



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:20 AM GMT

PDB ID : 3E9I  
Title : Lysyl-tRNA synthetase from *Bacillus stearothermophilus* complexed with L-Lysine hydroxamate-AMP  
Authors : Sakurama, H.; Takita, T.; Mikami, B.; Itoh, T.; Yasukawa, K.; Inouye, K.  
Deposited on : 2008-08-22  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

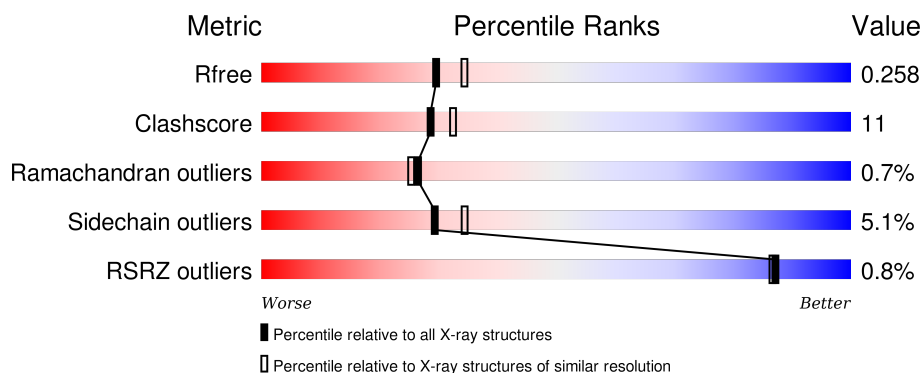
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	493	 75% 21% ..
1	B	493	 74% 22% ..
1	C	493	 75% 20% ...
1	D	493	 78% 18% ..

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
4	1PE	A	494	-	-	-	X
4	1PE	B	494	-	-	-	X
4	1PE	C	1202	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16520 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.

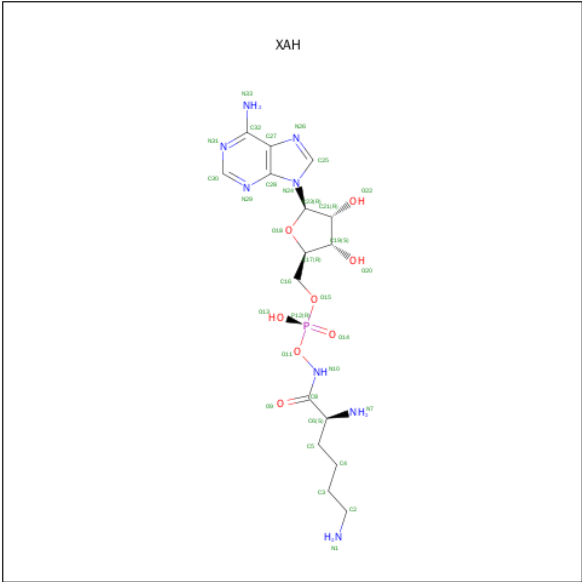
- Molecule 1 is a protein called Lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			
1	B	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			
1	C	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			
1	D	484	Total	C	N	O	S	0	0	0
			3956	2509	690	739	18			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

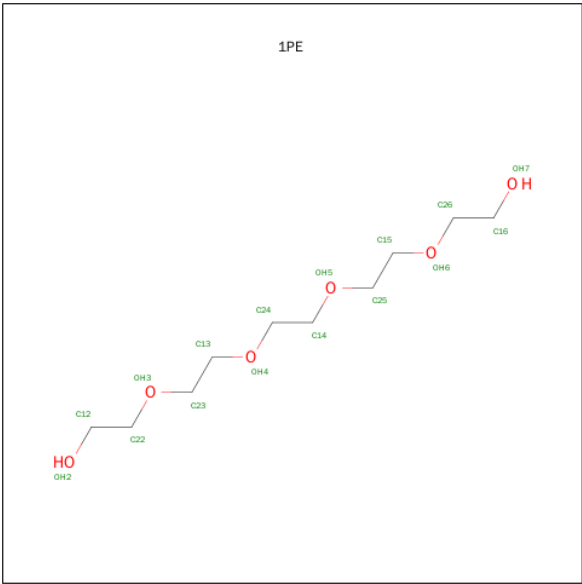
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 5'-O-{(R)-HYDROXY[(L-LYSYLAMINO)OXY]PHOSPHORYL}ADENOSINE (three-letter code: XAH) (formula: C<sub>16</sub>H<sub>27</sub>N<sub>8</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			33	16	8	8	1		
3	B	1	Total	C	N	O	P	0	0
			33	16	8	8	1		
3	C	1	Total	C	N	O	P	0	0
			33	16	8	8	1		
3	D	1	Total	C	N	O	P	0	0
			33	16	8	8	1		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	C	1	Total	C	O	0	0
			16	10	6		
4	C	1	Total	C	O	0	0
			16	10	6		

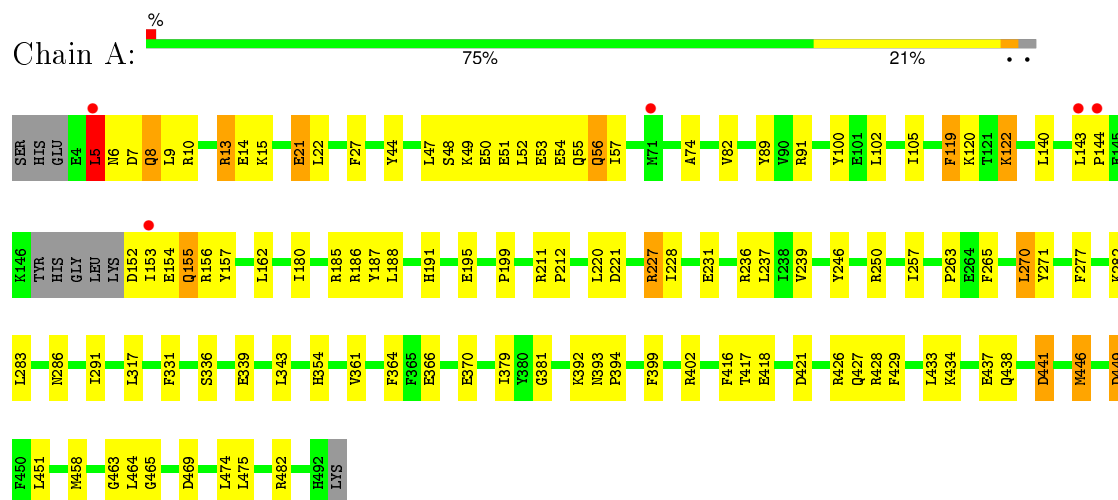
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	0
			111	111		
5	B	124	Total	O	0	0
			124	124		
5	C	128	Total	O	0	0
			128	128		
5	D	133	Total	O	0	0
			133	133		

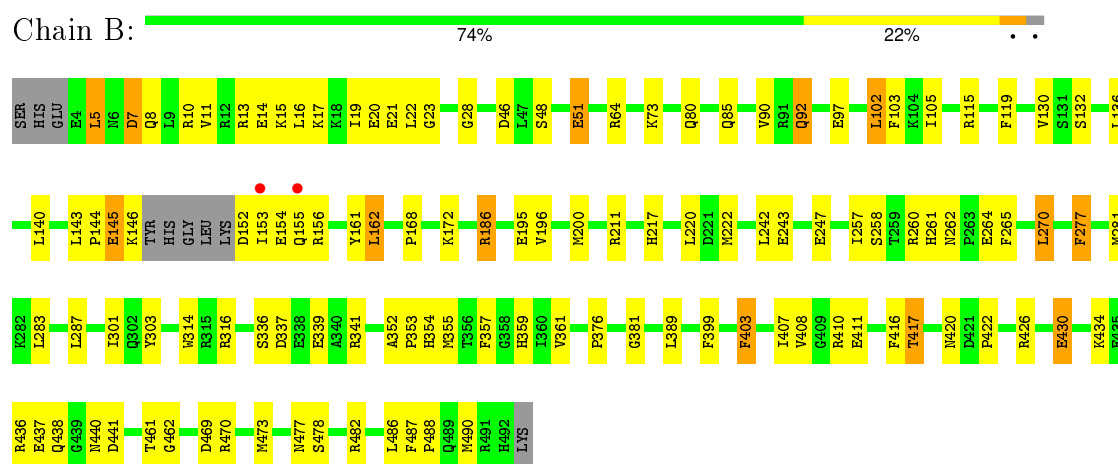
### 3 Residue-property plots

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.

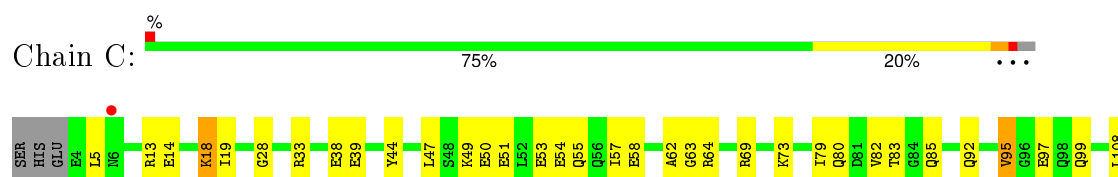
#### • Molecule 1: Lysyl-tRNA synthetase

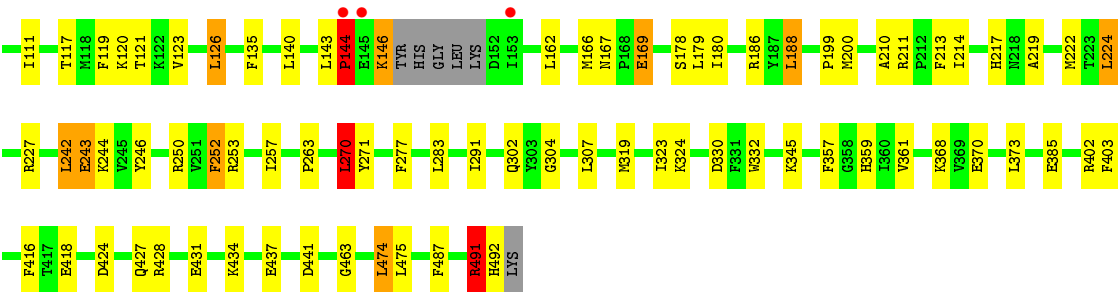


#### • Molecule 1: Lysyl-tRNA synthetase

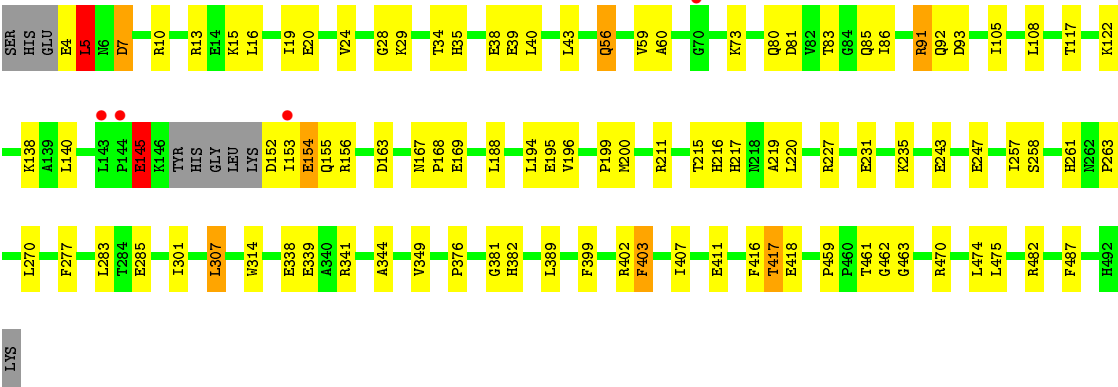
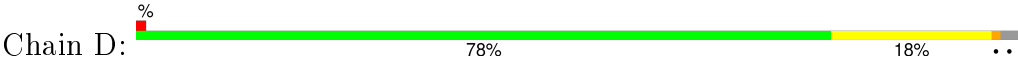


#### • Molecule 1: Lysyl-tRNA synthetase





● Molecule 1: Lysyl-tRNA synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.14Å 82.48Å 149.78Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	14.98 – 2.20 49.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	83.0 (14.98-2.20) 90.2 (49.93-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.45 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.182 , 0.246 0.197 , 0.258	Depositor DCC
$R_{free}$ test set	8789 reflections (10.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.021 for k,h,-l 0.020 for -k,-h,-l 0.479 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 92064 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: XAH, MG, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/4035	0.66	1/5433 (0.0%)
1	B	0.39	0/4035	0.65	1/5433 (0.0%)
1	C	0.39	0/4035	0.67	1/5433 (0.0%)
1	D	0.39	0/4035	0.66	1/5433 (0.0%)
All	All	0.39	0/16140	0.66	4/21732 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	THR	N-CA-C	-6.08	94.57	111.00
1	C	270	LEU	CA-CB-CG	5.52	128.00	115.30
1	D	417	THR	N-CA-C	-5.22	96.90	111.00
1	A	417	THR	N-CA-C	-5.00	97.49	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	3956	0	3921	105	0
1	B	3956	0	3921	105	0
1	C	3956	0	3921	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3956	0	3921	94	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	33	0	26	0	0
3	B	33	0	26	0	0
3	C	33	0	26	0	0
3	D	33	0	26	0	0
4	A	16	0	22	6	0
4	B	16	0	22	1	0
4	C	32	0	44	3	0
5	A	111	0	0	5	0
5	B	124	0	0	4	0
5	C	128	0	0	3	0
5	D	133	0	0	3	0
All	All	16520	0	15876	366	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 (366) 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:91:ARG:HH11	1:D:91:ARG:HB3	1.13	1.11
1:A:153:ILE:HG22	1:A:156:ARG:HH21	1.19	1.07
1:A:122:LYS:H	1:A:122:LYS:HE3	1.15	1.06
1:B:337:ASP:HB3	1:B:341:ARG:HH12	1.23	1.04
1:A:5:LEU:HD13	1:A:9:LEU:HG	1.45	0.96
1:D:217:HIS:HD2	1:D:220:LEU:H	1.09	0.93
1:D:73:LYS:HE3	1:D:92:GLN:HE22	1.32	0.92
1:B:73:LYS:HE3	1:B:92:GLN:HE21	1.36	0.91
1:C:213:PHE:HB3	1:D:215:THR:HG21	1.53	0.91
1:B:5:LEU:HB2	1:B:8:GLN:NE2	1.87	0.89
1:B:258:SER:HB3	1:B:261:HIS:HB2	1.55	0.88
1:D:217:HIS:CD2	1:D:220:LEU:H	1.92	0.87
1:C:144:PRO:HD3	1:C:162:LEU:HD22	1.58	0.85
1:A:122:LYS:H	1:A:122:LYS:CE	1.91	0.83
1:C:146:LYS:H	1:C:146:LYS:HD2	1.44	0.82
1:B:337:ASP:HB3	1:B:341:ARG:NH1	1.95	0.82
1:C:95:VAL:HG13	1:C:99:GLN:HB2	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PRO:HD3	1:A:162:LEU:HD22	1.62	0.81
1:B:5:LEU:HB2	1:B:8:GLN:HE21	1.46	0.80
1:A:153:ILE:HG22	1:A:156:ARG:NH2	1.96	0.80
1:A:153:ILE:HD12	1:A:482:ARG:HH11	1.46	0.79
1:B:217:HIS:HD2	1:B:220:LEU:H	1.28	0.79
1:B:73:LYS:HE3	1:B:92:GLN:NE2	1.97	0.79
1:A:153:ILE:HB	1:A:157:TYR:CE2	2.19	0.78
1:C:167:ASN:HB3	1:C:169:GLU:OE1	1.82	0.78
1:B:211:ARG:HH21	1:B:211:ARG:HG3	1.48	0.78
1:C:214:ILE:O	1:D:215:THR:HG23	1.83	0.77
1:C:427:GLN:O	1:C:431:GLU:HG2	1.85	0.77
1:A:8:GLN:HE21	1:A:8:GLN:HA	1.47	0.77
1:B:217:HIS:CD2	1:B:220:LEU:H	2.03	0.77
1:B:152:ASP:HB3	1:B:155:GLN:OE1	1.85	0.77
1:A:22:LEU:HD13	1:A:102:LEU:HD22	1.65	0.76
1:A:82:VAL:HB	1:B:243:GLU:HG3	1.67	0.76
1:A:270:LEU:HD12	1:A:271:TYR:N	2.01	0.76
1:D:91:ARG:HB3	1:D:91:ARG:NH1	1.96	0.75
1:A:154:GLU:HG3	1:A:155:GLN:H	1.52	0.75
1:B:7:ASP:O	1:B:11:VAL:HG23	1.87	0.74
1:C:38:GLU:HG2	1:C:83:THR:HB	1.68	0.74
1:D:91:ARG:HH11	1:D:91:ARG:CB	1.99	0.74
1:A:153:ILE:HD12	1:A:482:ARG:NH1	2.02	0.73
1:D:73:LYS:HG3	1:D:92:GLN:HE21	1.52	0.73
1:D:73:LYS:HG3	1:D:92:GLN:NE2	2.04	0.72
1:B:17:LYS:HE3	1:B:21:GLU:OE1	1.90	0.72
1:D:215:THR:HG22	1:D:216:HIS:H	1.55	0.72
1:D:56:GLN:HG3	1:D:117:THR:HG21	1.73	0.71
1:A:366:GLU:HA	1:A:370:GLU:HG3	1.72	0.71
1:D:73:LYS:HE3	1:D:92:GLN:NE2	2.06	0.71
1:B:152:ASP:HB2	1:B:155:GLN:HB2	1.73	0.70
1:C:424:ASP:O	1:C:428:ARG:HG2	1.92	0.70
1:D:153:ILE:HG13	1:D:154:GLU:N	2.07	0.69
1:C:140:LEU:HD23	5:C:710:HOH:O	1.91	0.68
1:A:8:GLN:HE21	1:A:8:GLN:CA	2.05	0.68
1:D:40:LEU:HD21	1:D:59:VAL:HG21	1.75	0.68
1:D:35:HIS:ND1	1:D:59:VAL:HG23	2.08	0.68
1:C:38:GLU:HG2	1:C:83:THR:CB	2.24	0.68
1:C:143:LEU:HB3	1:C:144:PRO:HD2	1.76	0.68
1:A:144:PRO:HG3	1:A:162:LEU:HD13	1.76	0.67
1:C:49:LYS:O	1:C:53:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:HG21	1:B:103:PHE:CG	2.29	0.67
1:A:143:LEU:HG	5:A:983:HOH:O	1.94	0.67
1:C:73:LYS:HD2	1:C:92:GLN:NE2	2.10	0.66
1:A:89:TYR:CE2	1:A:91:ARG:HD3	2.31	0.65
1:A:89:TYR:CZ	1:A:91:ARG:HD3	2.32	0.65
1:A:156:ARG:HD2	5:A:622:HOH:O	1.96	0.65
1:A:270:LEU:C	1:A:270:LEU:HD12	2.18	0.64
1:C:178:SER:OG	1:D:194:LEU:HD21	1.96	0.64
1:B:211:ARG:HG3	1:B:211:ARG:NH2	2.08	0.64
1:A:428:ARG:HD2	5:A:604:HOH:O	1.97	0.64
1:C:92:GLN:OE1	1:C:97:GLU:HG2	1.97	0.64
1:D:257:ILE:HG23	1:D:261:HIS:O	1.97	0.64
1:D:7:ASP:HA	1:D:10:ARG:NH1	2.13	0.63
1:D:301:ILE:HD11	1:D:474:LEU:HG	1.79	0.63
1:A:22:LEU:HD13	1:A:102:LEU:CD2	2.27	0.63
1:D:194:LEU:HD22	1:D:196:VAL:CG1	2.29	0.63
1:D:38:GLU:HB2	1:D:83:THR:HB	1.80	0.63
1:C:64:ARG:HD3	1:C:143:LEU:HD11	1.79	0.63
1:C:95:VAL:HG13	1:C:99:GLN:CB	2.28	0.63
1:C:418:GLU:OE1	1:C:463:GLY:HA3	1.99	0.62
1:A:236:ARG:HH21	1:A:449:ASP:HB3	1.64	0.62
1:A:49:LYS:O	1:A:53:GLU:HG3	1.99	0.62
1:C:270:LEU:C	1:C:270:LEU:HD12	2.20	0.62
1:B:301:ILE:HA	5:B:662:HOH:O	1.99	0.61
1:A:186:ARG:HH11	1:A:186:ARG:HG2	1.65	0.61
1:B:17:LYS:C	1:B:17:LYS:HD3	2.20	0.61
1:C:180:ILE:HG23	1:C:291:ILE:HG21	1.83	0.61
1:D:155:GLN:HA	1:D:155:GLN:HE21	1.66	0.61
1:D:155:GLN:HA	1:D:155:GLN:NE2	2.16	0.61
1:A:52:LEU:HD13	1:A:119:PHE:HA	1.82	0.61
1:D:16:LEU:HD22	1:D:140:LEU:HD21	1.82	0.61
1:C:63:GLY:HA3	1:C:79:ILE:HG23	1.82	0.61
1:C:257:ILE:HG22	1:C:263:PRO:HD3	1.83	0.60
1:A:122:LYS:HE3	1:A:122:LYS:N	2.01	0.60
1:B:341:ARG:HH11	1:B:341:ARG:HG3	1.66	0.60
1:C:38:GLU:HG3	1:C:39:GLU:N	2.16	0.60
1:C:18:LYS:HE2	1:C:18:LYS:HA	1.83	0.60
1:D:217:HIS:CD2	1:D:220:LEU:HG	2.36	0.60
1:B:13:ARG:HH11	1:B:13:ARG:HG2	1.66	0.59
1:B:7:ASP:HB3	1:B:10:ARG:NH2	2.17	0.59
1:A:282:LYS:HE3	1:A:286:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HG12	1:C:491:ARG:NH2	2.18	0.59
1:B:381:GLY:O	1:B:399:PHE:HB3	2.03	0.59
1:A:186:ARG:HH11	4:B:494:1PE:H161	1.67	0.59
1:C:434:LYS:O	1:C:437:GLU:HB2	2.03	0.59
1:D:39:GLU:O	1:D:43:LEU:HG	2.03	0.58
1:A:57:ILE:HG12	1:C:491:ARG:HH22	1.68	0.58
1:A:426:ARG:NH1	1:A:451:LEU:HD13	2.18	0.58
1:D:80:GLN:HB2	1:D:85:GLN:HG2	1.85	0.58
1:A:50:GLU:O	1:A:54:GLU:HG3	2.04	0.57
1:A:15:LYS:HE2	1:A:105:ILE:HG13	1.86	0.57
1:C:58:GLU:HG3	1:C:117:THR:HG22	1.85	0.57
1:A:429:PHE:HB3	1:A:446:MET:HG2	1.86	0.57
1:B:80:GLN:HB2	1:B:85:GLN:HG2	1.87	0.57
1:B:426:ARG:O	1:B:430:GLU:HG2	2.04	0.57
1:A:227:ARG:HD2	1:A:250:ARG:O	2.04	0.57
1:B:482:ARG:HH12	1:B:490:MET:HE2	1.70	0.56
1:C:38:GLU:HG3	1:C:39:GLU:H	1.71	0.56
1:D:194:LEU:HD22	1:D:196:VAL:HG13	1.87	0.56
1:A:185:ARG:HH22	1:B:195:GLU:CD	2.09	0.56
1:D:152:ASP:OD2	1:D:154:GLU:HG3	2.04	0.56
1:C:144:PRO:HD2	1:C:166:MET:HE2	1.88	0.55
1:B:13:ARG:HG2	1:B:13:ARG:NH1	2.22	0.55
1:C:199:PRO:CG	1:D:487:PHE:HB2	2.36	0.55
1:D:376:PRO:HA	1:D:407:ILE:HG12	1.88	0.55
1:C:319:MET:O	1:C:323:ILE:HG12	2.05	0.55
1:B:220:LEU:O	1:B:222:MET:HG3	2.06	0.55
1:D:153:ILE:HA	1:D:156:ARG:NH1	2.22	0.55
1:D:154:GLU:OE2	1:D:155:GLN:HG2	2.06	0.55
1:B:186:ARG:HB3	1:B:186:ARG:HH11	1.71	0.54
1:C:487:PHE:HB2	1:D:199:PRO:CG	2.37	0.54
1:D:19:ILE:HG22	1:D:24:VAL:HG13	1.90	0.54
1:B:90:VAL:HG21	1:B:103:PHE:CD2	2.43	0.54
1:B:217:HIS:CD2	1:B:220:LEU:HG	2.43	0.54
1:A:180:ILE:HG23	1:A:291:ILE:HG21	1.89	0.54
1:B:355:MET:HB3	1:B:359:HIS:HB2	1.90	0.54
1:A:185:ARG:NH2	1:B:195:GLU:OE2	2.41	0.53
1:A:9:LEU:O	1:A:13:ARG:HB2	2.08	0.53
1:B:258:SER:HB3	1:B:261:HIS:CB	2.32	0.53
1:D:156:ARG:HD3	1:D:163:ASP:OD1	2.08	0.53
1:A:186:ARG:HE	4:A:494:1PE:H232	1.72	0.53
1:B:434:LYS:O	1:B:437:GLU:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HG22	1:A:263:PRO:HD3	1.90	0.53
1:A:27:PHE:CZ	1:B:422:PRO:HD2	2.45	0.52
1:A:211:ARG:CZ	1:A:441:ASP:OD2	2.58	0.52
1:D:153:ILE:N	1:D:156:ARG:NH1	2.58	0.52
1:C:146:LYS:N	1:C:146:LYS:HD2	2.21	0.52
1:A:10:ARG:O	1:A:14:GLU:HG3	2.09	0.52
1:D:56:GLN:CA	1:D:56:GLN:HE21	2.23	0.52
1:D:34:THR:HG1	1:D:59:VAL:HG23	1.75	0.52
1:A:188:LEU:HD23	1:A:246:TYR:CD1	2.45	0.52
1:D:411:GLU:HG2	1:D:470:ARG:NH1	2.25	0.52
1:C:143:LEU:HB3	1:C:144:PRO:CD	2.39	0.51
1:A:152:ASP:HB3	1:A:154:GLU:HG2	1.90	0.51
1:B:260:ARG:HH11	1:B:260:ARG:HG2	1.74	0.51
1:B:172:LYS:HE3	5:B:637:HOH:O	2.09	0.51
1:A:48:SER:N	1:A:51:GLU:OE1	2.34	0.51
1:D:338:GLU:HA	1:D:338:GLU:OE1	2.10	0.51
1:D:35:HIS:HB3	1:D:39:GLU:HG3	1.92	0.51
1:C:357:PHE:O	1:C:361:VAL:HG23	2.11	0.51
1:B:336:SER:OG	1:B:339:GLU:HG3	2.11	0.51
1:B:217:HIS:NE2	1:B:220:LEU:HG	2.26	0.51
1:B:211:ARG:NH1	1:B:441:ASP:OD2	2.43	0.51
1:A:186:ARG:NE	4:A:494:1PE:H232	2.26	0.51
1:A:429:PHE:O	1:A:433:LEU:HD13	2.10	0.51
1:C:222:MET:HG3	1:C:224:LEU:HD13	1.91	0.51
1:A:418:GLU:OE1	1:A:463:GLY:HA3	2.10	0.51
1:B:341:ARG:HG3	1:B:341:ARG:NH1	2.26	0.51
1:B:115:ARG:HB2	1:B:132:SER:HB3	1.92	0.51
1:B:403:PHE:C	1:B:403:PHE:CD1	2.84	0.50
1:D:215:THR:HG22	1:D:216:HIS:N	2.23	0.50
1:D:257:ILE:HG12	1:D:263:PRO:HD3	1.92	0.50
1:A:211:ARG:NH2	1:A:441:ASP:OD2	2.44	0.50
1:A:186:ARG:NH1	1:A:186:ARG:HG2	2.26	0.50
1:C:359:HIS:CE1	1:C:385:GLU:HB3	2.45	0.50
1:D:211:ARG:HG2	5:D:866:HOH:O	2.11	0.50
1:A:5:LEU:HD21	5:A:532:HOH:O	2.11	0.50
1:A:186:ARG:HE	4:A:494:1PE:C22	2.25	0.50
1:B:90:VAL:HG12	1:B:130:VAL:HB	1.94	0.50
1:A:434:LYS:O	1:A:437:GLU:HB2	2.12	0.50
1:D:418:GLU:OE1	1:D:463:GLY:HA3	2.11	0.50
1:C:211:ARG:NE	1:C:441:ASP:OD2	2.44	0.50
1:A:48:SER:OG	1:A:51:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LYS:HD3	1:D:105:ILE:HG23	1.94	0.49
1:A:153:ILE:CG2	1:A:156:ARG:HH21	2.07	0.49
1:A:55:GLN:O	1:A:56:GLN:C	2.50	0.49
1:A:250:ARG:HB2	1:B:200:MET:HE3	1.94	0.49
1:C:47:LEU:O	1:C:120:LYS:HE2	2.13	0.49
1:B:352:ALA:HB3	1:B:355:MET:HG3	1.94	0.49
1:A:5:LEU:HB2	1:A:8:GLN:HB3	1.94	0.49
1:A:187:TYR:O	1:A:191:HIS:HD2	1.96	0.49
1:B:461:THR:HG22	1:B:462:GLY:N	2.27	0.49
1:A:5:LEU:O	1:A:6:ASN:C	2.50	0.49
1:C:13:ARG:HH11	1:C:13:ARG:HG2	1.78	0.49
1:B:408:VAL:HG23	1:B:408:VAL:O	2.13	0.48
1:B:172:LYS:HB3	5:B:637:HOH:O	2.13	0.48
1:D:417:THR:HG23	5:D:711:HOH:O	2.13	0.48
1:C:270:LEU:HD12	1:C:271:TYR:N	2.29	0.48
1:A:239:VAL:HG22	1:A:458:MET:HB2	1.95	0.48
1:D:19:ILE:CG2	1:D:24:VAL:HG13	2.42	0.48
1:D:7:ASP:HA	1:D:10:ARG:HH12	1.76	0.48
1:B:270:LEU:C	1:B:270:LEU:HD23	2.34	0.48
1:C:50:GLU:O	1:C:54:GLU:HG2	2.13	0.48
1:B:46:ASP:OD1	1:C:73:LYS:NZ	2.47	0.48
1:D:16:LEU:O	1:D:20:GLU:HG3	2.13	0.48
1:C:402:ARG:HA	1:C:416:PHE:HB3	1.95	0.48
1:A:154:GLU:HG3	1:A:155:GLN:N	2.25	0.48
1:A:7:ASP:HB3	1:A:10:ARG:HH12	1.79	0.47
1:B:376:PRO:HA	1:B:407:ILE:HG12	1.96	0.47
1:C:63:GLY:CA	1:C:79:ILE:HG23	2.45	0.47
1:C:82:VAL:HB	1:D:243:GLU:HG3	1.97	0.47
1:D:217:HIS:NE2	1:D:220:LEU:HG	2.29	0.47
1:A:152:ASP:CG	1:A:154:GLU:HG2	2.35	0.47
1:B:354:HIS:CD2	1:B:440:ASN:HB2	2.49	0.47
1:B:420:ASN:O	1:B:422:PRO:HD3	2.15	0.47
1:A:199:PRO:CG	1:B:487:PHE:HB2	2.45	0.47
1:C:330:ASP:OD1	1:C:332:TRP:HB2	2.15	0.47
1:B:303:TYR:HA	1:B:477:ASN:OD1	2.13	0.47
1:C:200:MET:HA	1:C:227:ARG:HD3	1.96	0.47
1:B:257:ILE:CG2	1:B:258:SER:N	2.77	0.47
1:D:153:ILE:HG13	1:D:154:GLU:H	1.78	0.47
1:B:16:LEU:C	1:B:16:LEU:HD23	2.34	0.47
1:B:15:LYS:HD3	1:B:105:ILE:HG23	1.97	0.47
1:D:194:LEU:HD23	1:D:194:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ALA:HB1	1:C:253:ARG:HG2	1.96	0.47
1:C:243:GLU:OE2	1:D:81:ASP:HB2	2.15	0.47
1:A:265:PHE:HB2	1:A:469:ASP:OD2	2.15	0.47
1:C:250:ARG:HB2	1:D:200:MET:HE3	1.97	0.47
1:D:196:VAL:O	1:D:247:GLU:HG3	2.14	0.46
1:A:186:ARG:HE	4:A:494:1PE:H221	1.78	0.46
1:C:44:TYR:HB2	1:C:126:LEU:HD11	1.96	0.46
1:B:196:VAL:O	1:B:247:GLU:HG3	2.15	0.46
1:D:301:ILE:CD1	1:D:474:LEU:HG	2.46	0.46
1:D:403:PHE:C	1:D:403:PHE:CD1	2.88	0.46
1:B:17:LYS:O	1:B:17:LYS:HD3	2.14	0.46
1:D:194:LEU:HD23	1:D:195:GLU:N	2.31	0.46
1:C:18:LYS:CA	1:C:18:LYS:HE2	2.44	0.46
1:C:80:GLN:HB2	1:C:85:GLN:HG2	1.98	0.46
1:B:436:ARG:HA	1:B:440:ASN:O	2.16	0.46
1:C:33:ARG:HD3	1:C:62:ALA:HB3	1.96	0.46
1:A:231:GLU:HG3	1:A:271:TYR:OH	2.15	0.46
1:C:403:PHE:CD1	1:C:403:PHE:C	2.89	0.46
1:B:48:SER:OG	1:B:51:GLU:HB3	2.16	0.45
1:C:111:ILE:HD13	1:D:459:PRO:HB3	1.98	0.45
1:C:79:ILE:O	1:C:85:GLN:HA	2.16	0.45
1:C:51:GLU:O	1:C:55:GLN:HG3	2.16	0.45
1:D:145:GLU:HG3	1:D:145:GLU:H	1.48	0.45
1:B:161:TYR:CD1	1:B:162:LEU:HD13	2.52	0.45
1:B:488:PRO:O	1:B:490:MET:HE3	2.16	0.45
1:C:188:LEU:HD23	1:C:246:TYR:CD1	2.51	0.45
1:C:178:SER:OG	1:D:194:LEU:CD2	2.63	0.45
1:D:211:ARG:HH11	1:D:211:ARG:HG3	1.82	0.45
1:D:4:GLU:HB3	1:D:5:LEU:H	1.59	0.45
1:C:186:ARG:CZ	4:C:1202:1PE:H222	2.47	0.45
1:D:59:VAL:HG22	1:D:60:ALA:N	2.32	0.45
5:C:825:HOH:O	1:D:29:LYS:HE3	2.17	0.45
1:B:352:ALA:HB1	1:B:353:PRO:HD2	1.99	0.44
1:D:56:GLN:HA	1:D:56:GLN:HE21	1.81	0.44
1:B:90:VAL:HG21	1:B:103:PHE:CD1	2.52	0.44
1:B:90:VAL:O	1:B:90:VAL:HG23	2.17	0.44
1:C:402:ARG:HB2	1:C:416:PHE:HB3	1.98	0.44
1:A:381:GLY:O	1:A:399:PHE:HB3	2.17	0.44
1:A:331:PHE:CG	1:A:361:VAL:HG22	2.53	0.44
1:A:44:TYR:CE1	1:A:57:ILE:HG21	2.52	0.44
1:B:16:LEU:HD12	1:B:140:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:HB3	1:A:228:ILE:CG2	2.47	0.44
1:A:52:LEU:HD13	1:A:119:PHE:CA	2.47	0.44
1:C:47:LEU:HA	1:C:51:GLU:OE2	2.18	0.44
1:B:277:PHE:O	1:B:281:MET:HG3	2.16	0.44
1:A:270:LEU:CD1	1:A:271:TYR:N	2.75	0.44
1:B:153:ILE:HG23	1:B:154:GLU:N	2.32	0.44
1:A:52:LEU:CD1	1:A:119:PHE:HA	2.48	0.44
1:C:242:LEU:O	1:C:244:LYS:N	2.46	0.44
1:A:464:LEU:HD12	1:A:465:GLY:H	1.83	0.44
1:C:323:ILE:HB	5:C:807:HOH:O	2.18	0.43
1:D:231:GLU:OE1	1:D:235:LYS:NZ	2.49	0.43
1:D:382:HIS:HB2	1:D:402:ARG:HD3	1.99	0.43
1:B:152:ASP:O	1:B:156:ARG:HG3	2.18	0.43
1:B:482:ARG:NH1	1:B:490:MET:HE2	2.32	0.43
1:B:19:ILE:O	1:B:22:LEU:HB3	2.19	0.43
1:D:341:ARG:HG2	1:D:341:ARG:HH21	1.83	0.43
1:D:217:HIS:HD2	1:D:220:LEU:N	1.93	0.43
1:B:5:LEU:HD13	1:B:8:GLN:NE2	2.34	0.43
1:D:153:ILE:CA	1:D:156:ARG:NH1	2.82	0.43
1:B:7:ASP:CB	1:B:10:ARG:NH2	2.81	0.43
1:B:301:ILE:HD12	1:B:301:ILE:O	2.17	0.43
4:A:494:1PE:H151	5:A:545:HOH:O	2.19	0.43
1:B:265:PHE:HB2	1:B:469:ASP:OD2	2.18	0.43
1:A:270:LEU:C	1:A:270:LEU:CD1	2.86	0.43
1:A:393:ASN:HA	1:A:394:PRO:HD3	1.88	0.43
1:D:270:LEU:HD23	1:D:270:LEU:C	2.39	0.43
1:A:421:ASP:C	1:A:421:ASP:OD2	2.57	0.43
1:A:122:LYS:CE	1:A:122:LYS:N	2.70	0.43
1:D:152:ASP:CG	1:D:153:ILE:N	2.71	0.43
1:D:153:ILE:HA	1:D:156:ARG:HH11	1.83	0.43
1:D:257:ILE:HG22	1:D:258:SER:N	2.34	0.42
1:C:121:THR:OG1	1:C:123:VAL:HG22	2.19	0.42
1:B:5:LEU:HD13	1:B:8:GLN:HE22	1.84	0.42
1:A:446:MET:SD	1:A:451:LEU:HD11	2.59	0.42
1:C:474:LEU:HD13	1:C:475:LEU:HD12	2.02	0.42
1:D:461:THR:HG22	1:D:462:GLY:N	2.34	0.42
1:D:91:ARG:NH1	1:D:93:ASP:OD2	2.52	0.42
1:B:488:PRO:HG2	1:B:490:MET:CE	2.49	0.42
1:A:47:LEU:HA	1:A:51:GLU:OE1	2.20	0.42
1:B:473:MET:HA	1:B:478:SER:HB2	2.00	0.42
1:D:56:GLN:NE2	1:D:56:GLN:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LYS:HE2	1:C:18:LYS:O	2.18	0.42
1:B:417:THR:HG23	5:B:503:HOH:O	2.19	0.42
1:D:122:LYS:HD2	5:D:998:HOH:O	2.20	0.42
1:B:436:ARG:C	1:B:438:GLN:N	2.72	0.42
1:D:167:ASN:HA	1:D:168:PRO:HD2	1.81	0.42
1:B:14:GLU:HA	1:B:14:GLU:OE2	2.19	0.42
1:B:64:ARG:HD3	1:B:143:LEU:HD21	2.01	0.42
1:B:301:ILE:HD12	1:B:301:ILE:C	2.39	0.42
1:B:314:TRP:CD2	1:B:376:PRO:HB2	2.55	0.42
1:B:357:PHE:O	1:B:361:VAL:HG23	2.20	0.42
1:A:354:HIS:HA	1:A:438:GLN:HE21	1.84	0.42
1:A:317:LEU:O	1:A:379:ILE:HA	2.20	0.42
1:B:260:ARG:HG3	1:B:470:ARG:NH2	2.35	0.42
1:A:220:LEU:O	1:A:221:ASP:C	2.57	0.42
1:A:152:ASP:CB	1:A:154:GLU:HG2	2.50	0.41
1:C:186:ARG:HD2	4:C:494:1PE:OH7	2.20	0.41
1:A:402:ARG:HB2	1:A:416:PHE:HB3	2.00	0.41
1:A:195:GLU:HB2	1:A:246:TYR:CZ	2.55	0.41
1:C:307:LEU:HD12	1:C:307:LEU:N	2.35	0.41
1:A:74:ALA:N	1:A:100:TYR:OH	2.53	0.41
1:C:402:ARG:CB	1:C:416:PHE:HB3	2.51	0.41
1:D:200:MET:HA	1:D:227:ARG:HD3	2.03	0.41
1:B:20:GLU:O	1:B:23:GLY:N	2.50	0.41
1:A:21:GLU:OE2	1:A:21:GLU:HA	2.19	0.41
1:C:217:HIS:HE1	1:C:219:ALA:HB3	1.84	0.41
1:C:252:PHE:CD1	1:C:252:PHE:N	2.88	0.41
1:A:336:SER:OG	1:A:339:GLU:HG3	2.19	0.41
1:B:145:GLU:OE2	1:B:146:LYS:N	2.53	0.41
1:A:143:LEU:HB3	1:A:144:PRO:CD	2.50	0.41
1:A:186:ARG:HH21	4:A:494:1PE:H221	1.86	0.41
1:D:307:LEU:HA	1:D:307:LEU:HD22	1.83	0.41
1:A:199:PRO:HG2	1:B:487:PHE:HB2	2.02	0.41
1:D:285:GLU:HA	1:D:314:TRP:CH2	2.55	0.41
1:A:49:LYS:HE3	1:A:120:LYS:O	2.21	0.41
1:C:57:ILE:O	1:C:117:THR:HA	2.20	0.41
1:B:407:ILE:O	1:B:408:VAL:C	2.59	0.41
1:A:339:GLU:O	1:A:343:LEU:HG	2.20	0.41
1:C:302:GLN:NE2	1:C:304:GLY:O	2.49	0.41
1:C:144:PRO:CD	1:C:166:MET:HE2	2.49	0.41
1:B:17:LYS:CD	1:B:17:LYS:C	2.89	0.41
1:C:19:ILE:HD13	1:C:135:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:N	1:C:140:LEU:HD22	2.35	0.41
1:A:392:LYS:HG3	1:A:428:ARG:NH1	2.36	0.41
1:B:168:PRO:O	1:B:172:LYS:HG2	2.21	0.41
1:A:152:ASP:C	1:A:154:GLU:H	2.24	0.40
1:D:301:ILE:HD13	1:D:475:LEU:HD23	2.03	0.40
1:B:430:GLU:H	1:B:430:GLU:HG2	1.49	0.40
1:D:381:GLY:O	1:D:399:PHE:HB3	2.20	0.40
1:B:5:LEU:HD12	1:B:5:LEU:O	2.20	0.40
1:D:194:LEU:HD22	1:D:196:VAL:HG12	2.03	0.40
1:C:199:PRO:HG2	1:D:487:PHE:HB2	2.03	0.40
1:B:102:LEU:HA	1:B:102:LEU:HD12	1.84	0.40
1:B:145:GLU:HA	1:B:145:GLU:OE2	2.21	0.40
1:D:344:ALA:HB1	1:D:349:VAL:O	2.21	0.40
1:A:237:LEU:HD21	1:B:486:LEU:HD13	2.03	0.40
1:B:7:ASP:HB3	1:B:10:ARG:CZ	2.51	0.40
1:B:420:ASN:N	1:B:420:ASN:OD1	2.54	0.40
1:D:217:HIS:NE2	1:D:219:ALA:HB3	2.37	0.40
1:D:40:LEU:HD12	1:D:86:ILE:CD1	2.52	0.40
1:A:89:TYR:OH	1:A:91:ARG:HD3	2.22	0.40
1:C:186:ARG:HD2	4:C:494:1PE:C16	2.51	0.40
1:B:262:ASN:ND2	1:B:264:GLU:O	2.52	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	480/493 (97%)	456 (95%)	22 (5%)	2 (0%)	39	42
1	B	480/493 (97%)	456 (95%)	21 (4%)	3 (1%)	30	29
1	C	480/493 (97%)	454 (95%)	21 (4%)	5 (1%)	19	16
1	D	480/493 (97%)	462 (96%)	15 (3%)	3 (1%)	30	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1920/1972 (97%)	1828 (95%)	79 (4%)	13 (1%)	26	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	PRO
1	A	56	GLN
1	B	28	GLY
1	D	28	GLY
1	D	145	GLU
1	C	243	GLU
1	C	491	ARG
1	A	5	LEU
1	C	28	GLY
1	B	145	GLU
1	C	370	GLU
1	D	5	LEU
1	C	144	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	425/433 (98%)	406 (96%)	19 (4%)	34	41
1	B	425/433 (98%)	403 (95%)	22 (5%)	29	33
1	C	425/433 (98%)	399 (94%)	26 (6%)	23	26
1	D	425/433 (98%)	406 (96%)	19 (4%)	34	41
All	All	1700/1732 (98%)	1614 (95%)	86 (5%)	29	34

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	8	GLN

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Mol	Chain	Res	Type
1	A	13	ARG
1	A	21	GLU
1	A	119	PHE
1	A	122	LYS
1	A	140	LEU
1	A	155	GLN
1	A	227	ARG
1	A	270	LEU
1	A	277	PHE
1	A	283	LEU
1	A	364	PHE
1	A	427	GLN
1	A	441	ASP
1	A	446	MET
1	A	449	ASP
1	A	474	LEU
1	A	475	LEU
1	B	5	LEU
1	B	7	ASP
1	B	51	GLU
1	B	92	GLN
1	B	97	GLU
1	B	102	LEU
1	B	119	PHE
1	B	136	LEU
1	B	162	LEU
1	B	186	ARG
1	B	242	LEU
1	B	270	LEU
1	B	277	PHE
1	B	283	LEU
1	B	287	LEU
1	B	316	ARG
1	B	389	LEU
1	B	403	PHE
1	B	410	ARG
1	B	411	GLU
1	B	416	PHE
1	B	430	GLU
1	C	5	LEU
1	C	14	GLU
1	C	18	LYS

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Mol	Chain	Res	Type
1	C	69	ARG
1	C	95	VAL
1	C	108	LEU
1	C	119	PHE
1	C	126	LEU
1	C	144	PRO
1	C	146	LYS
1	C	169	GLU
1	C	179	LEU
1	C	188	LEU
1	C	224	LEU
1	C	242	LEU
1	C	252	PHE
1	C	270	LEU
1	C	277	PHE
1	C	283	LEU
1	C	324	LYS
1	C	345	LYS
1	C	368	LYS
1	C	373	LEU
1	C	474	LEU
1	C	491	ARG
1	C	492	HIS
1	D	5	LEU
1	D	7	ASP
1	D	13	ARG
1	D	56	GLN
1	D	91	ARG
1	D	108	LEU
1	D	138	LYS
1	D	145	GLU
1	D	154	GLU
1	D	169	GLU
1	D	188	LEU
1	D	277	PHE
1	D	283	LEU
1	D	307	LEU
1	D	339	GLU
1	D	389	LEU
1	D	403	PHE
1	D	416	PHE
1	D	482	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	155	GLN
1	A	191	HIS
1	A	218	ASN
1	A	233	HIS
1	A	286	ASN
1	A	334	GLN
1	A	427	GLN
1	A	438	GLN
1	B	8	GLN
1	B	55	GLN
1	B	159	GLN
1	B	217	HIS
1	B	218	ASN
1	B	427	GLN
1	B	438	GLN
1	C	55	GLN
1	C	56	GLN
1	C	92	GLN
1	C	218	ASN
1	C	233	HIS
1	C	334	GLN
1	C	438	GLN
1	C	444	HIS
1	C	492	HIS
1	D	56	GLN
1	D	92	GLN
1	D	155	GLN
1	D	182	GLN
1	D	217	HIS
1	D	218	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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$
3	XAH	A	1001	-	28,35,35	0.93	2 (7%)	30,50,50	2.02	2 (6%)
4	1PE	A	494	-	15,15,15	0.97	0	14,14,14	0.99	0
3	XAH	B	1101	-	28,35,35	0.93	2 (7%)	30,50,50	2.08	2 (6%)
4	1PE	B	494	-	15,15,15	1.13	0	14,14,14	0.87	0
3	XAH	C	1201	-	28,35,35	0.93	2 (7%)	30,50,50	2.03	2 (6%)
4	1PE	C	1202	-	15,15,15	0.92	0	14,14,14	1.00	1 (7%)
4	1PE	C	494	-	15,15,15	1.05	0	14,14,14	0.86	0
3	XAH	D	1301	-	28,35,35	0.92	2 (7%)	30,50,50	2.10	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XAH	A	1001	-	-	0/16/41/41	0/3/3/3
4	1PE	A	494	-	-	0/13/13/13	0/0/0/0
3	XAH	B	1101	-	-	0/16/41/41	0/3/3/3
4	1PE	B	494	-	-	0/13/13/13	0/0/0/0
3	XAH	C	1201	-	-	0/16/41/41	0/3/3/3
4	1PE	C	1202	-	-	0/13/13/13	0/0/0/0
4	1PE	C	494	-	-	0/13/13/13	0/0/0/0
3	XAH	D	1301	-	-	0/16/41/41	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	XAH	O11-N10	-2.83	1.36	1.41
3	C	1201	XAH	O11-N10	-2.81	1.36	1.41
3	D	1301	XAH	O11-N10	-2.76	1.36	1.41
3	A	1001	XAH	O11-N10	-2.75	1.36	1.41
3	B	1101	XAH	O18-C23	2.49	1.44	1.41
3	D	1301	XAH	O18-C23	2.50	1.44	1.41
3	C	1201	XAH	O18-C23	2.50	1.44	1.41
3	A	1001	XAH	O18-C23	2.59	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1301	XAH	N29-C30-N31	-10.35	120.97	128.89
3	B	1101	XAH	N29-C30-N31	-10.33	120.98	128.89
3	A	1001	XAH	N29-C30-N31	-10.11	121.15	128.89
3	C	1201	XAH	N29-C30-N31	-10.09	121.17	128.89
3	D	1301	XAH	C28-C27-N26	-2.29	107.37	109.48
4	C	1202	1PE	OH3-C23-C13	-2.23	100.46	110.36
3	B	1101	XAH	C28-C27-N26	-2.19	107.46	109.48
3	A	1001	XAH	C28-C27-N26	-2.18	107.47	109.48
3	C	1201	XAH	C28-C27-N26	-2.07	107.57	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	494	1PE	6	0
4	B	494	1PE	1	0
4	C	1202	1PE	1	0
4	C	494	1PE	2	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	484/493 (98%)	-0.45	5 (1%) 84 83	7, 18, 39, 59	0
1	B	484/493 (98%)	-0.44	2 (0%) 93 93	8, 18, 40, 55	0
1	C	484/493 (98%)	-0.42	4 (0%) 87 87	8, 18, 39, 57	0
1	D	484/493 (98%)	-0.44	4 (0%) 87 87	7, 17, 40, 55	0
All	All	1936/1972 (98%)	-0.44	15 (0%) 87 87	7, 18, 40, 59	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	144	PRO	9.4
1	A	144	PRO	5.9
1	A	153	ILE	4.3
1	D	153	ILE	4.3
1	B	153	ILE	3.3
1	C	145	GLU	3.2
1	A	5	LEU	3.0
1	C	153	ILE	2.8
1	D	143	LEU	2.7
1	D	144	PRO	2.4
1	A	71	MET	2.4
1	C	6	ASN	2.4
1	A	143	LEU	2.3
1	D	70	GLY	2.1
1	B	155	GLN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no 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
4	1PE	A	494	16/16	0.92	0.21	8.32	15,30,55,55	0
4	1PE	B	494	16/16	0.91	0.16	3.77	18,23,41,42	0
4	1PE	C	1202	16/16	0.93	0.16	2.87	11,21,48,49	0
3	XAH	B	1101	33/33	0.96	0.11	0.91	9,14,17,18	0
3	XAH	A	1001	33/33	0.97	0.11	0.63	6,16,18,23	0
4	1PE	C	494	16/16	0.89	0.15	0.59	13,26,37,39	0
3	XAH	D	1301	33/33	0.96	0.10	0.25	6,16,20,21	0
3	XAH	C	1201	33/33	0.97	0.10	0.01	11,14,18,21	0
2	MG	D	1300	1/1	0.99	0.09	-	19,19,19,19	0
2	MG	A	1000	1/1	0.98	0.10	-	17,17,17,17	0
2	MG	B	1100	1/1	0.97	0.07	-	21,21,21,21	0
2	MG	C	1200	1/1	0.98	0.07	-	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.