



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:24 am GMT

PDB ID : 1PMM  
Title : Crystal structure of Escherichia coli GadB (low pH)  
Authors : Capitani, G.; De Biase, D.; Aurizi, C.; Gut, H.; Bossa, F.; Grutter, M.G.  
Deposited on : 2003-06-11  
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

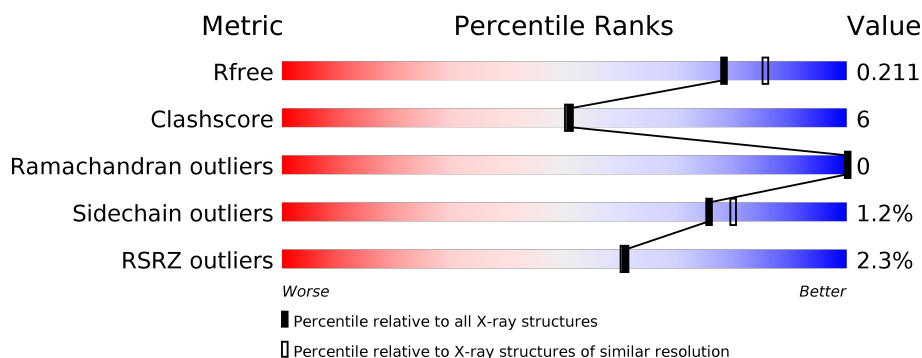
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	466	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	B	466	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div></div> </div> <div></div> </div>
1	C	466	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div></div> </div> <div></div> </div>
1	D	466	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	E	466	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	F	466	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div></div> </div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	B	6518	-	-	-	X

## 2 Entry composition [i](#)

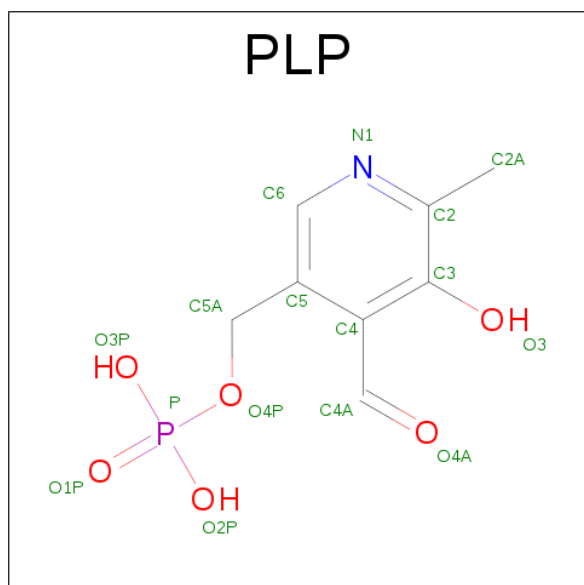
There are 4 unique types of molecules in this entry. The entry contains 23447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate decarboxylase beta.

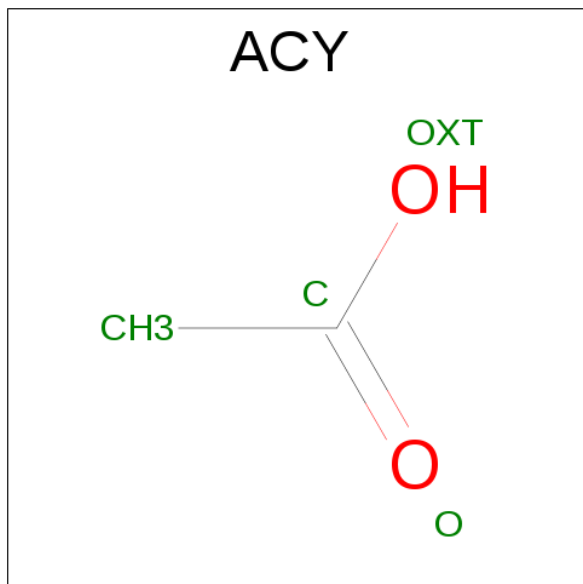
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	3	0
			3584	2287	610	661	26			
1	B	450	Total	C	N	O	S	0	3	0
			3585	2287	611	662	25			
1	C	449	Total	C	N	O	S	0	4	0
			3579	2282	608	664	25			
1	D	450	Total	C	N	O	S	0	3	0
			3584	2287	610	661	26			
1	E	449	Total	C	N	O	S	0	3	0
			3575	2281	608	660	26			
1	F	450	Total	C	N	O	S	0	3	0
			3584	2287	610	661	26			

- 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 ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

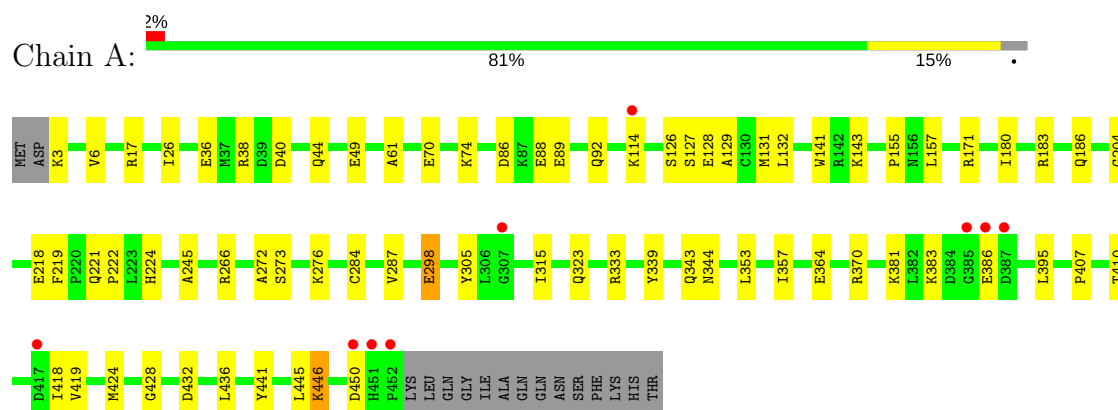
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	309	Total 309	O 309	0	0
4	B	320	Total 320	O 320	0	0
4	C	284	Total 284	O 284	0	0
4	D	333	Total 333	O 333	0	0
4	E	292	Total 292	O 292	0	0
4	F	304	Total 304	O 304	0	0

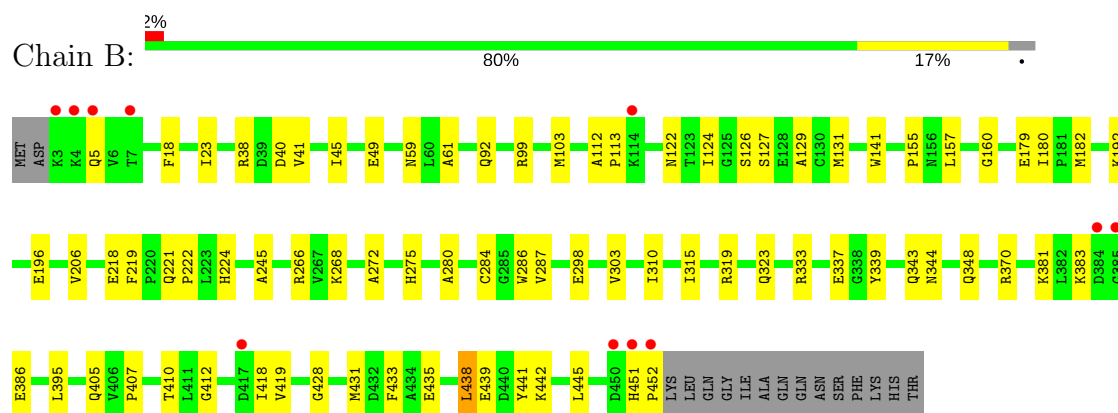
### 3 Residue-property plots [i](#)

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

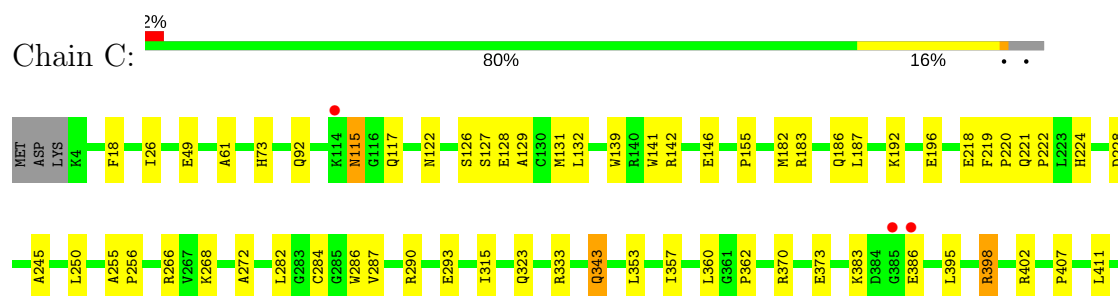
#### • Molecule 1: Glutamate decarboxylase beta

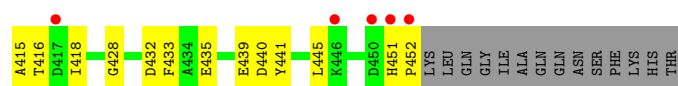


#### • Molecule 1: Glutamate decarboxylase beta

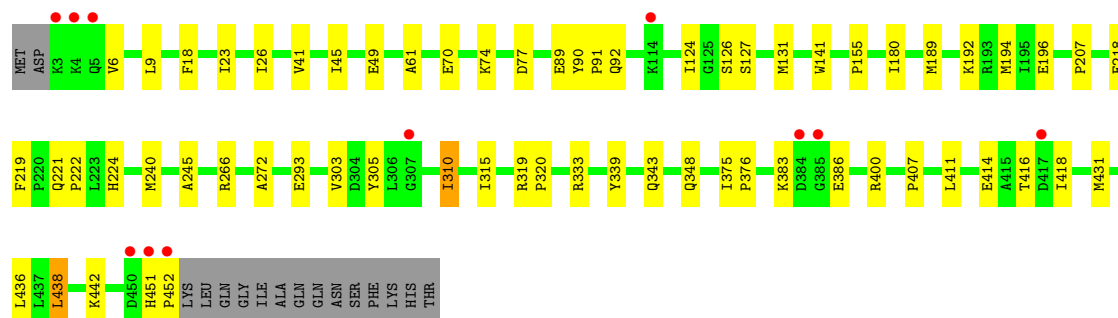
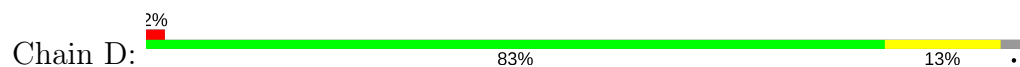


#### • Molecule 1: Glutamate decarboxylase beta

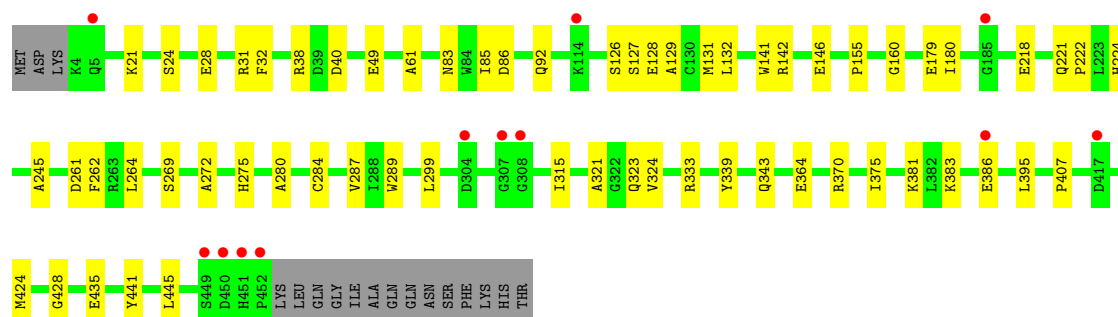
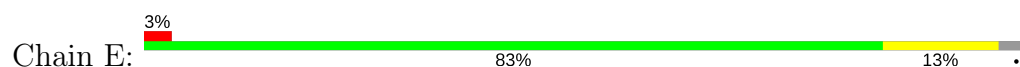




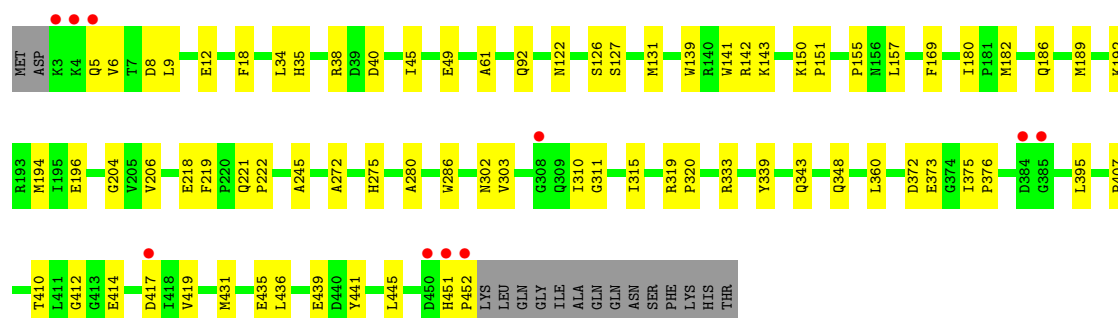
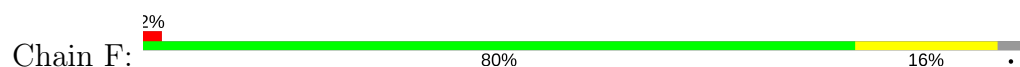
● Molecule 1: Glutamate decarboxylase beta



● Molecule 1: Glutamate decarboxylase beta



● Molecule 1: Glutamate decarboxylase beta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.78Å 91.41Å 93.69Å 76.80° 77.10° 78.24°	Depositor
Resolution (Å)	24.62 – 2.00 24.64 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.62-2.00) 89.2 (24.64-2.01)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.10 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.182 , 0.213 0.181 , 0.211	Depositor DCC
$R_{free}$ test set	5238 reflections (2.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.146 for k,l,h 0.146 for l,h,k 0.019 for -k,-h,-l 0.012 for -l,-k,-h 0.012 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, 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	0.32	0/3691	0.58	1/5002 (0.0%)
1	B	0.32	0/3692	0.58	1/5004 (0.0%)
1	C	0.31	0/3691	0.57	1/5004 (0.0%)
1	D	0.32	0/3691	0.58	1/5002 (0.0%)
1	E	0.31	0/3682	0.58	1/4991 (0.0%)
1	F	0.32	0/3691	0.58	1/5002 (0.0%)
All	All	0.32	0/22138	0.58	6/30005 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	GLU	N-CA-C	-5.64	95.78	111.00
1	A	218	GLU	N-CA-C	-5.50	96.15	111.00
1	F	218	GLU	N-CA-C	-5.47	96.23	111.00
1	D	218	GLU	N-CA-C	-5.42	96.36	111.00
1	E	218	GLU	N-CA-C	-5.41	96.39	111.00
1	C	218	GLU	N-CA-C	-5.28	96.74	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3584	0	3494	56	0
1	B	3585	0	3493	56	0
1	C	3579	0	3478	56	0
1	D	3584	0	3494	51	0
1	E	3575	0	3481	43	0
1	F	3584	0	3494	52	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
2	C	15	0	6	1	0
2	D	15	0	6	1	0
2	E	15	0	6	1	0
2	F	15	0	6	1	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	E	8	0	6	1	0
4	A	309	0	0	2	0
4	B	320	0	0	0	0
4	C	284	0	0	1	0
4	D	333	0	0	1	0
4	E	292	0	0	0	0
4	F	304	0	0	1	0
All	All	23447	0	20988	277	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 6.

All (277) 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:139:TRP:HE1	1:F:143:LYS:HE3	1.33	0.93
1:B:23:ILE:HG13	1:B:45:ILE:HD11	1.61	0.82
1:D:23:ILE:HG13	1:D:45:ILE:HD11	1.60	0.81
1:F:139:TRP:NE1	1:F:143:LYS:HE3	1.94	0.81
1:C:131[B]:MET:SD	1:D:315:ILE:HG23	2.22	0.80
1:D:310:ILE:HD13	1:D:310:ILE:H	1.48	0.78
1:F:127:SER:O	1:F:131[B]:MET:HG2	1.85	0.76
1:E:131[B]:MET:SD	1:F:315:ILE:HG23	2.28	0.74
1:E:127:SER:O	1:E:131[A]:MET:HG2	1.86	0.74
1:F:348:GLN:HE21	1:F:431:MET:HE3	1.53	0.72
1:D:438:LEU:HD22	1:D:442:LYS:HE3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:SER:O	1:B:131[B]:MET:HG2	1.90	0.71
1:E:395:LEU:HD21	1:E:441:TYR:CZ	2.25	0.71
1:A:131[B]:MET:SD	1:B:315:ILE:HG23	2.30	0.71
1:C:127:SER:O	1:C:131[A]:MET:HG2	1.91	0.71
1:B:370:ARG:HH11	1:B:370:ARG:HG2	1.56	0.70
1:F:348:GLN:HE21	1:F:431:MET:CE	2.03	0.70
1:F:339:TYR:O	1:F:343:GLN:HG2	1.91	0.70
1:B:221:GLN:HB3	1:B:222:PRO:HD3	1.74	0.69
1:E:339:TYR:O	1:E:343:GLN:HG2	1.92	0.69
1:D:339:TYR:O	1:D:343:GLN:HG2	1.93	0.69
1:D:127:SER:O	1:D:131[B]:MET:HG2	1.93	0.68
1:C:395:LEU:HD21	1:C:441:TYR:CZ	2.27	0.68
1:F:395:LEU:HD21	1:F:441:TYR:CZ	2.29	0.68
1:C:192:LYS:O	1:C:196:GLU:HG3	1.94	0.68
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.76	0.68
1:A:395:LEU:HD21	1:A:441:TYR:CZ	2.28	0.68
1:B:339:TYR:O	1:B:343:GLN:HG2	1.94	0.68
1:C:250:LEU:HD23	1:C:343:GLN:HG3	1.75	0.67
1:A:127:SER:O	1:A:131[B]:MET:HG3	1.96	0.66
1:C:142:ARG:O	1:C:146:GLU:HG3	1.96	0.66
1:B:438:LEU:HD22	1:B:442:LYS:HE3	1.78	0.65
1:A:383:LYS:HB2	1:A:386:GLU:HG3	1.77	0.65
1:A:127:SER:O	1:A:131[A]:MET:HG2	1.97	0.65
1:A:339:TYR:O	1:A:343:GLN:HG2	1.97	0.63
1:A:26:ILE:HD13	1:F:435:GLU:HG3	1.81	0.63
1:E:364:GLU:OE1	1:E:381:LYS:HE3	1.99	0.63
1:A:441:TYR:HE1	1:A:445:LEU:HD11	1.64	0.62
1:B:383:LYS:HB2	1:B:386:GLU:HG3	1.81	0.62
1:E:32:PHE:HB2	4:F:741:HOH:O	2.00	0.61
1:B:344:ASN:O	1:B:348[A]:GLN:HG3	2.01	0.61
1:B:245:ALA:HA	1:B:272:ALA:HA	1.82	0.60
1:D:348:GLN:HE21	1:D:431:MET:CE	2.14	0.60
1:C:441:TYR:HE1	1:C:445:LEU:HD11	1.66	0.60
1:D:6:VAL:HG11	1:F:5:GLN:HG2	1.84	0.60
1:C:61:ALA:HB2	1:C:407:PRO:HD3	1.84	0.59
1:F:180:ILE:HD12	1:F:189:MET:HG3	1.83	0.59
1:C:183:ARG:HD2	1:C:186:GLN:OE1	2.02	0.59
1:A:126:SER:HB2	2:A:500:PLP:O4P	2.03	0.59
1:D:89:GLU:C	1:D:91:PRO:HD3	2.24	0.59
1:C:435:GLU:O	1:C:439:GLU:HG3	2.03	0.58
1:B:435:GLU:HG3	1:C:26:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:TYR:HB2	1:D:310:ILE:HD12	1.85	0.58
1:E:28:GLU:HG2	1:E:31:ARG:O	2.02	0.58
1:A:3:LYS:O	1:A:6:VAL:HG12	2.04	0.58
1:B:395:LEU:HD21	1:B:441:TYR:CZ	2.39	0.58
1:A:221:GLN:HB3	1:A:222:PRO:HD3	1.87	0.57
1:E:49:GLU:O	1:F:92:GLN:HG2	2.05	0.57
1:D:310:ILE:HD13	1:D:310:ILE:N	2.19	0.57
1:F:435:GLU:O	1:F:439:GLU:HG3	2.05	0.57
1:C:115:ASN:ND2	1:C:117:GLN:H	2.03	0.56
1:E:126:SER:HB2	2:E:502:PLP:O4P	2.05	0.56
1:D:303:VAL:HG23	1:D:310:ILE:HD11	1.86	0.56
1:C:221:GLN:HB3	1:C:222:PRO:HD3	1.87	0.56
1:F:139:TRP:CD1	1:F:143:LYS:HE3	2.41	0.56
1:D:124:ILE:HD11	1:D:319:ARG:HD2	1.87	0.56
1:E:142:ARG:O	1:E:146:GLU:HG3	2.06	0.56
1:D:180:ILE:HD12	1:D:189:MET:HG3	1.88	0.55
1:A:70:GLU:HG2	1:A:74:LYS:HE3	1.88	0.55
1:F:182:MET:CE	1:F:412:GLY:H	2.19	0.55
1:A:61:ALA:HB2	1:A:407:PRO:HD3	1.87	0.55
1:C:395:LEU:HD21	1:C:441:TYR:CE2	2.42	0.54
1:E:315:ILE:HG21	1:F:315:ILE:HG21	1.90	0.54
1:D:418:ILE:HD12	1:D:418:ILE:N	2.22	0.54
1:A:441:TYR:CE1	1:A:445:LEU:HD11	2.43	0.54
1:E:92:GLN:HG2	1:F:49:GLU:O	2.07	0.54
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.73	0.54
1:F:410:THR:HG22	1:F:419:VAL:HG22	1.90	0.54
1:F:8:ASP:O	1:F:12:GLU:HG3	2.08	0.53
1:B:370:ARG:NH1	1:B:370:ARG:HG2	2.23	0.53
1:D:126:SER:HB2	2:D:501:PLP:O4P	2.07	0.53
1:C:126:SER:HB2	2:C:501:PLP:O4P	2.08	0.53
1:D:305:TYR:CB	1:D:310:ILE:HD12	2.38	0.53
1:A:395:LEU:HD21	1:A:441:TYR:CE2	2.44	0.53
1:A:315:ILE:HG21	1:B:315:ILE:HG21	1.90	0.53
1:C:245:ALA:HA	1:C:272:ALA:HA	1.89	0.53
1:F:180:ILE:HD11	1:F:194:MET:HA	1.91	0.53
1:F:126:SER:HB2	2:F:502:PLP:O4P	2.09	0.53
1:D:245:ALA:HA	1:D:272:ALA:HA	1.90	0.53
1:D:383:LYS:HB2	1:D:386:GLU:HG3	1.91	0.52
1:E:61:ALA:HB2	1:E:407:PRO:HD3	1.89	0.52
1:E:441:TYR:HE1	1:E:445:LEU:HD11	1.73	0.52
1:A:92:GLN:HG2	1:B:49:GLU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TRP:CZ3	1:C:155:PRO:HB3	2.45	0.52
1:B:348[B]:GLN:HG2	1:B:431:MET:CE	2.39	0.52
1:C:73:HIS:HD2	1:D:77:ASP:OD1	1.93	0.51
1:D:293:GLU:HG3	4:D:7807:HOH:O	2.10	0.51
1:A:315:ILE:HG23	1:B:131[A]:MET:SD	2.51	0.51
1:E:129:ALA:HB1	1:E:287:VAL:HB	1.92	0.51
1:C:411:LEU:O	1:C:416:THR:HA	2.10	0.51
1:B:303:VAL:CG2	1:B:310:ILE:HG23	2.41	0.51
1:A:128:GLU:O	1:A:132:LEU:HG	2.11	0.50
1:C:315:ILE:HD13	1:D:315:ILE:HG21	1.92	0.50
1:A:143:LYS:NZ	1:A:298:GLU:OE2	2.33	0.50
1:A:171:ARG:NH1	1:B:298:GLU:O	2.42	0.50
1:B:160:GLY:O	1:B:179:GLU:HG3	2.12	0.50
1:B:129:ALA:HB1	1:B:287:VAL:HB	1.93	0.50
1:C:284:CYS:HB2	1:C:323:GLN:HB3	1.94	0.50
1:A:245:ALA:HA	1:A:272:ALA:HA	1.94	0.49
1:C:250:LEU:CD2	1:C:343:GLN:HG3	2.42	0.49
1:D:221:GLN:HB3	1:D:222:PRO:HD3	1.95	0.49
1:B:126:SER:HB2	2:B:500:PLP:O4P	2.12	0.49
1:C:250:LEU:HD23	1:C:343:GLN:CG	2.40	0.49
1:D:436:LEU:HD11	1:E:49:GLU:HB3	1.93	0.49
1:B:395:LEU:HD21	1:B:441:TYR:CE2	2.48	0.49
1:A:36:GLU:HG2	1:B:337:GLU:CD	2.33	0.49
1:C:129:ALA:HB1	1:C:287:VAL:HB	1.94	0.49
1:D:180:ILE:HD11	1:D:194:MET:HA	1.94	0.49
1:D:207:PRO:HG2	1:D:240:MET:HE2	1.95	0.49
1:F:372:ASP:OD1	1:F:373:GLU:HG3	2.13	0.49
1:E:38:ARG:HB3	1:E:40:ASP:OD1	2.13	0.48
1:B:192:LYS:O	1:B:196:GLU:HG3	2.12	0.48
1:C:441:TYR:CE1	1:C:445:LEU:HD11	2.48	0.48
1:D:224:HIS:CD2	1:D:266:ARG:HB2	2.49	0.48
1:B:438:LEU:CD2	1:B:442:LYS:HE3	2.43	0.48
1:A:298:GLU:H	1:A:298:GLU:CD	2.16	0.48
1:A:428:GLY:HA2	1:F:18:PHE:CE1	2.49	0.48
1:E:383:LYS:HB2	1:E:386:GLU:HG3	1.94	0.48
1:F:302:ASN:HD22	1:F:311:GLY:HA2	1.78	0.48
1:D:90:TYR:N	1:D:91:PRO:HD3	2.28	0.48
1:D:9:LEU:HG	1:F:9:LEU:HD21	1.94	0.47
1:E:321:ALA:O	1:E:324:VAL:HG12	2.14	0.47
1:F:245:ALA:HA	1:F:272:ALA:HA	1.95	0.47
1:A:219:PHE:O	1:A:222:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ARG:HD3	1:A:44:GLN:HB2	1.96	0.47
1:A:141:TRP:CZ3	1:A:155:PRO:HB3	2.49	0.47
1:C:315:ILE:HG23	1:D:131[A]:MET:SD	2.54	0.47
1:F:141:TRP:CZ3	1:F:155:PRO:HB3	2.49	0.47
1:A:157:LEU:HD13	1:A:157:LEU:C	2.34	0.47
1:C:182:MET:CE	1:C:187:LEU:HB3	2.44	0.47
1:C:255:ALA:N	1:C:256:PRO:HD3	2.30	0.47
1:F:186:GLN:O	1:F:186:GLN:HG3	2.15	0.47
1:A:446:LYS:HE3	1:A:450:ASP:OD2	2.15	0.47
1:A:36:GLU:HG2	1:B:337:GLU:OE1	2.14	0.47
1:A:129:ALA:HB1	1:A:287:VAL:HB	1.97	0.47
1:C:370:ARG:HD3	1:C:373:GLU:OE1	2.15	0.47
1:E:141:TRP:CZ3	1:E:155:PRO:HB3	2.50	0.47
1:F:34:LEU:O	1:F:34:LEU:HD23	2.14	0.47
1:D:26:ILE:HD13	1:E:435:GLU:HG2	1.96	0.46
1:B:451:HIS:N	1:B:452:PRO:HD3	2.30	0.46
1:B:428:GLY:HA2	1:C:18:PHE:CE1	2.51	0.46
1:B:348[B]:GLN:HG2	1:B:431:MET:HE2	1.96	0.46
1:C:398:ARG:HH11	1:C:398:ARG:CG	2.29	0.46
1:E:284:CYS:HB2	1:E:323:GLN:HB3	1.98	0.46
1:C:128:GLU:O	1:C:132:LEU:HG	2.15	0.46
1:B:435:GLU:O	1:B:439:GLU:HG3	2.14	0.46
1:E:180:ILE:N	1:E:180:ILE:HD12	2.31	0.46
1:A:114:LYS:HG2	4:A:5816:HOH:O	2.15	0.45
1:D:436:LEU:HD11	1:E:49:GLU:CB	2.46	0.45
1:E:395:LEU:HD21	1:E:441:TYR:CE2	2.51	0.45
1:B:141:TRP:CZ3	1:B:155:PRO:HB3	2.51	0.45
1:C:402:ARG:HE	1:C:440:ASP:CG	2.19	0.45
1:D:41:VAL:O	1:D:45:ILE:HG12	2.16	0.45
1:D:61:ALA:HB2	1:D:407:PRO:HD3	1.98	0.45
1:C:92:GLN:HG2	1:D:49:GLU:O	2.16	0.45
1:A:446:LYS:HA	1:A:446:LYS:NZ	2.31	0.45
1:C:228:ASP:HA	1:C:266:ARG:HH21	1.82	0.45
1:F:303:VAL:CG2	1:F:310:ILE:HG23	2.47	0.45
1:B:182:MET:CE	1:B:412:GLY:H	2.29	0.45
1:E:160:GLY:O	1:E:179:GLU:HG3	2.17	0.45
1:A:186:GLN:O	1:A:186:GLN:HG3	2.17	0.45
1:A:183:ARG:NH2	1:A:186:GLN:OE1	2.49	0.45
1:C:451:HIS:N	1:C:452:PRO:HD3	2.32	0.45
1:C:398:ARG:HG3	1:C:398:ARG:NH1	2.31	0.45
1:D:70:GLU:HG2	1:D:74:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLN:HG2	1:F:6:VAL:HG11	1.98	0.44
1:B:180:ILE:HD12	1:B:180:ILE:N	2.32	0.44
1:D:348:GLN:HE21	1:D:431:MET:HE3	1.81	0.44
1:A:273:SER:CB	1:A:276:LYS:HG3	2.48	0.44
1:D:451:HIS:N	1:D:452:PRO:HD3	2.32	0.44
1:A:88:GLU:OE1	1:A:305:TYR:HA	2.18	0.44
1:B:219:PHE:O	1:B:222:PRO:HD2	2.18	0.44
1:C:343:GLN:HA	1:C:343:GLN:OE1	2.17	0.44
1:D:348:GLN:HE21	1:D:431:MET:HE2	1.83	0.44
1:E:245:ALA:HA	1:E:272:ALA:HA	1.98	0.44
1:B:157:LEU:HD11	1:B:206:VAL:HG23	1.98	0.44
1:A:49:GLU:O	1:B:92:GLN:HG2	2.18	0.44
1:C:383:LYS:HB2	1:C:386:GLU:HG3	1.99	0.44
1:C:415:ALA:HB1	1:C:418:ILE:HD12	1.99	0.44
1:E:83:ASN:OD1	1:E:85:ILE:HG22	2.18	0.44
1:B:18:PHE:CE1	1:C:428:GLY:HA2	2.53	0.44
1:C:370:ARG:HD3	1:C:373:GLU:CD	2.38	0.43
1:D:192:LYS:O	1:D:196:GLU:HG3	2.17	0.43
1:D:219:PHE:O	1:D:222:PRO:HD2	2.18	0.43
1:E:370:ARG:HH11	1:E:370:ARG:HG2	1.83	0.43
1:F:45:ILE:O	1:F:49:GLU:HG3	2.18	0.43
1:A:364:GLU:OE1	1:A:381:LYS:HE3	2.18	0.43
1:A:381:LYS:HD2	1:A:418:ILE:HG23	1.99	0.43
1:C:122:ASN:HB2	1:C:286:TRP:CZ3	2.53	0.43
1:C:362:PRO:HA	4:C:8790:HOH:O	2.17	0.43
1:F:61:ALA:HB2	1:F:407:PRO:HD3	1.98	0.43
1:B:38:ARG:HB3	1:B:40:ASP:OD1	2.19	0.43
1:B:61:ALA:HB2	1:B:407:PRO:HD3	1.99	0.43
1:D:375:ILE:HB	1:D:376:PRO:CD	2.49	0.43
1:F:131[B]:MET:SD	1:F:169:PHE:HB2	2.58	0.43
1:A:273:SER:HB2	1:A:276:LYS:HG3	2.01	0.43
1:D:348:GLN:HE22	1:E:24:SER:HB2	1.83	0.43
1:D:141:TRP:CZ3	1:D:155:PRO:HB3	2.53	0.43
1:F:139:TRP:CE3	1:F:142:ARG:NH2	2.87	0.43
1:F:38:ARG:HB3	1:F:40:ASP:OD1	2.18	0.43
1:B:224:HIS:CD2	1:B:266:ARG:HB2	2.54	0.43
1:B:441:TYR:HE1	1:B:445:LEU:HD11	1.82	0.43
1:C:353:LEU:O	1:C:357:ILE:HG13	2.18	0.43
1:B:284:CYS:HB2	1:B:323:GLN:HB3	1.99	0.43
1:D:411:LEU:O	1:D:416:THR:HA	2.19	0.43
1:A:157:LEU:HD22	1:A:204:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:O	1:C:222:PRO:HD2	2.19	0.43
1:E:343:GLN:OE1	1:E:343:GLN:HA	2.19	0.43
1:F:375:ILE:HB	1:F:376:PRO:CD	2.49	0.43
1:A:224:HIS:CD2	1:A:266:ARG:HB2	2.54	0.42
1:A:353:LEU:O	1:A:357:ILE:HG13	2.19	0.42
1:F:219:PHE:O	1:F:222:PRO:HD2	2.19	0.42
1:F:360:LEU:HB3	1:F:445:LEU:CD1	2.49	0.42
1:A:410:THR:HG22	1:A:419:VAL:HG22	2.00	0.42
1:B:59:ASN:HA	1:B:405:GLN:HB2	2.01	0.42
1:C:115:ASN:C	1:C:115:ASN:HD22	2.22	0.42
1:F:34:LEU:HD22	1:F:35:HIS:CE1	2.54	0.42
1:A:424[A]:MET:HG2	4:A:5632:HOH:O	2.19	0.42
1:A:180:ILE:N	1:A:180:ILE:HD12	2.34	0.42
1:C:219:PHE:HA	1:C:220:PRO:HD3	1.91	0.42
1:B:112:ALA:HA	1:B:113:PRO:HD3	1.86	0.42
1:B:410:THR:HG22	1:B:419:VAL:HG22	2.01	0.42
1:B:23:ILE:CG1	1:B:45:ILE:HD11	2.39	0.42
1:C:360:LEU:HB3	1:C:445:LEU:CD1	2.49	0.42
1:F:221:GLN:HB3	1:F:222:PRO:HD3	2.01	0.42
1:C:315:ILE:HG21	1:D:315:ILE:HG21	2.02	0.42
1:F:157:LEU:HD11	1:F:206:VAL:HG23	2.02	0.42
1:A:86:ASP:HB3	1:A:89:GLU:HB2	2.00	0.42
1:E:28:GLU:CG	1:E:31:ARG:O	2.67	0.42
1:F:157:LEU:HD12	1:F:204:GLY:O	2.20	0.42
1:B:124:ILE:HD11	1:B:319:ARG:HD2	2.02	0.41
1:E:315:ILE:HG23	1:F:131[A]:MET:SD	2.60	0.41
1:A:38:ARG:HB3	1:A:40:ASP:OD1	2.20	0.41
1:E:128:GLU:O	1:E:132:LEU:HG	2.21	0.41
1:E:441:TYR:CE1	1:E:445:LEU:HD11	2.54	0.41
1:E:275:HIS:HA	1:E:280:ALA:O	2.21	0.41
1:E:86:ASP:OD2	3:E:9518:ACY:OXT	2.39	0.41
1:C:182:MET:HE1	1:C:187:LEU:HB3	2.01	0.41
1:B:122:ASN:HB2	1:B:286:TRP:CZ3	2.56	0.41
1:E:269:SER:HB3	1:E:289:TRP:CD1	2.56	0.41
1:B:381:LYS:HD2	1:B:418:ILE:HG23	2.03	0.41
1:D:124:ILE:CD1	1:D:319:ARG:HD2	2.48	0.41
1:E:261:ASP:HB2	1:E:262:PHE:H	1.64	0.41
1:F:122:ASN:HB2	1:F:286:TRP:CZ3	2.56	0.41
1:F:150:LYS:HB3	1:F:151:PRO:HD2	2.03	0.41
1:A:344:ASN:HA	1:A:344:ASN:HD22	1.68	0.41
1:C:49:GLU:O	1:D:92:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:ILE:HD12	1:E:424[A]:MET:HE1	2.02	0.41
1:F:319:ARG:HB2	1:F:320:PRO:HD2	2.03	0.40
1:A:284:CYS:HB2	1:A:323:GLN:HB3	2.04	0.40
1:A:49:GLU:HG2	1:F:436:LEU:HD11	2.03	0.40
1:B:41:VAL:O	1:B:45:ILE:HG12	2.21	0.40
1:B:99:ARG:O	1:B:103:MET:HG3	2.21	0.40
1:C:282:LEU:O	1:D:320:PRO:HG3	2.21	0.40
1:F:275:HIS:HA	1:F:280:ALA:O	2.21	0.40
1:A:432:ASP:O	1:A:436:LEU:HD23	2.21	0.40
1:B:441:TYR:CE1	1:B:445:LEU:HD11	2.56	0.40
1:C:186:GLN:O	1:C:186:GLN:HG3	2.21	0.40
1:C:224:HIS:CD2	1:C:266:ARG:HB2	2.56	0.40
1:F:192:LYS:O	1:F:196:GLU:HG3	2.20	0.40
1:F:451:HIS:N	1:F:452:PRO:HD3	2.36	0.40
1:A:432:ASP:OD2	1:F:49:GLU:OE2	2.40	0.40
1:B:275:HIS:HA	1:B:280:ALA:O	2.22	0.40
1:D:18:PHE:CE1	1:E:428:GLY:HA2	2.56	0.40
1:B:49:GLU:OE2	1:C:432:ASP:OD2	2.40	0.40
1:D:303:VAL:CG2	1:D:310:ILE:HD11	2.50	0.40
1:E:224:HIS:CD2	1:E:264:LEU:HB3	2.56	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	451/466 (97%)	440 (98%)	11 (2%)	0	100	100
1	B	451/466 (97%)	440 (98%)	11 (2%)	0	100	100
1	C	451/466 (97%)	439 (97%)	12 (3%)	0	100	100
1	D	451/466 (97%)	438 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	450/466 (97%)	439 (98%)	11 (2%)	0	100	100
1	F	451/466 (97%)	440 (98%)	11 (2%)	0	100	100
All	All	2705/2796 (97%)	2636 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	379/390 (97%)	376 (99%)	3 (1%)	85	88
1	B	379/390 (97%)	375 (99%)	4 (1%)	78	82
1	C	379/390 (97%)	370 (98%)	9 (2%)	54	56
1	D	379/390 (97%)	374 (99%)	5 (1%)	73	78
1	E	378/390 (97%)	375 (99%)	3 (1%)	85	88
1	F	379/390 (97%)	376 (99%)	3 (1%)	85	88
All	All	2273/2340 (97%)	2246 (99%)	27 (1%)	75	80

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	333	ARG
1	A	446	LYS
1	B	268	LYS
1	B	333	ARG
1	B	433	PHE
1	B	438	LEU
1	C	115	ASN
1	C	139	TRP
1	C	268	LYS
1	C	290	ARG
1	C	293	GLU

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Mol	Chain	Res	Type
1	C	333	ARG
1	C	343	GLN
1	C	398	ARG
1	C	433	PHE
1	D	310	ILE
1	D	333	ARG
1	D	400	ARG
1	D	414	GLU
1	D	438	LEU
1	E	21	LYS
1	E	299	LEU
1	E	333	ARG
1	F	333	ARG
1	F	414	GLU
1	F	417	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	35	HIS
1	A	81	ASN
1	A	344	ASN
1	B	5	GLN
1	B	81	ASN
1	B	297	GLN
1	B	302	ASN
1	B	344	ASN
1	C	5	GLN
1	C	73	HIS
1	C	81	ASN
1	C	115	ASN
1	C	297	GLN
1	C	344	ASN
1	D	81	ASN
1	D	109	HIS
1	D	201	ASN
1	D	221	GLN
1	D	297	GLN
1	D	348	GLN
1	E	81	ASN
1	F	221	GLN

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Mol	Chain	Res	Type
1	F	297	GLN
1	F	302	ASN
1	F	344	ASN
1	F	348	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PLP	A	500	1	15,15,16	0.91	0	20,22,23	1.45	5 (25%)
3	ACY	A	5518	-	1,3,3	2.88	1 (100%)	0,3,3	0.00	-
2	PLP	B	500	1	15,15,16	0.80	0	20,22,23	1.48	6 (30%)
3	ACY	B	6518	-	1,3,3	2.55	1 (100%)	0,3,3	0.00	-
2	PLP	C	501	1	15,15,16	0.90	0	20,22,23	1.47	6 (30%)
3	ACY	C	8518	-	1,3,3	2.82	1 (100%)	0,3,3	0.00	-
2	PLP	D	501	1	15,15,16	0.83	0	20,22,23	1.48	6 (30%)
3	ACY	D	7518	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PLP	E	502	1	15,15,16	0.91	1 (6%)	20,22,23	1.48	6 (30%)
3	ACY	E	9518	-	1,3,3	2.85	1 (100%)	0,3,3	0.00	-
3	ACY	E	9519	-	1,3,3	2.79	1 (100%)	0,3,3	0.00	-
2	PLP	F	502	1	15,15,16	0.84	0	20,22,23	1.48	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	A	500	1	-	0/6/6/8	0/1/1/1
3	ACY	A	5518	-	-	0/0/0/0	0/0/0/0
2	PLP	B	500	1	-	0/6/6/8	0/1/1/1
3	ACY	B	6518	-	-	0/0/0/0	0/0/0/0
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1
3	ACY	C	8518	-	-	0/0/0/0	0/0/0/0
2	PLP	D	501	1	-	0/6/6/8	0/1/1/1
3	ACY	D	7518	-	-	0/0/0/0	0/0/0/0
2	PLP	E	502	1	-	0/6/6/8	0/1/1/1
3	ACY	E	9518	-	-	0/0/0/0	0/0/0/0
3	ACY	E	9519	-	-	0/0/0/0	0/0/0/0
2	PLP	F	502	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	502	PLP	C3-C2	2.09	1.42	1.40
3	B	6518	ACY	CH3-C	2.55	1.52	1.48
3	D	7518	ACY	CH3-C	2.68	1.52	1.48
3	E	9519	ACY	CH3-C	2.79	1.52	1.48
3	C	8518	ACY	CH3-C	2.82	1.52	1.48
3	E	9518	ACY	CH3-C	2.85	1.52	1.48
3	A	5518	ACY	CH3-C	2.88	1.52	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	PLP	C3-C2-N1	-2.47	117.50	120.75
2	C	501	PLP	C3-C2-N1	-2.45	117.53	120.75
2	A	500	PLP	C3-C2-N1	-2.45	117.53	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	502	PLP	C3-C2-N1	-2.44	117.55	120.75
2	E	502	PLP	C3-C2-N1	-2.43	117.56	120.75
2	B	500	PLP	C3-C2-N1	-2.42	117.57	120.75
2	D	501	PLP	C4A-C4-C3	-2.12	116.88	120.54
2	B	500	PLP	C4A-C4-C3	-2.10	116.91	120.54
2	F	502	PLP	C4A-C4-C3	-2.08	116.94	120.54
2	C	501	PLP	C4A-C4-C3	-2.08	116.95	120.54
2	E	502	PLP	C4A-C4-C3	-2.08	116.96	120.54
2	A	500	PLP	O3P-P-O1P	2.07	118.59	110.50
2	A	500	PLP	C2A-C2-C3	2.07	123.43	120.96
2	F	502	PLP	O3P-P-O1P	2.09	118.68	110.50
2	F	502	PLP	C2A-C2-C3	2.09	123.46	120.96
2	B	500	PLP	O3P-P-O1P	2.10	118.73	110.50
2	C	501	PLP	C2A-C2-C3	2.10	123.47	120.96
2	B	500	PLP	C2A-C2-C3	2.11	123.48	120.96
2	E	502	PLP	O3P-P-O1P	2.12	118.78	110.50
2	D	501	PLP	C2A-C2-C3	2.13	123.50	120.96
2	D	501	PLP	O3P-P-O1P	2.13	118.84	110.50
2	C	501	PLP	O3P-P-O1P	2.14	118.89	110.50
2	E	502	PLP	C2A-C2-C3	2.18	123.57	120.96
2	A	500	PLP	C6-N1-C2	2.38	123.85	119.26
2	E	502	PLP	C6-N1-C2	2.39	123.86	119.26
2	C	501	PLP	C6-N1-C2	2.39	123.86	119.26
2	F	502	PLP	C6-N1-C2	2.40	123.88	119.26
2	D	501	PLP	C6-N1-C2	2.42	123.91	119.26
2	B	500	PLP	C6-N1-C2	2.44	123.95	119.26
2	A	500	PLP	C4A-C4-C5	3.01	123.89	120.86
2	D	501	PLP	C4A-C4-C5	3.08	123.97	120.86
2	B	500	PLP	C4A-C4-C5	3.10	123.99	120.86
2	F	502	PLP	C4A-C4-C5	3.13	124.02	120.86
2	E	502	PLP	C4A-C4-C5	3.13	124.02	120.86
2	C	501	PLP	C4A-C4-C5	3.27	124.16	120.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLP	1	0
2	B	500	PLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	PLP	1	0
2	D	501	PLP	1	0
2	E	502	PLP	1	0
3	E	9518	ACY	1	0
2	F	502	PLP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	450/466 (96%)	-0.20	9 (2%) 65 65	7, 13, 25, 44	0
1	B	450/466 (96%)	-0.19	11 (2%) 59 59	7, 13, 26, 44	0
1	C	449/466 (96%)	-0.14	8 (1%) 69 68	9, 15, 26, 44	0
1	D	450/466 (96%)	-0.19	11 (2%) 59 59	5, 13, 27, 42	0
1	E	449/466 (96%)	-0.18	12 (2%) 55 54	7, 14, 26, 46	0
1	F	450/466 (96%)	-0.18	10 (2%) 62 61	6, 13, 26, 44	0
All	All	2698/2796 (96%)	-0.18	61 (2%) 61 60	5, 14, 26, 46	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	452	PRO	6.8
1	D	452	PRO	6.4
1	E	452	PRO	6.2
1	A	452	PRO	5.0
1	F	385	GLY	4.9
1	B	452	PRO	4.9
1	A	114	LYS	4.7
1	C	452	PRO	4.6
1	D	385	GLY	4.6
1	E	114	LYS	4.4
1	C	114	LYS	4.3
1	B	385	GLY	4.0
1	D	5	GLN	3.7
1	F	4	LYS	3.7
1	D	4	LYS	3.6
1	F	5	GLN	3.5
1	B	3	LYS	3.4
1	C	451	HIS	3.4
1	B	5	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	450	ASP	3.3
1	E	451	HIS	3.3
1	B	114	LYS	3.2
1	B	451	HIS	3.1
1	A	307	GLY	3.1
1	F	450	ASP	3.0
1	D	3	LYS	3.0
1	A	385	GLY	2.9
1	B	417	ASP	2.9
1	F	451	HIS	2.9
1	C	450	ASP	2.8
1	A	450	ASP	2.8
1	A	451	HIS	2.7
1	D	384	ASP	2.7
1	F	417	ASP	2.7
1	C	386	GLU	2.7
1	F	384	ASP	2.7
1	D	114	LYS	2.6
1	B	450	ASP	2.6
1	A	417	ASP	2.6
1	E	307	GLY	2.6
1	A	386	GLU	2.6
1	D	450	ASP	2.6
1	B	4	LYS	2.6
1	D	307	GLY	2.6
1	C	385	GLY	2.5
1	E	449	SER	2.4
1	B	384	ASP	2.4
1	D	417	ASP	2.4
1	A	387	ASP	2.4
1	E	417	ASP	2.3
1	F	3	LYS	2.2
1	F	308	GLY	2.2
1	B	7	THR	2.2
1	E	5	GLN	2.2
1	E	304	ASP	2.2
1	E	308	GLY	2.1
1	D	451	HIS	2.1
1	E	386	GLU	2.1
1	E	185	GLY	2.1
1	C	417	ASP	2.0
1	C	446	LYS	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( $\text{\AA}^2$ )	Q<0.9
3	ACY	B	6518	4/4	0.97	0.13	2.18	14,15,15,15	0
3	ACY	E	9518	4/4	0.97	0.13	1.22	19,20,20,20	0
3	ACY	E	9519	4/4	0.96	0.11	0.78	17,17,17,17	0
2	PLP	A	500	15/16	0.97	0.09	0.33	11,12,13,13	0
3	ACY	D	7518	4/4	0.97	0.11	0.29	19,19,19,20	0
2	PLP	F	502	15/16	0.97	0.09	0.22	10,11,11,12	0
2	PLP	D	501	15/16	0.97	0.09	0.13	10,10,10,11	0
3	ACY	A	5518	4/4	0.98	0.09	-0.18	18,18,19,19	0
3	ACY	C	8518	4/4	0.97	0.10	-0.31	17,18,18,18	0
2	PLP	E	502	15/16	0.98	0.08	-0.33	11,12,13,13	0
2	PLP	C	501	15/16	0.96	0.09	-0.36	12,13,14,15	0
2	PLP	B	500	15/16	0.97	0.08	-0.58	11,11,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.