0.59
1:A:375:ASP:HB3	4:A:733:HOH:O	2.02	0.59
1:A:140:LEU:HD13	1:A:161:GLU:HG2	1.80	0.58
1:B:271:PRO:HB2	1:B:274:ASN:ND2	2.17	0.58
1:E:317:ARG:HB2	1:E:317:ARG:HH21	1.68	0.58
1:C:304:MET:CE	1:C:379:ILE:HG23	2.33	0.58
1:A:42:PRO:HG2	1:A:242:PRO:HG3	1.86	0.58
1:E:151:LEU:HD13	1:E:187:ARG:HG2	1.85	0.58
1:B:20:SER:HA	1:D:264:GLN:HE22	1.69	0.57
1:B:23:ARG:HH12	1:D:257:GLN:HE21	1.50	0.57
1:A:92:GLU:HG2	4:A:737:HOH:O	2.03	0.57
1:A:112:LEU:HD22	1:A:118:VAL:HG22	1.87	0.57
1:E:22:ILE:HB	1:F:264:GLN:NE2	2.18	0.57
1:B:87:ILE:O	1:B:223:ARG:NH1	2.37	0.57
1:B:384:ARG:HH22	1:B:388:ARG:NH1	2.01	0.57
1:D:342:ARG:HH11	1:D:342:ARG:HG2	1.69	0.57
1:E:140:LEU:HD11	1:E:161:GLU:CG	2.29	0.57
1:A:112:LEU:CD2	1:A:118:VAL:HG22	2.34	0.57
1:F:120:LEU:O	1:F:141:THR:HA	2.05	0.57
1:D:304:MET:HE3	1:D:379:ILE:HG23	1.87	0.56
1:D:28:LEU:HD11	1:D:41:LEU:HD13	1.87	0.56
1:C:269:HIS:HD2	1:C:270:THR:O	1.88	0.56
1:A:257:GLN:HE22	1:C:23:ARG:CZ	2.16	0.56
1:A:23:ARG:HH12	1:C:257:GLN:HE21	1.52	0.56
1:C:65:GLU:CD	1:C:65:GLU:H	2.08	0.56
1:D:342:ARG:CG	1:D:342:ARG:HH11	2.20	0.55
1:B:300:LYS:HE2	1:B:372:ALA:O	2.07	0.55
1:E:274:ASN:ND2	1:E:274:ASN:H	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:HA	1:C:30:GLN:OE1	2.07	0.55
1:D:257:GLN:O	1:D:261:GLN:HG3	2.06	0.55
1:C:274:ASN:N	1:C:274:ASN:HD22	2.02	0.55
1:A:110:VAL:HG13	1:A:111:PHE:CD2	2.41	0.55
1:E:20:SER:HB3	1:E:23:ARG:HG2	1.88	0.55
1:E:106:LEU:O	1:E:110:VAL:HG12	2.08	0.54
1:F:306:HIS:HD2	4:F:657:HOH:O	1.90	0.54
1:B:264:GLN:NE2	1:D:22:ILE:HD13	2.23	0.54
3:A:700:LEU:HD22	1:C:268:LEU:HD13	1.89	0.54
1:E:140:LEU:HD13	1:E:161:GLU:HG2	1.84	0.54
1:F:92:GLU:HG2	4:F:639:HOH:O	2.08	0.54
1:D:140:LEU:CD1	1:D:161:GLU:HG2	2.36	0.53
1:C:151:LEU:HD13	1:C:187:ARG:HG2	1.90	0.53
1:D:22:ILE:HG13	1:D:126:MET:CE	2.39	0.53
1:D:21:THR:HB	1:D:126:MET:HE1	1.89	0.53
1:F:23:ARG:HG3	4:F:638:HOH:O	2.08	0.53
1:A:384:ARG:NH1	1:A:388:ARG:HD3	2.24	0.53
1:A:64:GLY:O	1:A:68:LEU:HB2	2.09	0.53
1:B:164:ARG:CZ	4:B:783:HOH:O	2.47	0.53
1:D:28:LEU:C	1:D:30:GLN:H	2.12	0.53
1:E:348:ASN:HB2	4:E:769:HOH:O	2.07	0.53
1:C:310:ARG:NH2	1:C:311:GLU:OE2	2.41	0.53
1:D:269:HIS:HD2	1:D:270:THR:O	1.92	0.53
1:B:274:ASN:N	1:B:274:ASN:HD22	2.05	0.53
1:A:202:ASP:OD2	2:A:600:PLP:N1	2.41	0.52
1:E:118:VAL:CG2	4:E:786:HOH:O	2.46	0.52
1:C:332:PRO:HD2	1:C:335:LEU:HD12	1.91	0.52
1:F:306:HIS:CD2	4:F:657:HOH:O	2.61	0.52
1:E:63:LYS:O	1:E:66:VAL:HG12	2.10	0.52
1:E:120:LEU:HD23	1:E:141:THR:HG22	1.92	0.52
1:C:160:ARG:HG2	4:C:806:HOH:O	2.10	0.52
1:D:190:GLN:OE1	1:D:193:MET:HE3	2.10	0.52
1:D:100:SER:HB2	2:D:600:PLP:H5A2	1.92	0.52
4:B:778:HOH:O	2:D:600:PLP:C4A	2.58	0.52
3:E:700:LEU:HD23	1:F:268:LEU:HD13	1.90	0.52
1:B:62:GLU:OE2	1:E:138:ARG:NH1	2.43	0.51
1:A:269:HIS:HD2	1:A:270:THR:O	1.93	0.51
1:E:375:ASP:O	1:E:379:ILE:HG12	2.11	0.51
1:E:189:LEU:O	1:E:193:MET:HG3	2.10	0.51
1:B:182:LEU:HD13	1:B:216:PRO:HG2	1.92	0.51
1:E:43:ALA:HB3	1:E:46:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:HIS:HB3	4:F:633:HOH:O	2.11	0.51
1:E:71:SER:HB2	1:E:72:PRO:CD	2.41	0.51
1:D:28:LEU:HD21	1:D:41:LEU:HD21	1.93	0.51
1:F:189:LEU:HD22	1:F:221:LEU:HB3	1.93	0.51
1:D:209:TYR:CD2	1:D:214:ARG:HB3	2.46	0.51
1:D:271:PRO:HB2	1:D:274:ASN:ND2	2.26	0.51
1:D:189:LEU:HD22	1:D:221:LEU:HB3	1.93	0.51
1:F:107:VAL:HG11	1:F:200:VAL:HG21	1.93	0.50
1:D:22:ILE:HG13	1:D:126:MET:HE2	1.94	0.50
1:A:342:ARG:HH11	1:A:342:ARG:CG	2.20	0.50
1:E:46:LEU:HD23	1:E:293:VAL:HG22	1.94	0.50
1:C:25:LEU:HD22	1:C:26:LEU:HD12	1.93	0.50
1:C:344:ALA:HB1	1:C:349:VAL:HG13	1.93	0.50
1:A:61:ARG:HG3	1:C:53:ALA:CB	2.41	0.50
1:A:206:ARG:HG2	1:A:207:GLU:HG2	1.92	0.50
1:A:317:ARG:HH12	1:A:332:PRO:CA	2.23	0.50
1:B:170:PRO:HG2	1:B:218:LEU:HD22	1.94	0.50
1:B:32:PRO:HD2	1:B:33:GLY:H	1.75	0.50
1:C:39:GLY:H	1:C:368:ARG:HH21	1.58	0.50
1:A:120:LEU:O	1:A:141:THR:HA	2.10	0.50
1:C:74:GLU:HB3	1:C:80:ARG:CZ	2.42	0.50
1:D:372:ALA:HB3	4:D:656:HOH:O	2.11	0.50
1:E:138:ARG:NH2	1:E:161:GLU:OE1	2.41	0.49
1:A:264:GLN:NE2	1:C:22:ILE:HB	2.27	0.49
1:F:83:VAL:O	1:F:87:ILE:HG13	2.12	0.49
1:E:176:THR:HA	1:E:328:TRP:HB2	1.95	0.49
1:E:189:LEU:HD22	1:E:221:LEU:HB3	1.93	0.49
1:E:64:GLY:O	1:E:68:LEU:HB2	2.12	0.49
1:C:170:PRO:HG2	1:C:218:LEU:HD13	1.94	0.49
1:D:87:ILE:O	1:D:223:ARG:NH1	2.46	0.49
1:A:168:LEU:HD13	1:A:188:LEU:HD21	1.94	0.49
1:E:209:TYR:O	1:E:294:ARG:HG3	2.13	0.49
1:F:22:ILE:HD13	1:F:130:GLN:HE21	1.78	0.49
1:A:107:VAL:HG11	1:A:200:VAL:HG21	1.93	0.49
1:C:42:PRO:HG2	1:C:242:PRO:HD3	1.95	0.48
1:D:95:LEU:HD13	1:D:260:VAL:HG22	1.95	0.48
1:F:95:LEU:HD13	1:F:260:VAL:HG22	1.95	0.48
1:C:71:SER:OG	1:C:72:PRO:HD2	2.13	0.48
1:B:264:GLN:HG3	4:D:713:HOH:O	2.13	0.48
1:D:304:MET:HE2	1:D:379:ILE:HG23	1.96	0.48
1:A:31:ARG:N	1:A:32:PRO:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:THR:HA	1:F:328:TRP:HB2	1.95	0.48
1:B:28:LEU:C	1:B:30:GLN:N	2.65	0.48
1:C:207:GLU:O	1:C:294:ARG:HD3	2.13	0.48
1:A:274:ASN:HD22	1:A:274:ASN:N	2.09	0.48
1:A:30:GLN:HG3	4:A:767:HOH:O	2.14	0.48
1:D:139:PHE:HB2	1:D:360:ASN:HD21	1.79	0.48
1:C:271:PRO:HB2	1:C:274:ASN:ND2	2.29	0.48
1:A:20:SER:HA	1:C:264:GLN:HE22	1.79	0.47
1:D:106:LEU:O	1:D:110:VAL:HG12	2.14	0.47
1:E:87:ILE:O	1:E:223:ARG:NH1	2.47	0.47
1:D:300:LYS:HE2	1:D:372:ALA:O	2.15	0.47
1:F:358:PHE:CE2	1:F:363:GLY:HA3	2.50	0.47
1:B:381:GLU:O	1:B:385:ARG:HG3	2.15	0.47
1:F:344:ALA:HB1	1:F:349:VAL:HG13	1.96	0.47
1:C:121:GLU:HB3	1:C:144:ALA:HB2	1.97	0.47
1:D:231:ILE:HD12	1:D:251:ALA:HB1	1.96	0.47
1:A:347:GLU:O	1:A:385:ARG:HD3	2.14	0.47
1:F:121:GLU:OE2	4:F:620:HOH:O	2.20	0.47
1:C:120:LEU:O	1:C:141:THR:HA	2.15	0.47
1:E:112:LEU:HD21	1:E:118:VAL:CG2	2.41	0.47
1:E:312:VAL:HA	1:E:313:PRO:HD2	1.67	0.47
1:B:342:ARG:H	1:B:342:ARG:HG2	1.38	0.47
1:E:112:LEU:CD2	1:E:118:VAL:CG2	2.91	0.47
1:F:209:TYR:CE2	1:F:214:ARG:HB3	2.50	0.47
1:C:181:PRO:HD2	1:C:184:ALA:HB3	1.97	0.47
1:B:263:LYS:HE3	1:B:269:HIS:HA	1.97	0.47
1:E:65:GLU:H	1:E:65:GLU:CD	2.19	0.47
1:E:182:LEU:HD13	1:E:216:PRO:HD2	1.97	0.47
1:E:282:LEU:HG	1:E:286:PHE:CD1	2.50	0.47
1:A:119:LEU:HD11	1:A:154:LEU:CD1	2.46	0.46
1:C:285:GLY:HA2	1:C:288:GLU:OE1	2.16	0.46
1:D:43:ALA:HB3	1:D:46:LEU:HD22	1.97	0.46
1:A:320:ARG:HD2	1:B:288:GLU:HG3	1.97	0.46
1:B:27:LYS:C	1:B:29:THR:N	2.68	0.46
1:C:271:PRO:HG2	4:C:831:HOH:O	2.14	0.46
1:B:146:GLU:HG3	4:B:736:HOH:O	2.16	0.46
1:F:300:LYS:HE3	1:F:374:LEU:O	2.15	0.46
1:F:55:ALA:O	1:F:59:ILE:HG12	2.16	0.46
1:F:272:MET:HB2	4:F:642:HOH:O	2.16	0.46
1:A:26:LEU:HD13	3:A:700:LEU:HD21	1.98	0.46
1:B:384:ARG:NH2	1:B:388:ARG:NH1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:LEU:HD11	1:E:390:LEU:HD23	1.97	0.46
1:C:64:GLY:O	1:C:68:LEU:HB2	2.16	0.45
1:D:387:GLY:O	1:D:391:LYS:HG2	2.17	0.45
1:C:21:THR:HB	1:C:126:MET:HE1	1.98	0.45
1:C:199:VAL:HG11	1:C:218:LEU:HD23	1.97	0.45
4:A:792:HOH:O	1:C:261:GLN:CD	2.54	0.45
1:C:274:ASN:N	1:C:274:ASN:ND2	2.64	0.45
1:E:26:LEU:HB3	1:F:72:PRO:HA	1.99	0.45
1:B:95:LEU:HD13	1:B:260:VAL:HG22	1.98	0.45
3:B:700:LEU:HD22	1:D:268:LEU:HD13	1.98	0.45
1:A:384:ARG:HH12	1:A:388:ARG:HD3	1.81	0.45
1:E:347:GLU:HB2	1:E:349:VAL:HG12	1.99	0.45
1:F:65:GLU:CD	1:F:65:GLU:H	2.20	0.45
1:C:292:ARG:CG	1:C:292:ARG:HH21	2.28	0.45
1:B:133:ARG:NH2	1:B:359:ALA:O	2.50	0.45
1:B:30:GLN:CB	1:B:34:ILE:HG21	2.47	0.45
1:E:202:ASP:OD2	2:E:600:PLP:N1	2.51	0.44
1:E:112:LEU:HD22	1:E:118:VAL:HG22	1.96	0.44
1:E:210:PHE:HB3	1:E:298:ARG:HG3	1.98	0.44
1:A:77:ALA:HB3	1:A:78:PRO:HD3	1.98	0.44
1:B:58:ARG:HD3	1:E:161:GLU:OE1	2.18	0.44
1:D:329:MET:HB3	1:D:367:LEU:HD22	1.98	0.44
1:E:107:VAL:HG11	1:E:200:VAL:HG21	1.98	0.44
1:D:203:ASP:CG	1:D:206:ARG:HB2	2.38	0.44
1:B:288:GLU:H	1:B:288:GLU:CD	2.20	0.44
1:A:170:PRO:HD2	4:A:714:HOH:O	2.18	0.44
1:C:358:PHE:CE2	1:C:363:GLY:HA3	2.52	0.44
1:A:30:GLN:HB3	1:A:31:ARG:H	1.52	0.44
1:E:87:ILE:HD13	1:E:248:PHE:CE1	2.53	0.44
1:D:240:LEU:HG	1:D:282:LEU:HD11	2.00	0.44
1:B:136:GLY:N	1:B:137:PRO:CD	2.81	0.44
1:A:342:ARG:NH1	1:A:342:ARG:CG	2.78	0.44
1:A:176:THR:HA	1:A:328:TRP:HB2	2.00	0.43
1:E:87:ILE:CD1	1:E:248:PHE:CE1	3.01	0.43
1:D:227:TYR:HA	1:D:228:PRO:HD3	1.87	0.43
1:A:300:LYS:HE2	1:A:372:ALA:O	2.18	0.43
1:B:107:VAL:HG11	1:B:200:VAL:HG21	2.00	0.43
1:F:274:ASN:N	1:F:274:ASN:HD22	2.12	0.43
1:D:209:TYR:O	1:D:294:ARG:HG3	2.18	0.43
1:C:312:VAL:HA	1:C:313:PRO:HD2	1.85	0.43
1:E:34:ILE:HG23	1:E:34:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLN:HA	1:F:266:ALA:O	2.18	0.43
1:F:79:LEU:HD12	1:F:275:GLN:HB3	1.99	0.43
1:B:285:GLY:HA2	1:B:288:GLU:OE1	2.19	0.43
1:B:310:ARG:NH2	4:B:739:HOH:O	2.45	0.43
1:D:202:ASP:OD2	2:D:600:PLP:N1	2.51	0.43
1:C:118:VAL:HG22	1:C:137:PRO:HB2	2.01	0.43
1:A:375:ASP:CG	1:A:376:ARG:N	2.70	0.43
1:B:38:ALA:O	1:B:39:GLY:O	2.36	0.43
1:E:174:ASN:HB3	2:E:600:PLP:H2A1	2.00	0.43
1:C:212:GLU:H	1:C:212:GLU:HG2	1.67	0.43
1:E:269:HIS:HD2	1:E:270:THR:O	2.01	0.43
1:E:109:LYS:HE2	1:F:134:LEU:HD11	2.00	0.43
1:A:166:LEU:HD12	1:A:166:LEU:N	2.34	0.43
1:C:210:PHE:HB3	1:C:298:ARG:HG3	2.01	0.43
1:D:164:ARG:NH2	4:D:667:HOH:O	2.52	0.42
1:F:17:ILE:C	1:F:19:ALA:H	2.22	0.42
1:A:46:LEU:HD11	1:A:296:VAL:HG21	1.99	0.42
1:B:335:LEU:HD11	1:B:394:LEU:HD13	2.01	0.42
1:E:328:TRP:CZ2	1:E:366:THR:HB	2.54	0.42
1:E:238:LYS:HD2	1:E:325:MET:CE	2.50	0.42
1:B:102:GLN:O	1:B:106:LEU:HG	2.19	0.42
1:A:203:ASP:CG	1:A:206:ARG:HB2	2.40	0.42
1:C:102:GLN:O	1:C:106:LEU:HG	2.19	0.42
1:B:274:ASN:N	1:B:274:ASN:ND2	2.67	0.42
1:F:384:ARG:NH2	1:F:388:ARG:NH1	2.63	0.42
1:B:70:TYR:HB3	1:D:26:LEU:HD13	2.01	0.42
1:F:182:LEU:HB3	1:F:183:PRO:HD3	2.01	0.42
1:D:46:LEU:CD1	1:D:296:VAL:HG21	2.50	0.42
1:F:63:LYS:O	1:F:66:VAL:HG13	2.20	0.42
1:A:95:LEU:HD13	1:A:260:VAL:HG22	2.01	0.42
1:D:64:GLY:O	1:D:68:LEU:HB2	2.19	0.42
1:E:101:GLN:HE22	1:E:127:GLY:HA3	1.85	0.42
1:C:176:THR:HA	1:C:328:TRP:HB2	2.00	0.42
1:B:278:VAL:HG13	1:B:282:LEU:HD22	2.01	0.42
1:B:151:LEU:HD13	1:B:187:ARG:HG2	2.02	0.42
1:D:42:PRO:HD2	1:D:242:PRO:HG3	2.01	0.42
1:A:391:LYS:HD3	4:A:763:HOH:O	2.20	0.42
1:A:227:TYR:HA	1:A:228:PRO:HD3	1.82	0.42
1:D:102:GLN:O	1:D:106:LEU:HG	2.20	0.42
1:F:87:ILE:HD12	1:F:250:VAL:HG21	2.02	0.42
1:B:31:ARG:HA	1:B:32:PRO:HA	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:GLU:HA	1:E:179:LEU:O	2.19	0.42
1:B:51:GLU:HG3	4:B:729:HOH:O	2.19	0.42
1:F:258:LYS:HA	1:F:258:LYS:HD3	1.86	0.42
1:D:231:ILE:HD12	1:D:251:ALA:CB	2.50	0.41
1:D:312:VAL:HA	1:D:313:PRO:HD3	1.97	0.41
1:A:212:GLU:H	1:A:212:GLU:HG2	1.65	0.41
1:A:312:VAL:HA	1:A:313:PRO:HD2	1.93	0.41
1:A:274:ASN:ND2	1:A:274:ASN:N	2.68	0.41
1:D:358:PHE:CE2	1:D:363:GLY:HA3	2.55	0.41
1:F:121:GLU:HB3	1:F:144:ALA:HB2	2.03	0.41
1:A:63:LYS:O	1:A:66:VAL:HG13	2.19	0.41
1:E:152:ASP:OD1	4:E:772:HOH:O	2.22	0.41
1:B:28:LEU:N	4:B:776:HOH:O	2.53	0.41
1:A:102:GLN:O	1:A:106:LEU:HG	2.20	0.41
1:C:29:THR:O	1:C:30:GLN:C	2.58	0.41
1:D:190:GLN:OE1	1:D:193:MET:CE	2.68	0.41
1:C:227:TYR:HA	1:C:228:PRO:HD3	1.89	0.41
1:A:209:TYR:CD2	1:A:214:ARG:HB3	2.56	0.41
1:F:241:SER:HA	1:F:242:PRO:HD2	1.95	0.41
1:D:289:ARG:O	1:D:293:VAL:HG13	2.20	0.41
1:B:120:LEU:O	1:B:141:THR:HA	2.20	0.41
1:C:151:LEU:HD21	4:C:841:HOH:O	2.20	0.41
1:C:22:ILE:O	1:C:25:LEU:HB3	2.20	0.41
1:B:30:GLN:HB2	1:B:34:ILE:HG21	2.03	0.41
1:D:256:LEU:O	1:D:260:VAL:HG23	2.21	0.41
1:E:312:VAL:CG1	1:E:316:VAL:HG22	2.51	0.41
1:C:106:LEU:O	1:C:110:VAL:HG13	2.21	0.41
1:B:313:PRO:HG3	1:B:391:LYS:HG2	2.02	0.41
1:B:74:GLU:O	1:B:80:ARG:HD3	2.21	0.41
1:A:258:LYS:HA	1:A:258:LYS:HD3	1.88	0.41
1:A:207:GLU:O	1:A:294:ARG:HD3	2.21	0.41
1:A:342:ARG:NH1	1:A:342:ARG:HG3	2.23	0.40
1:D:384:ARG:NH1	4:D:701:HOH:O	2.53	0.40
1:F:64:GLY:O	1:F:68:LEU:HB2	2.20	0.40
1:A:84:ALA:HB1	1:A:89:VAL:O	2.22	0.40
1:E:42:PRO:HG3	1:E:325:MET:HE1	2.03	0.40
1:D:22:ILE:HD12	1:D:22:ILE:N	2.36	0.40
1:A:102:GLN:HA	1:C:266:ALA:O	2.21	0.40
1:E:261:GLN:NE2	1:F:18:GLN:HA	2.35	0.40
1:F:70:TYR:HA	1:F:269:HIS:CE1	2.57	0.40
1:C:77:ALA:HB3	1:C:78:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:CG	1:D:342:ARG:NH1	2.81	0.40
1:C:112:LEU:HD21	1:C:118:VAL:CG1	2.41	0.40
1:B:358:PHE:CE2	1:B:363:GLY:HA3	2.57	0.40
1:D:21:THR:HG21	1:D:356:PRO:HG2	2.02	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	389/397 (98%)	369 (95%)	18 (5%)	2 (0%)	34	34
1	B	389/397 (98%)	371 (95%)	13 (3%)	5 (1%)	15	10
1	C	389/397 (98%)	370 (95%)	16 (4%)	3 (1%)	24	21
1	D	389/397 (98%)	370 (95%)	18 (5%)	1 (0%)	46	52
1	E	389/397 (98%)	373 (96%)	12 (3%)	4 (1%)	19	16
1	F	389/397 (98%)	376 (97%)	11 (3%)	2 (0%)	34	34
All	All	2334/2382 (98%)	2229 (96%)	88 (4%)	17 (1%)	26	26

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	B	28	LEU
1	B	39	GLY
1	E	32	PRO
1	A	33	GLY
1	E	39	GLY
1	F	18	GLN
1	C	18	GLN

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Mol	Chain	Res	Type
1	C	30	GLN
1	F	39	GLY
1	B	333	LYS
1	E	348	ASN
1	C	32	PRO
1	D	32	PRO
1	E	29	THR
1	B	355	GLY
1	B	32	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	307/316 (97%)	272 (89%)	35 (11%)	7	5
1	B	307/316 (97%)	270 (88%)	37 (12%)	6	4
1	C	307/316 (97%)	273 (89%)	34 (11%)	8	5
1	D	307/316 (97%)	274 (89%)	33 (11%)	8	6
1	E	307/316 (97%)	278 (91%)	29 (9%)	11	8
1	F	307/316 (97%)	268 (87%)	39 (13%)	5	3
All	All	1842/1896 (97%)	1635 (89%)	207 (11%)	7	5

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	23	ARG
1	A	24	GLU
1	A	26	LEU
1	A	28	LEU
1	A	46	LEU
1	A	65	GLU
1	A	68	LEU
1	A	71	SER

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Mol	Chain	Res	Type
1	A	79	LEU
1	A	120	LEU
1	A	134	LEU
1	A	142	VAL
1	A	158	LEU
1	A	179	LEU
1	A	190	GLN
1	A	192	VAL
1	A	212	GLU
1	A	218	LEU
1	A	221	LEU
1	A	239	VAL
1	A	240	LEU
1	A	256	LEU
1	A	273	LEU
1	A	274	ASN
1	A	282	LEU
1	A	290	LEU
1	A	291	GLU
1	A	316	VAL
1	A	317	ARG
1	A	336	SER
1	A	340	LEU
1	A	367	LEU
1	A	384	ARG
1	A	391	LYS
1	B	5	SER
1	B	20	SER
1	B	24	GLU
1	B	26	LEU
1	B	28	LEU
1	B	29	THR
1	B	54	GLU
1	B	66	VAL
1	B	68	LEU
1	B	71	SER
1	B	79	LEU
1	B	120	LEU
1	B	134	LEU
1	B	142	VAL
1	B	158	LEU
1	B	160	ARG

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Mol	Chain	Res	Type
1	B	162	ARG
1	B	179	LEU
1	B	187	ARG
1	B	218	LEU
1	B	221	LEU
1	B	256	LEU
1	B	273	LEU
1	B	274	ASN
1	B	282	LEU
1	B	288	GLU
1	B	290	LEU
1	B	316	VAL
1	B	317	ARG
1	B	340	LEU
1	B	342	ARG
1	B	345	LEU
1	B	349	VAL
1	B	367	LEU
1	B	377	GLU
1	B	386	LEU
1	B	394	LEU
1	C	5	SER
1	C	17	ILE
1	C	20	SER
1	C	28	LEU
1	C	36	SER
1	C	46	LEU
1	C	68	LEU
1	C	79	LEU
1	C	110	VAL
1	C	116	SER
1	C	118	VAL
1	C	120	LEU
1	C	134	LEU
1	C	158	LEU
1	C	179	LEU
1	C	187	ARG
1	C	212	GLU
1	C	214	ARG
1	C	221	LEU
1	C	240	LEU
1	C	246	VAL

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Mol	Chain	Res	Type
1	C	273	LEU
1	C	274	ASN
1	C	282	LEU
1	C	290	LEU
1	C	304	MET
1	C	316	VAL
1	C	333	LYS
1	C	340	LEU
1	C	367	LEU
1	C	384	ARG
1	C	386	LEU
1	C	391	LYS
1	C	394	LEU
1	D	21	THR
1	D	22	ILE
1	D	28	LEU
1	D	30	GLN
1	D	46	LEU
1	D	66	VAL
1	D	68	LEU
1	D	71	SER
1	D	79	LEU
1	D	116	SER
1	D	118	VAL
1	D	119	LEU
1	D	120	LEU
1	D	134	LEU
1	D	158	LEU
1	D	160	ARG
1	D	188	LEU
1	D	221	LEU
1	D	240	LEU
1	D	273	LEU
1	D	290	LEU
1	D	294	ARG
1	D	304	MET
1	D	316	VAL
1	D	333	LYS
1	D	338	GLU
1	D	340	LEU
1	D	342	ARG
1	D	367	LEU

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Mol	Chain	Res	Type
1	D	375	ASP
1	D	376	ARG
1	D	386	LEU
1	D	394	LEU
1	E	21	THR
1	E	23	ARG
1	E	24	GLU
1	E	26	LEU
1	E	65	GLU
1	E	68	LEU
1	E	79	LEU
1	E	119	LEU
1	E	120	LEU
1	E	126	MET
1	E	134	LEU
1	E	158	LEU
1	E	160	ARG
1	E	179	LEU
1	E	187	ARG
1	E	221	LEU
1	E	240	LEU
1	E	256	LEU
1	E	273	LEU
1	E	274	ASN
1	E	282	LEU
1	E	289	ARG
1	E	290	LEU
1	E	317	ARG
1	E	347	GLU
1	E	367	LEU
1	E	375	ASP
1	E	376	ARG
1	E	391	LYS
1	F	5	SER
1	F	8	GLU
1	F	20	SER
1	F	28	LEU
1	F	29	THR
1	F	34	ILE
1	F	46	LEU
1	F	66	VAL
1	F	68	LEU

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Mol	Chain	Res	Type
1	F	71	SER
1	F	79	LEU
1	F	85	GLU
1	F	118	VAL
1	F	120	LEU
1	F	130	GLN
1	F	134	LEU
1	F	142	VAL
1	F	158	LEU
1	F	160	ARG
1	F	162	ARG
1	F	179	LEU
1	F	187	ARG
1	F	188	LEU
1	F	212	GLU
1	F	218	LEU
1	F	221	LEU
1	F	240	LEU
1	F	256	LEU
1	F	273	LEU
1	F	274	ASN
1	F	282	LEU
1	F	290	LEU
1	F	291	GLU
1	F	316	VAL
1	F	340	LEU
1	F	342	ARG
1	F	367	LEU
1	F	384	ARG
1	F	386	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	101	GLN
1	A	257	GLN
1	A	261	GLN
1	A	264	GLN
1	A	269	HIS
1	A	274	ASN
1	A	360	ASN

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Mol	Chain	Res	Type
1	B	101	GLN
1	B	135	GLN
1	B	257	GLN
1	B	261	GLN
1	B	264	GLN
1	B	269	HIS
1	B	274	ASN
1	B	302	GLN
1	B	306	HIS
1	B	360	ASN
1	C	101	GLN
1	C	135	GLN
1	C	257	GLN
1	C	264	GLN
1	C	269	HIS
1	C	274	ASN
1	C	360	ASN
1	D	101	GLN
1	D	257	GLN
1	D	264	GLN
1	D	269	HIS
1	D	274	ASN
1	D	360	ASN
1	E	101	GLN
1	E	257	GLN
1	E	261	GLN
1	E	264	GLN
1	E	269	HIS
1	E	274	ASN
1	E	360	ASN
1	F	101	GLN
1	F	130	GLN
1	F	264	GLN
1	F	269	HIS
1	F	274	ASN
1	F	360	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
2	PLP	A	600	1	15,15,16	1.12	1 (6%)	21,22,23	1.58	3 (14%)
3	LEU	A	700	-	5,8,8	0.27	0	5,10,10	1.76	1 (20%)
2	PLP	B	600	1	15,15,16	1.25	1 (6%)	21,22,23	1.59	5 (23%)
3	LEU	B	700	-	5,8,8	0.25	0	5,10,10	0.98	0
2	PLP	C	600	1	15,15,16	1.69	2 (13%)	21,22,23	1.73	7 (33%)
2	PLP	D	600	1	15,15,16	1.31	2 (13%)	21,22,23	1.85	5 (23%)
2	PLP	E	600	1	15,15,16	2.66	3 (20%)	21,22,23	1.39	5 (23%)
3	LEU	E	700	-	5,8,8	0.22	0	5,10,10	1.19	1 (20%)
2	PLP	F	600	1	15,15,16	2.58	7 (46%)	21,22,23	2.28	6 (28%)

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	A	600	1	-	0/6/6/8	0/1/1/1
3	LEU	A	700	-	-	0/4/8/8	0/0/0/0
2	PLP	B	600	1	-	0/6/6/8	0/1/1/1
3	LEU	B	700	-	-	0/4/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	600	1	-	0/6/6/8	0/1/1/1
2	PLP	D	600	1	-	0/6/6/8	0/1/1/1
2	PLP	E	600	1	-	0/6/6/8	0/1/1/1
3	LEU	E	700	-	-	0/4/8/8	0/0/0/0
2	PLP	F	600	1	-	0/6/6/8	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	PLP	C4A-C4	-9.36	1.32	1.51
2	F	600	PLP	C4A-C4	-5.45	1.40	1.51
2	F	600	PLP	O3-C3	-3.75	1.28	1.37
2	F	600	PLP	P-O3P	-3.67	1.41	1.54
2	F	600	PLP	P-O2P	-3.49	1.42	1.54
2	A	600	PLP	C3-C2	-3.44	1.38	1.40
2	C	600	PLP	C3-C2	-3.43	1.38	1.40
2	D	600	PLP	C3-C2	-3.39	1.38	1.40
2	F	600	PLP	C3-C2	-3.19	1.38	1.40
2	F	600	PLP	P-O1P	-2.77	1.42	1.51
2	E	600	PLP	C3-C2	-2.55	1.39	1.40
2	F	600	PLP	P-O4P	-2.21	1.52	1.60
2	E	600	PLP	C2-N1	2.25	1.38	1.34
2	D	600	PLP	C4A-C4	2.31	1.56	1.51
2	B	600	PLP	C2-N1	2.79	1.40	1.34
2	C	600	PLP	C4A-C4	4.66	1.61	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	PLP	C4A-C4-C5	-5.94	114.69	120.88
2	C	600	PLP	C4A-C4-C5	-4.45	116.24	120.88
2	D	600	PLP	C4A-C4-C5	-4.17	116.54	120.88
2	D	600	PLP	C5A-C5-C6	-3.76	112.17	119.28
2	F	600	PLP	C5A-C5-C6	-3.69	112.29	119.28
2	B	600	PLP	O4P-C5A-C5	-3.46	103.28	108.99
2	F	600	PLP	C5A-C5-C4	-2.87	117.85	121.65
2	A	600	PLP	C5-C6-N1	-2.79	119.01	123.86
2	C	600	PLP	C5-C6-N1	-2.78	119.03	123.86
2	E	600	PLP	C4A-C4-C3	-2.74	115.40	120.36
2	C	600	PLP	O4P-C5A-C5	-2.39	105.05	108.99
2	B	600	PLP	C5A-C5-C4	-2.29	118.62	121.65
2	B	600	PLP	C5-C6-N1	-2.22	120.01	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	PLP	C5-C6-N1	-2.19	120.06	123.86
2	B	600	PLP	C4A-C4-C3	-2.13	116.50	120.36
2	C	600	PLP	C5A-C5-C4	-2.01	118.98	121.65
2	E	600	PLP	O2P-P-O4P	2.06	112.51	106.56
2	A	600	PLP	C3-C4-C5	2.10	121.07	118.78
2	E	600	PLP	C6-C5-C4	2.24	120.04	118.15
2	C	600	PLP	C4A-C4-C3	2.25	124.42	120.36
2	D	600	PLP	C3-C4-C5	2.30	121.29	118.78
2	C	600	PLP	O2P-P-O4P	2.36	113.36	106.56
3	E	700	LEU	CG-CB-CA	2.63	120.42	114.80
2	D	600	PLP	O4P-P-O1P	2.69	113.98	107.14
2	B	600	PLP	O3-C3-C2	2.79	122.50	117.66
2	F	600	PLP	O3-C3-C2	2.80	122.53	117.66
2	C	600	PLP	C6-C5-C4	2.85	120.56	118.15
2	E	600	PLP	C4A-C4-C5	2.86	123.86	120.88
2	F	600	PLP	C4A-C4-C3	3.47	126.63	120.36
3	A	700	LEU	CG-CB-CA	3.74	122.78	114.80
2	D	600	PLP	O4P-C5A-C5	3.76	115.21	108.99
2	F	600	PLP	O4P-P-O1P	3.86	116.98	107.14
2	A	600	PLP	O4P-P-O1P	3.98	117.27	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	PLP	1	0
3	A	700	LEU	2	0
2	B	600	PLP	1	0
3	B	700	LEU	2	0
2	D	600	PLP	7	0
2	E	600	PLP	3	0
3	E	700	LEU	1	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	391/397 (98%)	0.01	14 (3%)	46	50	14, 25, 46, 66	0
1	B	391/397 (98%)	0.12	15 (3%)	44	48	15, 27, 46, 60	0
1	C	391/397 (98%)	0.29	25 (6%)	23	25	14, 27, 54, 77	0
1	D	391/397 (98%)	0.27	23 (5%)	26	28	15, 29, 49, 84	0
1	E	391/397 (98%)	0.44	30 (7%)	16	18	17, 31, 70, 90	0
1	F	391/397 (98%)	0.30	23 (5%)	26	28	18, 32, 45, 81	0
All	All	2346/2382 (98%)	0.24	130 (5%)	29	32	14, 29, 54, 90	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	THR	13.5
1	F	28	LEU	12.5
1	D	25	LEU	10.4
1	E	26	LEU	10.2
1	E	32	PRO	8.9
1	E	25	LEU	8.7
1	F	32	PRO	8.7
1	E	33	GLY	8.5
1	D	32	PRO	8.5
1	D	20	SER	8.5
1	A	32	PRO	8.4
1	E	30	GLN	8.3
1	F	29	THR	8.3
1	F	25	LEU	8.2
1	C	26	LEU	7.6
1	D	26	LEU	7.6
1	F	26	LEU	7.6
1	C	25	LEU	7.5
1	F	31	ARG	7.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	28	LEU	7.1
1	C	29	THR	7.1
1	D	28	LEU	6.7
1	F	21	THR	6.5
1	A	31	ARG	6.2
1	E	29	THR	6.2
1	D	23	ARG	6.2
1	C	32	PRO	6.2
1	B	33	GLY	6.1
1	C	22	ILE	6.1
1	F	22	ILE	5.9
1	B	32	PRO	5.8
1	F	23	ARG	5.8
1	E	34	ILE	5.8
1	B	34	ILE	5.2
1	C	20	SER	5.0
1	D	31	ARG	5.0
1	B	29	THR	4.9
1	E	28	LEU	4.8
1	F	19	ALA	4.8
1	B	334	GLY	4.6
1	C	31	ARG	4.6
1	C	21	THR	4.6
1	E	350	ALA	4.5
1	E	31	ARG	4.5
1	C	23	ARG	4.5
1	A	28	LEU	4.1
1	D	22	ILE	4.0
1	E	345	LEU	4.0
1	E	348	ASN	4.0
1	A	34	ILE	4.0
1	E	23	ARG	3.9
1	F	30	GLN	3.8
1	E	349	VAL	3.8
1	E	21	THR	3.5
1	F	20	SER	3.5
1	F	24	GLU	3.5
1	C	333	LYS	3.5
1	D	21	THR	3.4
1	F	334	GLY	3.4
1	E	342	ARG	3.4
1	D	27	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	18	GLN	3.4
1	E	346	GLU	3.2
1	A	33	GLY	3.2
1	E	19	ALA	3.2
1	E	388	ARG	3.2
1	E	390	LEU	3.1
1	C	30	GLN	3.1
1	E	384	ARG	3.1
1	C	387	GLY	3.1
1	A	20	SER	3.1
1	E	308	LEU	3.1
1	B	348	ASN	3.0
1	E	343	ARG	3.0
1	C	24	GLU	2.9
1	E	35	LEU	2.9
1	B	395	ALA	2.9
1	E	22	ILE	2.8
1	E	377	GLU	2.8
1	A	26	LEU	2.7
1	D	38	ALA	2.7
1	D	24	GLU	2.7
1	A	345	LEU	2.6
1	E	334	GLY	2.6
1	F	126	MET	2.6
1	E	340	LEU	2.6
1	C	332	PRO	2.5
1	A	25	LEU	2.5
1	C	27	LYS	2.5
1	B	386	LEU	2.5
1	C	334	GLY	2.5
1	B	393	LEU	2.4
1	A	348	ASN	2.4
1	B	160	ARG	2.4
1	D	7	SER	2.4
1	D	288	GLU	2.4
1	A	342	ARG	2.4
1	D	160	ARG	2.4
1	F	284	GLU	2.3
1	B	35	LEU	2.3
1	C	317	ARG	2.3
1	F	316	VAL	2.3
1	C	33	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	31	ARG	2.3
1	D	33	GLY	2.3
1	F	27	LYS	2.3
1	F	342	ARG	2.2
1	C	391	LYS	2.2
1	D	34	ILE	2.2
1	A	38	ALA	2.2
1	D	19	ALA	2.2
1	D	212	GLU	2.2
1	B	26	LEU	2.2
1	C	160	ARG	2.2
1	F	292	ARG	2.1
1	C	314	LYS	2.1
1	C	146	GLU	2.1
1	F	299	GLU	2.1
1	C	335	LEU	2.1
1	D	346	GLU	2.1
1	F	317	ARG	2.1
1	D	18	GLN	2.1
1	D	284	GLU	2.0
1	B	266	ALA	2.0
1	A	316	VAL	2.0
1	E	386	LEU	2.0
1	E	20	SER	2.0
1	C	97	THR	2.0
1	A	347	GLU	2.0
1	B	342	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	LEU	B	700	9/9	0.89	0.31	3.58	34,36,38,39	0
2	PLP	A	600	15/16	0.96	0.17	1.50	18,27,30,32	0
2	PLP	D	600	15/16	0.96	0.16	0.78	20,27,31,34	0
2	PLP	F	600	15/16	0.94	0.14	0.76	22,30,32,34	0
2	PLP	B	600	15/16	0.97	0.17	0.74	21,35,38,38	0
3	LEU	A	700	9/9	0.93	0.20	0.61	33,34,35,35	0
3	LEU	E	700	9/9	0.82	0.33	0.59	62,62,63,63	0
2	PLP	E	600	15/16	0.96	0.16	0.30	18,31,36,36	0
2	PLP	C	600	15/16	0.97	0.16	0.22	16,27,29,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.