



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 08:14 pm GMT

PDB ID : 2EF5  
Title : Crystal structure of the arginase from thermus thermophilus  
Authors : Kumarevel, T.S.; Karthe, P.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-02-20  
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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

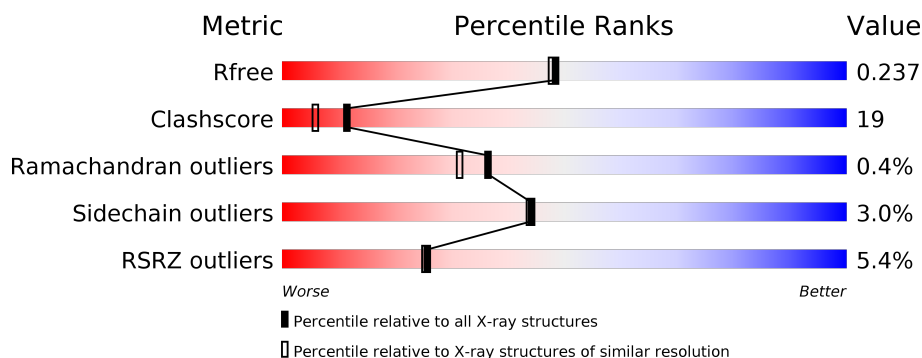
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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	290	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>6%</div> </div> </div>
1	B	290	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>6%</div> </div> </div>
1	D	290	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>6%</div> </div> </div>
1	E	290	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>6%</div> </div> </div>
1	F	290	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>6%</div> </div> </div>
1	G	290	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>6%</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
4	LYS	A	3001	-	-	X	X
4	LYS	B	3006	-	-	-	X
4	LYS	D	3002	-	-	-	X
4	LYS	E	3003	-	-	X	X
4	LYS	F	3004	-	-	X	X
4	LYS	G	3005	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13060 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.

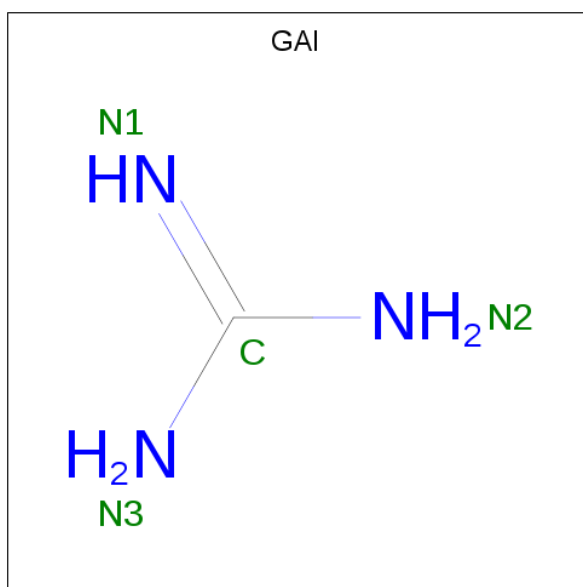
- Molecule 1 is a protein called Arginase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	B	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	D	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	E	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	F	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			
1	G	273	Total	C	N	O	S	0	0	0
			2052	1300	363	382	7			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

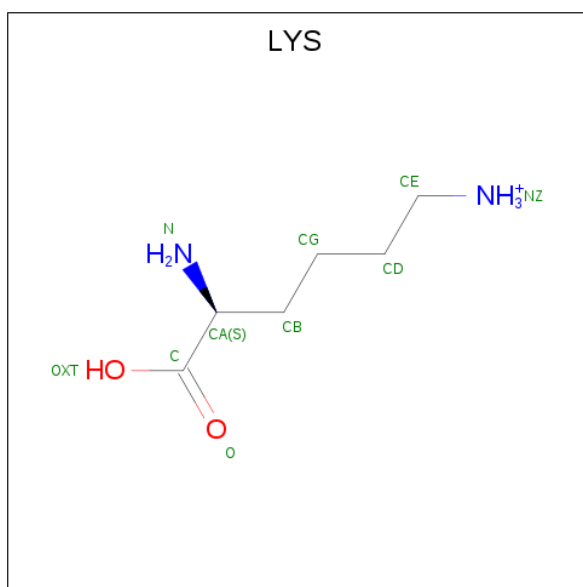
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is GUANIDINE (three-letter code: GAI) (formula: CH<sub>5</sub>N<sub>3</sub>).



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

- Molecule 4 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	2	2		
4	B	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	E	1	Total	C	N	O	0	0
			10	6	2	2		
4	F	1	Total	C	N	O	0	0
			10	6	2	2		
4	G	1	Total	C	N	O	0	0
			10	6	2	2		

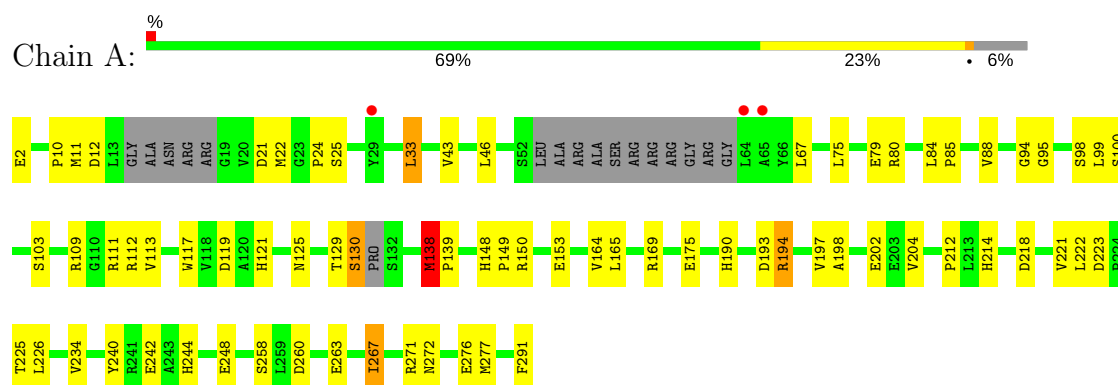
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total	O	0	0
			100	100		
5	B	116	Total	O	0	0
			116	116		
5	D	91	Total	O	0	0
			91	91		
5	E	132	Total	O	0	0
			132	132		
5	F	103	Total	O	0	0
			103	103		
5	G	110	Total	O	0	0
			110	110		

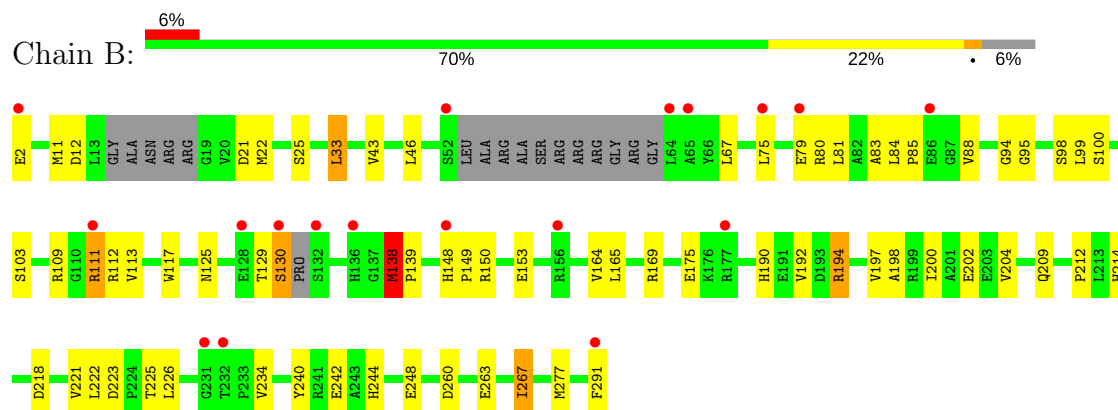
### 3 Residue-property plots [i](#)

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.

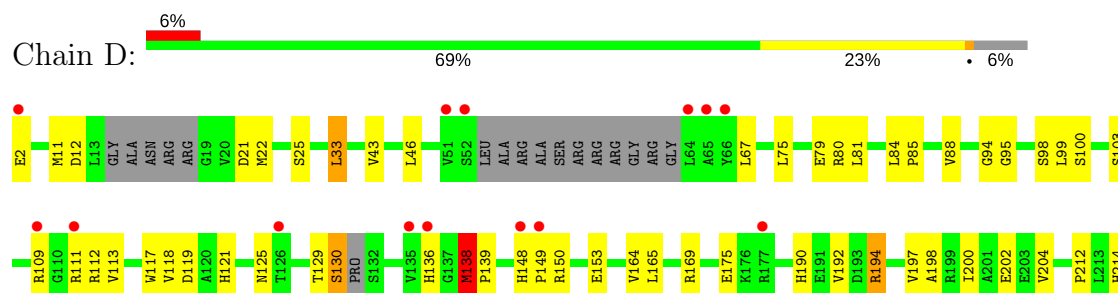
#### • Molecule 1: Arginase



#### • Molecule 1: Arginase

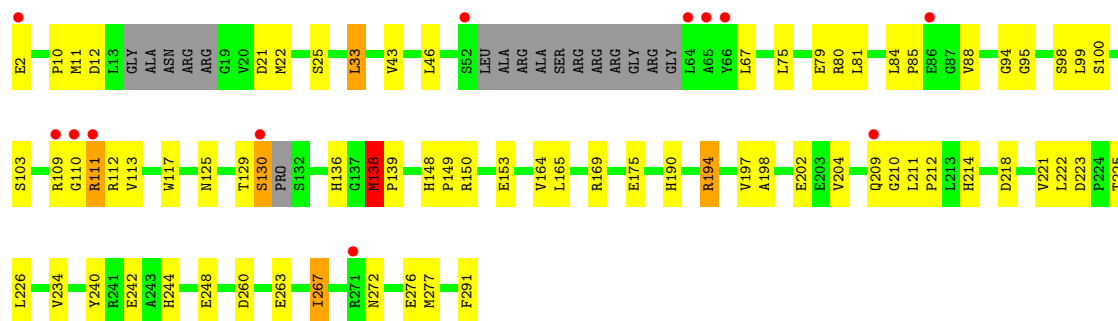


#### • Molecule 1: Arginase

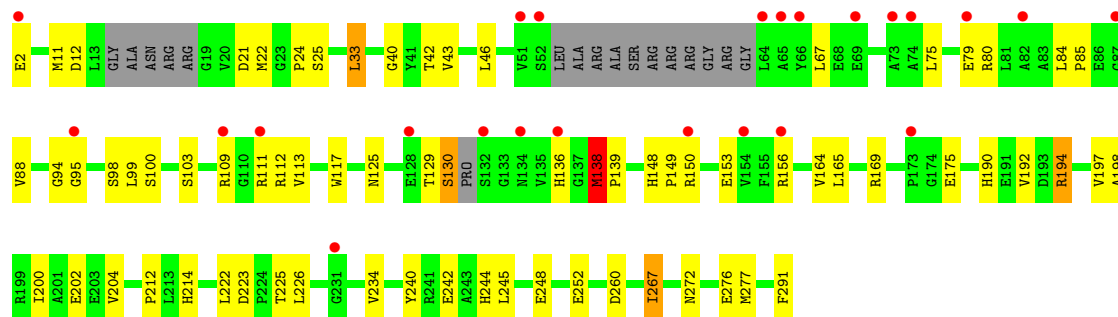




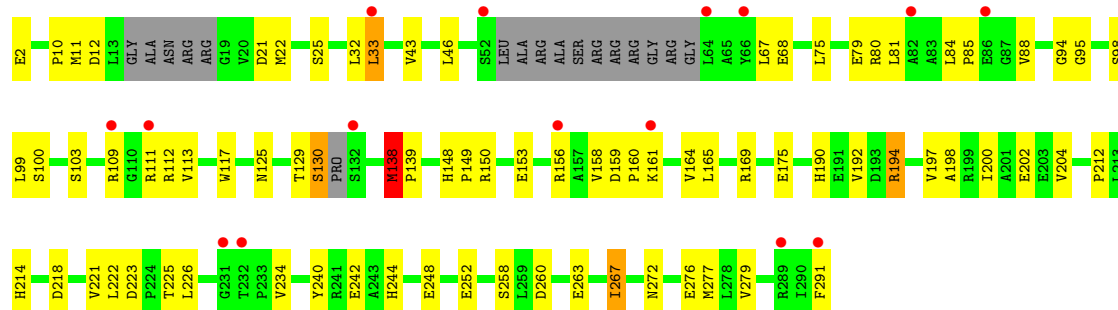
## ● Molecule 1: Arginase



## ● Molecule 1: Arginase



## ● Molecule 1: Arginase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.79Å 97.48Å 126.46Å 90.00° 108.66° 90.00°	Depositor
Resolution (Å)	19.98 – 2.00 45.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.98-2.00) 99.1 (45.15-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.236 0.233 , 0.237	Depositor DCC
$R_{free}$ test set	1150 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GAI

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	0/2083	0.66	1/2828 (0.0%)
1	B	0.33	0/2083	0.69	2/2828 (0.1%)
1	D	0.31	0/2083	0.66	1/2828 (0.0%)
1	E	0.35	0/2083	0.68	1/2828 (0.0%)
1	F	0.29	0/2083	0.66	1/2828 (0.0%)
1	G	0.34	0/2083	0.67	1/2828 (0.0%)
All	All	0.32	0/12498	0.67	7/16968 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	95	GLY	N-CA-C	-8.12	92.81	113.10
1	E	95	GLY	N-CA-C	-7.98	93.16	113.10
1	G	95	GLY	N-CA-C	-7.64	94.00	113.10
1	B	95	GLY	N-CA-C	-7.52	94.30	113.10
1	A	95	GLY	N-CA-C	-7.52	94.30	113.10
1	D	95	GLY	N-CA-C	-7.27	94.93	113.10
1	B	111	ARG	NE-CZ-NH2	-5.53	117.53	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2052	0	2101	70	0
1	B	2052	0	2101	69	2
1	D	2052	0	2101	59	0
1	E	2052	0	2101	120	0
1	F	2052	0	2101	78	0
1	G	2052	0	2101	138	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
3	A	8	0	8	0	0
3	B	4	0	4	0	0
3	D	4	0	4	0	0
3	E	4	0	4	0	0
3	G	4	0	4	0	0
4	A	10	0	12	16	0
4	B	10	0	12	3	0
4	D	10	0	12	3	0
4	E	10	0	12	9	0
4	F	10	0	12	12	2
4	G	10	0	12	11	2
5	A	100	0	0	6	0
5	B	116	0	0	2	0
5	D	91	0	0	1	0
5	E	132	0	0	5	0
5	F	103	0	0	6	0
5	G	110	0	0	3	0
All	All	13060	0	12702	474	4

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 19.

All (474) 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)
4:A:3001:LYS:NZ	4:A:3001:LYS:CE	1.69	1.52
1:E:111:ARG:HH22	1:G:161:LYS:N	0.99	1.40
4:E:3003:LYS:NZ	4:E:3003:LYS:CE	1.81	1.40
1:E:111:ARG:NH2	1:G:161:LYS:N	1.77	1.32
1:E:21:ASP:O	4:E:3003:LYS:HE2	1.42	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:LEU:HG	1:G:156:ARG:NH2	1.57	1.19
1:F:21:ASP:O	4:F:3004:LYS:HE2	1.44	1.18
1:G:22:MET:HA	4:G:3005:LYS:HD2	1.25	1.18
1:G:21:ASP:O	4:G:3005:LYS:HE2	1.42	1.16
1:B:25:SER:OG	4:B:3006:LYS:HG2	1.47	1.13
1:B:111:ARG:HD3	1:B:112:ARG:N	1.67	1.08
1:E:111:ARG:NH2	1:G:161:LYS:H	1.41	1.07
1:B:111:ARG:HD3	1:B:112:ARG:H	0.90	1.05
1:E:111:ARG:CZ	1:G:161:LYS:H	1.73	1.02
1:E:111:ARG:NH2	1:G:161:LYS:HG3	1.76	1.01
1:A:22:MET:HA	4:A:3001:LYS:HD2	1.38	1.01
1:B:111:ARG:CD	1:B:112:ARG:H	1.73	1.01
1:E:111:ARG:HH22	1:G:161:LYS:CA	1.75	0.99
1:E:209:GLN:OE1	1:G:153:GLU:O	1.81	0.97
1:A:21:ASP:O	4:A:3001:LYS:HE3	1.60	0.96
1:E:111:ARG:CD	1:G:159:ASP:OD1	2.14	0.96
1:A:21:ASP:O	4:A:3001:LYS:HE2	1.66	0.96
1:D:25:SER:OG	4:D:3002:LYS:HG2	1.64	0.96
1:E:211:LEU:HG	1:G:156:ARG:CZ	1.96	0.95
1:E:111:ARG:HG2	1:E:111:ARG:HH11	1.32	0.94
1:E:111:ARG:CZ	1:G:159:ASP:OD1	2.17	0.93
1:E:209:GLN:O	1:G:156:ARG:NH2	2.02	0.93
1:E:111:ARG:CD	1:E:112:ARG:H	1.81	0.92
1:G:21:ASP:O	4:G:3005:LYS:CE	2.20	0.89
1:E:111:ARG:HD2	1:G:159:ASP:OD1	1.70	0.89
1:A:129:THR:O	1:A:130:SER:HB2	1.70	0.89
1:E:129:THR:O	1:E:130:SER:HB2	1.73	0.88
1:D:129:THR:O	1:D:130:SER:HB2	1.74	0.88
1:E:111:ARG:HD3	1:E:112:ARG:N	1.88	0.87
1:G:129:THR:O	1:G:130:SER:HB2	1.74	0.86
1:G:111:ARG:HD3	1:G:112:ARG:H	1.41	0.85
1:A:21:ASP:C	4:A:3001:LYS:HE3	1.96	0.85
1:F:129:THR:O	1:F:130:SER:HB2	1.74	0.84
1:G:22:MET:HA	4:G:3005:LYS:CD	2.06	0.84
1:B:129:THR:O	1:B:130:SER:HB2	1.76	0.84
4:F:3004:LYS:C	5:F:3097:HOH:O	2.15	0.84
1:E:111:ARG:NH2	1:G:161:LYS:CG	2.38	0.84
1:E:111:ARG:HD3	1:E:112:ARG:H	1.38	0.83
1:D:111:ARG:HD3	1:D:112:ARG:H	1.42	0.83
1:E:111:ARG:NH1	1:G:161:LYS:H	1.76	0.82
1:F:111:ARG:HD3	1:F:112:ARG:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:LEU:HG	1:G:156:ARG:HH22	1.44	0.81
1:A:111:ARG:HD3	1:A:112:ARG:H	1.43	0.81
1:E:111:ARG:HG3	1:G:159:ASP:OD2	1.80	0.80
1:F:22:MET:HG2	4:F:3004:LYS:HD2	1.64	0.79
1:E:111:ARG:HD2	1:G:159:ASP:CG	2.02	0.79
1:E:111:ARG:NH1	1:G:159:ASP:OD1	2.15	0.79
1:E:21:ASP:O	4:E:3003:LYS:CE	2.26	0.79
1:E:111:ARG:NE	1:G:159:ASP:OD1	2.16	0.78
1:D:84:LEU:O	1:D:109:ARG:NH2	2.16	0.78
1:E:111:ARG:NH1	1:E:111:ARG:HG2	1.98	0.77
1:E:84:LEU:O	1:E:109:ARG:NH2	2.19	0.76
1:E:111:ARG:CG	1:E:111:ARG:HH11	1.98	0.75
1:A:22:MET:HA	4:A:3001:LYS:CD	2.15	0.75
1:F:2:GLU:CD	1:G:150:ARG:HD3	2.07	0.75
1:E:111:ARG:NH2	1:G:161:LYS:CB	2.50	0.75
1:B:75:LEU:O	1:B:79:GLU:HG3	1.87	0.74
1:E:111:ARG:NH1	1:G:161:LYS:HB2	2.02	0.74
1:B:209:GLN:NE2	1:F:156:ARG:HH22	1.86	0.73
1:E:209:GLN:O	1:G:156:ARG:CZ	2.34	0.73
1:E:111:ARG:CD	1:G:159:ASP:CG	2.56	0.73
1:A:117:TRP:HB3	1:A:165:LEU:HD23	1.71	0.72
1:E:117:TRP:HB3	1:E:165:LEU:HD23	1.70	0.72
1:G:159:ASP:OD1	1:G:160:PRO:HD2	1.90	0.72
1:A:22:MET:CA	4:A:3001:LYS:HD2	2.16	0.71
1:F:21:ASP:C	4:F:3004:LYS:HE2	2.11	0.70
4:F:3004:LYS:CA	5:F:3097:HOH:O	2.39	0.70
1:E:111:ARG:CZ	1:G:161:LYS:HB2	2.21	0.70
1:G:117:TRP:HB3	1:G:165:LEU:HD23	1.71	0.70
1:B:209:GLN:CD	1:F:156:ARG:HH22	1.95	0.70
1:F:2:GLU:OE2	1:G:150:ARG:NH1	2.23	0.70
1:F:84:LEU:O	1:F:109:ARG:NH2	2.25	0.69
1:E:111:ARG:CG	1:G:159:ASP:CG	2.60	0.69
1:E:111:ARG:CD	1:E:112:ARG:N	2.51	0.69
1:E:209:GLN:NE2	1:G:153:GLU:HA	2.08	0.69
1:G:22:MET:CA	4:G:3005:LYS:HD2	2.15	0.69
1:E:111:ARG:HD2	1:G:159:ASP:OD2	1.93	0.69
1:F:117:TRP:HB3	1:F:165:LEU:HD23	1.75	0.69
1:D:11:MET:HE3	1:D:98:SER:HB2	1.75	0.68
1:B:84:LEU:O	1:B:109:ARG:NH2	2.27	0.68
1:B:25:SER:OG	4:B:3006:LYS:CG	2.36	0.68
1:A:11:MET:CE	1:A:98:SER:HB2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:MET:HE3	1:E:98:SER:HB2	1.76	0.67
4:E:3003:LYS:HG2	5:E:3084:HOH:O	1.94	0.67
1:A:84:LEU:O	1:A:109:ARG:NH2	2.27	0.67
1:D:117:TRP:HB3	1:D:165:LEU:HD23	1.76	0.67
1:G:84:LEU:O	1:G:109:ARG:NH2	2.28	0.67
1:A:164:VAL:HG11	1:A:204:VAL:HG22	1.76	0.66
1:A:94:GLY:HA3	1:A:99:LEU:HD21	1.77	0.66
1:G:11:MET:HE3	1:G:98:SER:HB2	1.77	0.66
1:A:148:HIS:HD2	1:A:150:ARG:H	1.44	0.65
1:G:21:ASP:O	4:G:3005:LYS:HD2	1.96	0.65
1:G:21:ASP:O	4:G:3005:LYS:CD	2.44	0.65
1:B:190:HIS:HE1	1:B:194:ARG:HE	1.45	0.65
4:G:3005:LYS:HG3	5:G:3038:HOH:O	1.94	0.65
1:E:111:ARG:CZ	1:G:161:LYS:CB	2.75	0.65
1:E:111:ARG:HD2	1:E:112:ARG:H	1.59	0.65
1:F:198:ALA:O	1:F:202:GLU:HG2	1.97	0.65
1:G:25:SER:HG	4:G:3005:LYS:N	1.95	0.65
1:B:198:ALA:O	1:B:202:GLU:HG2	1.97	0.64
1:A:169:ARG:HG3	1:A:234:VAL:HG11	1.77	0.64
1:G:11:MET:CE	1:G:98:SER:HB2	2.27	0.64
1:B:11:MET:CE	1:B:98:SER:HB2	2.28	0.64
1:D:11:MET:CE	1:D:98:SER:HB2	2.27	0.64
1:G:75:LEU:O	1:G:79:GLU:HG3	1.98	0.64
1:E:94:GLY:HA3	1:E:99:LEU:HD21	1.79	0.63
1:B:117:TRP:HB3	1:B:165:LEU:HD23	1.80	0.63
1:E:211:LEU:HD23	1:G:156:ARG:NH1	2.13	0.63
1:F:129:THR:O	1:F:130:SER:CB	2.46	0.63
1:G:129:THR:O	1:G:130:SER:CB	2.46	0.63
1:E:111:ARG:HH21	1:G:161:LYS:HG3	1.62	0.63
1:D:149:PRO:O	1:D:153:GLU:HG2	1.99	0.63
1:G:198:ALA:O	1:G:202:GLU:HG2	1.98	0.63
1:G:169:ARG:HG3	1:G:234:VAL:HG11	1.80	0.63
1:E:110:GLY:O	1:G:161:LYS:NZ	2.31	0.63
1:E:129:THR:O	1:E:130:SER:CB	2.47	0.63
1:E:169:ARG:HG3	1:E:234:VAL:HG11	1.80	0.62
4:F:3004:LYS:HA	5:F:3097:HOH:O	1.96	0.62
1:B:169:ARG:HG3	1:B:234:VAL:HG11	1.81	0.62
1:B:209:GLN:OE1	1:F:156:ARG:NH1	2.31	0.62
1:F:94:GLY:HA3	1:F:99:LEU:HD21	1.82	0.62
1:D:169:ARG:HG3	1:D:234:VAL:HG11	1.82	0.62
1:B:129:THR:O	1:B:130:SER:CB	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:THR:O	1:D:130:SER:CB	2.46	0.62
1:G:22:MET:SD	1:G:267:ILE:HD13	2.40	0.62
1:A:129:THR:O	1:A:130:SER:CB	2.45	0.62
1:B:22:MET:SD	1:B:267:ILE:HD13	2.40	0.62
1:A:94:GLY:HA3	1:A:99:LEU:CD2	2.30	0.62
1:B:209:GLN:NE2	1:F:156:ARG:NH2	2.48	0.61
1:D:138:MET:N	1:D:139:PRO:HD2	2.16	0.61
1:F:169:ARG:HG3	1:F:234:VAL:HG11	1.81	0.61
1:A:149:PRO:O	1:A:153:GLU:HG2	2.00	0.61
1:E:2:GLU:HG3	5:E:3124:HOH:O	1.98	0.61
1:E:164:VAL:HG11	1:E:204:VAL:HG22	1.82	0.61
1:E:223:ASP:OD2	1:E:225:THR:HG22	2.00	0.61
1:D:164:VAL:HG11	1:D:204:VAL:HG22	1.82	0.61
1:E:111:ARG:CG	1:G:159:ASP:OD2	2.47	0.61
1:F:11:MET:CE	1:F:98:SER:HB2	2.30	0.61
1:F:138:MET:N	1:F:139:PRO:HD2	2.16	0.61
1:E:111:ARG:HG3	1:G:159:ASP:CG	2.22	0.61
1:B:94:GLY:HA3	1:B:99:LEU:HD21	1.82	0.60
1:E:75:LEU:O	1:E:79:GLU:HG3	2.01	0.60
1:F:42:THR:HG21	1:G:68:GLU:OE2	2.01	0.60
1:E:190:HIS:HE1	1:E:194:ARG:HE	1.49	0.60
1:F:138:MET:N	1:F:139:PRO:CD	2.65	0.60
1:E:111:ARG:HH22	1:G:160:PRO:C	1.94	0.60
1:D:138:MET:N	1:D:139:PRO:CD	2.65	0.60
1:B:111:ARG:HH11	1:B:111:ARG:HG2	1.67	0.60
1:F:244:HIS:O	1:F:248:GLU:HG3	2.02	0.60
1:D:198:ALA:O	1:D:202:GLU:HG2	2.01	0.60
4:E:3003:LYS:CA	5:E:3121:HOH:O	2.49	0.60
1:D:94:GLY:HA3	1:D:99:LEU:HD21	1.84	0.59
1:B:149:PRO:O	1:B:153:GLU:HG2	2.02	0.59
1:F:149:PRO:O	1:F:153:GLU:HG2	2.00	0.59
1:G:148:HIS:HD2	1:G:150:ARG:H	1.50	0.59
1:A:11:MET:HE3	1:A:98:SER:HB2	1.82	0.59
1:E:149:PRO:O	1:E:153:GLU:HG2	2.02	0.59
1:E:138:MET:N	1:E:139:PRO:CD	2.66	0.58
1:F:190:HIS:HE1	1:F:194:ARG:HE	1.51	0.58
1:E:138:MET:N	1:E:139:PRO:HD2	2.18	0.58
1:G:94:GLY:HA3	1:G:99:LEU:HD21	1.86	0.58
1:A:75:LEU:O	1:A:79:GLU:HG3	2.02	0.58
1:E:111:ARG:HH12	1:G:161:LYS:H	1.48	0.58
1:A:138:MET:N	1:A:139:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:VAL:HG22	1:G:159:ASP:N	2.17	0.58
1:A:148:HIS:CD2	1:A:150:ARG:HB2	2.39	0.58
1:G:138:MET:N	1:G:139:PRO:HD2	2.18	0.58
1:E:11:MET:CE	1:E:98:SER:HB2	2.34	0.58
1:A:148:HIS:CD2	1:A:150:ARG:H	2.22	0.57
1:D:109:ARG:HG2	1:D:109:ARG:NH1	2.18	0.57
1:G:138:MET:N	1:G:139:PRO:CD	2.67	0.57
1:A:223:ASP:OD2	1:A:225:THR:HG22	2.04	0.57
1:B:164:VAL:HG11	1:B:204:VAL:HG22	1.87	0.57
1:F:75:LEU:O	1:F:79:GLU:HG3	2.04	0.57
1:F:11:MET:HE3	1:F:98:SER:HB2	1.86	0.57
1:B:138:MET:N	1:B:139:PRO:CD	2.67	0.57
4:F:3004:LYS:O	5:F:3097:HOH:O	2.17	0.57
1:G:10:PRO:HB2	4:G:3005:LYS:NZ	2.20	0.57
1:G:190:HIS:HE1	1:G:194:ARG:HE	1.53	0.57
1:B:11:MET:HE3	1:B:98:SER:HB2	1.85	0.56
1:A:198:ALA:O	1:A:202:GLU:HG2	2.06	0.56
1:D:25:SER:CB	4:D:3002:LYS:HG2	2.34	0.56
1:D:75:LEU:O	1:D:79:GLU:HG3	2.04	0.56
1:F:12:ASP:HB2	1:F:21:ASP:HB3	1.87	0.56
1:B:138:MET:N	1:B:139:PRO:HD2	2.20	0.56
1:D:148:HIS:HD2	1:D:150:ARG:H	1.54	0.56
1:F:94:GLY:HA3	1:F:99:LEU:CD2	2.36	0.56
1:A:169:ARG:NH2	1:A:221:VAL:O	2.35	0.56
1:E:94:GLY:HA3	1:E:99:LEU:CD2	2.35	0.56
1:G:244:HIS:O	1:G:248:GLU:HG3	2.05	0.56
1:B:12:ASP:HB2	1:B:21:ASP:HB3	1.88	0.56
1:A:138:MET:N	1:A:139:PRO:HD2	2.21	0.55
1:F:2:GLU:OE1	1:G:150:ARG:HD2	2.05	0.55
1:B:190:HIS:CE1	1:B:194:ARG:HE	2.22	0.55
1:B:209:GLN:CD	1:F:156:ARG:NH2	2.59	0.55
1:B:209:GLN:HE22	1:F:156:ARG:HH22	1.55	0.55
1:D:109:ARG:HG2	1:D:109:ARG:HH11	1.70	0.55
1:F:21:ASP:O	4:F:3004:LYS:CE	2.37	0.55
1:G:190:HIS:CE1	1:G:194:ARG:HE	2.25	0.55
1:B:148:HIS:HD2	1:B:150:ARG:H	1.54	0.55
1:B:94:GLY:HA3	1:B:99:LEU:CD2	2.37	0.55
1:F:2:GLU:CD	1:G:150:ARG:CD	2.74	0.55
1:B:85:PRO:HG2	1:B:88:VAL:HG21	1.89	0.55
1:D:22:MET:SD	1:D:267:ILE:HD13	2.47	0.55
1:D:94:GLY:HA3	1:D:99:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:PRO:HB2	4:E:3003:LYS:NZ	2.21	0.55
1:F:109:ARG:HG2	1:F:109:ARG:NH1	2.21	0.55
1:E:209:GLN:CD	1:G:153:GLU:O	2.45	0.55
1:E:22:MET:SD	1:E:267:ILE:HD13	2.46	0.55
1:D:12:ASP:HB2	1:D:21:ASP:HB3	1.89	0.55
1:F:164:VAL:HG11	1:F:204:VAL:HG22	1.89	0.55
1:F:24:PRO:HD2	5:F:3034:HOH:O	2.06	0.55
1:F:25:SER:OG	4:F:3004:LYS:HA	2.07	0.55
1:E:211:LEU:CD2	1:G:156:ARG:NH1	2.70	0.54
1:D:111:ARG:CD	1:D:112:ARG:H	2.18	0.54
1:B:111:ARG:NH1	1:B:111:ARG:HG2	2.21	0.54
1:D:226:LEU:HD21	1:D:240:TYR:HB2	1.90	0.54
1:F:222:LEU:HD13	1:F:277:MET:HE2	1.89	0.54
1:G:148:HIS:CD2	1:G:150:ARG:HB2	2.43	0.54
1:A:111:ARG:CD	1:A:112:ARG:H	2.19	0.54
1:F:148:HIS:HD2	1:F:150:ARG:H	1.56	0.54
1:G:94:GLY:HA3	1:G:99:LEU:CD2	2.37	0.54
1:B:197:VAL:HG21	1:B:242:GLU:HB3	1.90	0.53
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.22	0.53
1:D:125:ASN:ND2	1:D:175:GLU:HG3	2.24	0.53
1:E:109:ARG:NH1	1:E:109:ARG:HG2	2.23	0.53
1:G:111:ARG:HD3	1:G:112:ARG:N	2.19	0.53
1:E:111:ARG:NH2	1:G:161:LYS:CA	2.49	0.53
1:A:190:HIS:HE1	1:A:194:ARG:HE	1.55	0.53
1:G:223:ASP:OD2	1:G:225:THR:HG22	2.08	0.53
1:B:226:LEU:HD21	1:B:240:TYR:HB2	1.89	0.53
1:E:148:HIS:HD2	1:E:150:ARG:H	1.55	0.53
1:A:10:PRO:HB2	4:A:3001:LYS:NZ	2.24	0.53
1:B:111:ARG:CD	1:B:112:ARG:N	2.48	0.53
1:D:222:LEU:HD13	1:D:277:MET:HE2	1.91	0.53
1:F:125:ASN:ND2	1:F:175:GLU:HG3	2.24	0.53
1:E:85:PRO:HG2	1:E:88:VAL:HG21	1.91	0.52
1:G:148:HIS:CD2	1:G:150:ARG:H	2.26	0.52
1:G:109:ARG:HG2	1:G:109:ARG:NH1	2.24	0.52
1:G:164:VAL:HG11	1:G:204:VAL:HG22	1.89	0.52
1:B:109:ARG:HG2	1:B:109:ARG:NH1	2.23	0.52
1:B:125:ASN:O	1:B:138:MET:HB3	2.10	0.52
1:E:222:LEU:HD13	1:E:277:MET:HE2	1.91	0.52
1:E:211:LEU:CG	1:G:156:ARG:HH22	2.19	0.52
1:B:223:ASP:OD2	1:B:225:THR:HG22	2.10	0.52
1:G:169:ARG:NH2	1:G:221:VAL:O	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.75	0.52
1:F:272:ASN:O	1:F:276:GLU:HG3	2.09	0.52
1:E:111:ARG:NH1	1:G:159:ASP:CG	2.63	0.52
1:E:111:ARG:NH2	1:G:160:PRO:C	2.59	0.52
1:D:25:SER:OG	4:D:3002:LYS:CG	2.50	0.51
1:G:226:LEU:HD21	1:G:240:TYR:HB2	1.92	0.51
1:E:198:ALA:O	1:E:202:GLU:HG2	2.10	0.51
1:A:22:MET:HG2	4:A:3001:LYS:HD2	1.92	0.51
1:B:209:GLN:OE1	1:F:156:ARG:NH2	2.44	0.51
1:E:125:ASN:ND2	1:E:175:GLU:HG3	2.25	0.51
1:B:169:ARG:NH2	1:B:221:VAL:O	2.34	0.51
1:D:148:HIS:CD2	1:D:150:ARG:HB2	2.45	0.51
1:E:111:ARG:HH11	1:G:159:ASP:CG	2.14	0.51
1:A:99:LEU:HD12	1:A:99:LEU:C	2.31	0.51
1:D:190:HIS:HE1	1:D:194:ARG:HE	1.58	0.51
1:F:190:HIS:CE1	1:F:194:ARG:HE	2.28	0.51
1:E:210:GLY:C	1:G:156:ARG:NH1	2.65	0.51
1:E:111:ARG:CD	1:G:159:ASP:OD2	2.57	0.51
1:F:214:HIS:HE1	1:F:260:ASP:OD2	1.94	0.51
1:E:210:GLY:C	1:G:156:ARG:HH12	2.13	0.51
1:F:226:LEU:HD21	1:F:240:TYR:HB2	1.94	0.50
1:G:21:ASP:C	4:G:3005:LYS:HE2	2.25	0.50
4:E:3003:LYS:HA	5:E:3121:HOH:O	2.11	0.50
1:A:244:HIS:O	1:A:248:GLU:HG3	2.11	0.50
1:F:109:ARG:HH11	1:F:109:ARG:HG2	1.75	0.50
1:G:149:PRO:O	1:G:153:GLU:HG2	2.10	0.50
1:E:111:ARG:CZ	1:G:161:LYS:CG	2.90	0.50
1:A:12:ASP:HB2	1:A:21:ASP:HB3	1.93	0.50
1:D:148:HIS:CD2	1:D:150:ARG:H	2.30	0.50
1:E:226:LEU:HD21	1:E:240:TYR:HB2	1.94	0.50
1:A:148:HIS:HD2	1:A:150:ARG:HB2	1.76	0.50
1:D:169:ARG:NH2	1:D:221:VAL:O	2.37	0.49
1:E:190:HIS:CE1	1:E:194:ARG:HE	2.27	0.49
1:F:2:GLU:OE1	1:G:150:ARG:CD	2.60	0.49
1:F:67:LEU:C	1:F:67:LEU:HD23	2.33	0.49
1:G:159:ASP:OD1	1:G:160:PRO:CD	2.58	0.49
1:D:223:ASP:OD2	1:D:225:THR:HG22	2.12	0.49
1:E:109:ARG:HG2	1:E:109:ARG:HH11	1.76	0.49
1:F:248:GLU:O	1:F:252:GLU:HG3	2.12	0.49
1:G:67:LEU:HD23	1:G:67:LEU:C	2.32	0.49
1:A:214:HIS:HD2	1:A:258:SER:OG	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:MET:H	1:F:139:PRO:CD	2.25	0.49
1:G:109:ARG:HG2	1:G:109:ARG:HH11	1.78	0.49
1:A:2:GLU:HG3	5:A:3079:HOH:O	2.10	0.49
1:D:2:GLU:HG3	5:D:3084:HOH:O	2.11	0.49
1:B:222:LEU:HD13	1:B:277:MET:HE2	1.93	0.49
1:B:33:LEU:HG	1:B:43:VAL:HG11	1.93	0.49
1:E:148:HIS:CD2	1:E:150:ARG:H	2.30	0.49
1:F:85:PRO:HG2	1:F:88:VAL:HG21	1.94	0.49
1:A:24:PRO:HD2	5:A:3009:HOH:O	2.12	0.49
1:F:148:HIS:CD2	1:F:150:ARG:HB2	2.47	0.49
1:G:222:LEU:HD13	1:G:277:MET:HE2	1.95	0.49
1:A:190:HIS:CE1	1:A:194:ARG:HE	2.30	0.49
1:A:11:MET:HE1	1:A:98:SER:HB2	1.95	0.49
1:G:33:LEU:HG	1:G:43:VAL:HG11	1.95	0.49
1:B:148:HIS:CD2	1:B:150:ARG:H	2.30	0.49
1:D:85:PRO:HG2	1:D:88:VAL:HG21	1.94	0.49
1:D:67:LEU:C	1:D:67:LEU:HD23	2.34	0.49
1:G:12:ASP:HB2	1:G:21:ASP:HB3	1.93	0.49
1:A:67:LEU:C	1:A:67:LEU:HD23	2.33	0.48
1:E:211:LEU:HG	1:G:156:ARG:NH1	2.27	0.48
1:B:244:HIS:O	1:B:248:GLU:HG3	2.13	0.48
1:D:244:HIS:O	1:D:248:GLU:HG3	2.13	0.48
4:E:3003:LYS:C	5:E:3121:HOH:O	2.51	0.48
1:F:113:VAL:HG12	1:F:212:PRO:HG2	1.96	0.48
1:B:125:ASN:ND2	1:B:175:GLU:HG3	2.28	0.48
1:A:226:LEU:HD21	1:A:240:TYR:HB2	1.96	0.48
1:G:148:HIS:HD2	1:G:150:ARG:HB2	1.79	0.48
1:A:169:ARG:HG3	1:A:234:VAL:CG1	2.42	0.48
1:F:111:ARG:CD	1:F:112:ARG:H	2.21	0.48
1:E:111:ARG:HH12	1:G:161:LYS:N	2.10	0.48
1:B:113:VAL:HG12	1:B:212:PRO:HG2	1.96	0.48
1:F:148:HIS:CD2	1:F:150:ARG:H	2.32	0.48
1:D:190:HIS:CE1	1:D:194:ARG:HE	2.32	0.48
1:A:214:HIS:CD2	1:A:258:SER:OG	2.67	0.48
1:B:109:ARG:HG2	1:B:109:ARG:HH11	1.78	0.48
1:B:248:GLU:OE1	1:E:190:HIS:HD2	1.97	0.48
1:D:197:VAL:HG21	1:D:242:GLU:HB3	1.96	0.48
1:E:209:GLN:C	1:G:156:ARG:NH2	2.67	0.48
1:G:85:PRO:HG2	1:G:88:VAL:HG21	1.95	0.48
1:A:22:MET:CG	4:A:3001:LYS:HD2	2.43	0.48
1:B:100:SER:HA	1:B:103:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:HIS:CD2	1:B:150:ARG:HB2	2.49	0.48
1:E:209:GLN:NE2	1:G:153:GLU:CA	2.75	0.47
1:G:214:HIS:HE1	1:G:260:ASP:OD2	1.97	0.47
1:E:209:GLN:HG3	1:E:209:GLN:O	2.14	0.47
1:F:223:ASP:OD2	1:F:225:THR:HG22	2.14	0.47
1:G:111:ARG:CD	1:G:112:ARG:H	2.17	0.47
1:G:272:ASN:O	1:G:276:GLU:HG3	2.14	0.47
1:A:125:ASN:ND2	1:A:175:GLU:HG3	2.29	0.47
1:A:46:LEU:HD22	1:A:80:ARG:NH2	2.30	0.47
1:A:25:SER:OG	4:A:3001:LYS:CA	2.62	0.47
1:B:99:LEU:HD12	1:B:99:LEU:C	2.35	0.47
1:F:169:ARG:HG3	1:F:234:VAL:CG1	2.44	0.47
1:G:2:GLU:HG3	5:G:3105:HOH:O	2.14	0.47
1:E:67:LEU:C	1:E:67:LEU:HD23	2.35	0.47
1:E:12:ASP:HB2	1:E:21:ASP:HB3	1.96	0.47
1:A:111:ARG:HD3	1:A:112:ARG:N	2.22	0.46
1:E:148:HIS:CD2	1:E:150:ARG:HB2	2.51	0.46
1:F:22:MET:SD	1:F:267:ILE:HD13	2.55	0.46
1:G:125:ASN:ND2	1:G:175:GLU:HG3	2.30	0.46
1:A:222:LEU:HD13	1:A:277:MET:HE2	1.98	0.46
4:A:3001:LYS:C	5:A:3076:HOH:O	2.53	0.46
1:D:138:MET:H	1:D:139:PRO:CD	2.27	0.46
1:E:214:HIS:HE1	1:E:260:ASP:OD2	1.98	0.46
1:G:100:SER:HA	1:G:103:SER:OG	2.16	0.46
1:A:197:VAL:HG21	1:A:242:GLU:HB3	1.98	0.46
1:B:67:LEU:HD23	1:B:67:LEU:C	2.35	0.46
1:F:99:LEU:C	1:F:99:LEU:HD12	2.36	0.46
1:B:169:ARG:HG3	1:B:234:VAL:CG1	2.46	0.46
1:D:192:VAL:HA	1:D:200:ILE:CD1	2.46	0.46
1:F:21:ASP:C	4:F:3004:LYS:CE	2.82	0.46
1:A:138:MET:H	1:A:139:PRO:CD	2.29	0.46
1:B:2:GLU:HG3	5:B:3112:HOH:O	2.15	0.46
1:D:214:HIS:HE1	1:D:260:ASP:OD2	1.99	0.46
1:E:99:LEU:HD12	1:E:99:LEU:C	2.35	0.46
1:A:271:ARG:N	5:A:3023:HOH:O	2.49	0.46
1:D:111:ARG:HD3	1:D:112:ARG:N	2.21	0.46
1:G:248:GLU:O	1:G:252:GLU:HG3	2.15	0.46
1:D:118:VAL:HG12	1:D:221:VAL:HG21	1.97	0.45
1:A:218:ASP:OD2	1:A:263:GLU:HG3	2.16	0.45
1:A:25:SER:OG	4:A:3001:LYS:CB	2.64	0.45
1:B:85:PRO:HG2	1:B:88:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:HIS:HD2	1:D:150:ARG:HB2	1.81	0.45
1:E:209:GLN:HE22	1:G:153:GLU:CA	2.30	0.45
1:G:218:ASP:OD2	1:G:263:GLU:HG3	2.16	0.45
1:D:81:LEU:HD12	1:D:103:SER:HA	1.98	0.45
1:E:98:SER:OG	1:E:136:HIS:HA	2.15	0.45
1:F:111:ARG:HD3	1:F:112:ARG:N	2.24	0.45
1:A:25:SER:OG	4:A:3001:LYS:HA	2.16	0.45
1:G:169:ARG:HG3	1:G:234:VAL:CG1	2.47	0.45
1:E:218:ASP:OD2	1:E:263:GLU:HG3	2.16	0.45
1:A:113:VAL:HG12	1:A:212:PRO:HG2	1.99	0.45
1:A:119:ASP:HB3	1:A:121:HIS:O	2.17	0.45
1:G:158:VAL:CG2	1:G:159:ASP:N	2.80	0.45
1:D:113:VAL:HG12	1:D:212:PRO:HG2	1.98	0.45
1:F:148:HIS:HD2	1:F:150:ARG:HB2	1.82	0.45
1:E:85:PRO:HG2	1:E:88:VAL:CG2	2.47	0.44
1:F:214:HIS:CE1	1:F:260:ASP:OD2	2.70	0.44
1:A:85:PRO:HG2	1:A:88:VAL:HG21	1.98	0.44
1:D:99:LEU:C	1:D:99:LEU:HD12	2.37	0.44
1:G:214:HIS:HD2	1:G:258:SER:OG	2.00	0.44
1:D:46:LEU:HD22	1:D:80:ARG:NH2	2.32	0.44
1:F:25:SER:OG	4:F:3004:LYS:CA	2.65	0.44
1:B:46:LEU:HD22	1:B:80:ARG:NH2	2.33	0.44
1:D:169:ARG:HG3	1:D:234:VAL:CG1	2.46	0.44
1:F:100:SER:HA	1:F:103:SER:OG	2.18	0.44
1:F:98:SER:OG	1:F:136:HIS:HA	2.18	0.44
1:F:33:LEU:HG	1:F:43:VAL:HG11	1.99	0.44
1:G:156:ARG:NH2	5:G:3031:HOH:O	2.42	0.44
1:E:169:ARG:HG3	1:E:234:VAL:CG1	2.46	0.44
1:F:197:VAL:HG21	1:F:242:GLU:HB3	2.00	0.44
1:E:197:VAL:HG21	1:E:242:GLU:HB3	2.00	0.43
1:F:2:GLU:HB2	1:G:150:ARG:HD3	1.99	0.43
1:G:22:MET:SD	1:G:267:ILE:CD1	3.06	0.43
1:G:214:HIS:CD2	1:G:258:SER:OG	2.71	0.43
1:A:272:ASN:O	1:A:276:GLU:HG3	2.19	0.43
1:D:33:LEU:HG	1:D:43:VAL:HG11	2.00	0.43
1:E:111:ARG:HA	1:E:111:ARG:HD3	1.31	0.43
4:A:3001:LYS:HE2	5:A:3009:HOH:O	2.18	0.43
1:E:169:ARG:NH2	1:E:221:VAL:O	2.40	0.43
1:E:33:LEU:HG	1:E:43:VAL:HG11	2.00	0.43
1:F:22:MET:HA	4:F:3004:LYS:HG3	2.00	0.43
1:F:40:GLY:O	1:G:148:HIS:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:LEU:N	1:G:156:ARG:HH22	2.16	0.43
1:F:277:MET:HG2	5:F:3026:HOH:O	2.19	0.43
1:G:99:LEU:HD12	1:G:99:LEU:C	2.39	0.43
1:B:81:LEU:HD12	1:B:103:SER:HA	2.00	0.43
1:D:214:HIS:HD2	1:D:258:SER:OG	2.01	0.43
1:E:25:SER:OG	4:E:3003:LYS:CG	2.67	0.43
1:D:100:SER:HA	1:D:103:SER:OG	2.18	0.43
1:G:192:VAL:HA	1:G:200:ILE:CD1	2.49	0.43
1:A:193:ASP:HB3	1:F:245:LEU:HD22	2.01	0.43
1:A:99:LEU:HD12	1:A:100:SER:N	2.34	0.43
1:D:218:ASP:OD2	1:D:263:GLU:HG3	2.19	0.43
1:E:113:VAL:HG12	1:E:212:PRO:HG2	2.00	0.42
1:D:85:PRO:HG2	1:D:88:VAL:CG2	2.49	0.42
1:G:214:HIS:CE1	1:G:260:ASP:OD2	2.72	0.42
1:B:11:MET:HE1	1:B:98:SER:HB2	1.98	0.42
1:E:272:ASN:O	1:E:276:GLU:HG3	2.19	0.42
1:G:85:PRO:HG2	1:G:88:VAL:CG2	2.50	0.42
1:A:33:LEU:HG	1:A:43:VAL:HG11	2.02	0.42
1:B:22:MET:SD	1:B:267:ILE:CD1	3.07	0.42
1:D:119:ASP:HB3	1:D:121:HIS:O	2.20	0.42
1:D:98:SER:OG	1:D:136:HIS:HA	2.20	0.42
1:D:214:HIS:CD2	1:D:258:SER:OG	2.73	0.42
1:E:100:SER:HA	1:E:103:SER:OG	2.18	0.42
1:E:138:MET:H	1:E:139:PRO:CD	2.32	0.42
1:E:211:LEU:N	1:G:156:ARG:HH12	2.18	0.42
1:E:211:LEU:CG	1:G:156:ARG:CZ	2.85	0.42
1:A:100:SER:HA	1:A:103:SER:OG	2.19	0.42
1:B:218:ASP:OD2	1:B:263:GLU:HG3	2.19	0.42
1:E:244:HIS:O	1:E:248:GLU:HG3	2.19	0.42
1:G:197:VAL:HG21	1:G:242:GLU:HB3	2.00	0.42
1:D:125:ASN:O	1:D:138:MET:HB3	2.19	0.42
1:G:81:LEU:HD12	1:G:103:SER:HA	2.01	0.41
1:G:113:VAL:HG12	1:G:212:PRO:HG2	2.02	0.41
1:B:148:HIS:HD2	1:B:150:ARG:HB2	1.84	0.41
1:E:81:LEU:HD12	1:E:103:SER:HA	2.03	0.41
1:A:214:HIS:HE1	1:A:260:ASP:OD2	2.04	0.41
4:A:3001:LYS:CA	5:A:3076:HOH:O	2.68	0.41
1:E:211:LEU:HD23	1:G:156:ARG:HH12	1.85	0.41
1:F:46:LEU:HD22	1:F:80:ARG:NH2	2.35	0.41
1:F:85:PRO:HG2	1:F:88:VAL:CG2	2.50	0.41
1:B:194:ARG:HD2	5:B:3121:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:ASN:O	1:F:138:MET:HB3	2.21	0.41
1:B:111:ARG:CG	1:B:112:ARG:N	2.84	0.41
1:B:138:MET:H	1:B:139:PRO:CD	2.33	0.41
1:B:192:VAL:HA	1:B:200:ILE:CD1	2.51	0.41
1:G:156:ARG:NH1	1:G:156:ARG:HG2	2.34	0.41
1:A:125:ASN:O	1:A:138:MET:HB3	2.21	0.41
1:E:46:LEU:HD22	1:E:80:ARG:NH2	2.34	0.41
1:G:46:LEU:HD22	1:G:80:ARG:NH2	2.36	0.41
1:A:22:MET:SD	1:A:267:ILE:HD13	2.61	0.41
1:G:32:LEU:HB2	1:G:279:VAL:HG22	2.03	0.41
1:B:214:HIS:HE1	1:B:260:ASP:OD2	2.04	0.40
1:A:148:HIS:HA	1:A:149:PRO:HD3	1.92	0.40
1:F:192:VAL:HA	1:F:200:ILE:CD1	2.51	0.40
1:F:148:HIS:HA	1:F:149:PRO:HD3	1.90	0.40
1:E:211:LEU:CG	1:G:156:ARG:NH1	2.85	0.40
1:G:192:VAL:HA	1:G:200:ILE:HD11	2.03	0.40
1:B:25:SER:OG	4:B:3006:LYS:HA	2.21	0.40
1:E:148:HIS:HD2	1:E:150:ARG:HB2	1.84	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:O	1:B:111:ARG:NH2[2_555]	1.79	0.41
1:B:83:ALA:N	1:B:111:ARG:NH2[2_555]	1.91	0.29
4:F:3004:LYS:NZ	4:G:3005:LYS:OXT[2_556]	2.08	0.12
4:F:3004:LYS:CB	4:G:3005:LYS:CB[2_556]	2.10	0.10

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	265/290 (91%)	258 (97%)	6 (2%)	1 (0%)	36	31
1	B	265/290 (91%)	259 (98%)	5 (2%)	1 (0%)	36	31
1	D	265/290 (91%)	258 (97%)	6 (2%)	1 (0%)	36	31
1	E	265/290 (91%)	260 (98%)	4 (2%)	1 (0%)	36	31
1	F	265/290 (91%)	259 (98%)	5 (2%)	1 (0%)	36	31
1	G	265/290 (91%)	258 (97%)	6 (2%)	1 (0%)	36	31
All	All	1590/1740 (91%)	1552 (98%)	32 (2%)	6 (0%)	36	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	MET
1	B	138	MET
1	D	138	MET
1	F	138	MET
1	E	138	MET
1	G	138	MET

### 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	218/231 (94%)	212 (97%)	6 (3%)	47	47
1	B	218/231 (94%)	212 (97%)	6 (3%)	47	47
1	D	218/231 (94%)	212 (97%)	6 (3%)	47	47
1	E	218/231 (94%)	211 (97%)	7 (3%)	42	41
1	F	218/231 (94%)	212 (97%)	6 (3%)	47	47
1	G	218/231 (94%)	212 (97%)	6 (3%)	47	47
All	All	1308/1386 (94%)	1271 (97%)	37 (3%)	44	47

All (37) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	33	LEU
1	A	130	SER
1	A	138	MET
1	A	194	ARG
1	A	267	ILE
1	A	291	PHE
1	B	33	LEU
1	B	130	SER
1	B	138	MET
1	B	194	ARG
1	B	267	ILE
1	B	291	PHE
1	D	33	LEU
1	D	130	SER
1	D	138	MET
1	D	194	ARG
1	D	267	ILE
1	D	291	PHE
1	E	33	LEU
1	E	111	ARG
1	E	130	SER
1	E	138	MET
1	E	194	ARG
1	E	267	ILE
1	E	291	PHE
1	F	33	LEU
1	F	130	SER
1	F	138	MET
1	F	194	ARG
1	F	267	ILE
1	F	291	PHE
1	G	33	LEU
1	G	130	SER
1	G	138	MET
1	G	194	ARG
1	G	267	ILE
1	G	291	PHE

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	125	ASN
1	A	134	ASN

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Mol	Chain	Res	Type
1	A	148	HIS
1	A	190	HIS
1	A	214	HIS
1	B	125	ASN
1	B	134	ASN
1	B	148	HIS
1	B	190	HIS
1	B	214	HIS
1	D	125	ASN
1	D	134	ASN
1	D	148	HIS
1	D	190	HIS
1	D	214	HIS
1	E	125	ASN
1	E	134	ASN
1	E	148	HIS
1	E	190	HIS
1	E	209	GLN
1	E	214	HIS
1	F	125	ASN
1	F	134	ASN
1	F	148	HIS
1	F	190	HIS
1	F	214	HIS
1	G	125	ASN
1	G	134	ASN
1	G	148	HIS
1	G	190	HIS
1	G	214	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	GAI	A	1001	-	3,3,3	1.47	0	3,3,3	1.14	0
3	GAI	A	1004	-	3,3,3	1.42	0	3,3,3	1.14	0
4	LYS	A	3001	1,4	4,9,9	2.95	3 (75%)	3,10,10	2.77	2 (66%)
3	GAI	B	1006	-	3,3,3	1.41	0	3,3,3	1.07	0
4	LYS	B	3006	-	4,9,9	0.72	0	3,10,10	3.10	1 (33%)
3	GAI	D	1002	-	3,3,3	1.46	0	3,3,3	1.10	0
4	LYS	D	3002	-	4,9,9	1.75	1 (25%)	3,10,10	3.01	1 (33%)
3	GAI	E	1003	-	3,3,3	1.54	0	3,3,3	1.14	0
4	LYS	E	3003	4	4,9,9	3.80	4 (100%)	3,10,10	2.29	2 (66%)
4	LYS	F	3004	4	4,9,9	1.76	1 (25%)	3,10,10	1.49	1 (33%)
3	GAI	G	1005	-	3,3,3	1.28	0	3,3,3	1.10	0
4	LYS	G	3005	4	4,9,9	3.59	4 (100%)	3,10,10	2.28	1 (33%)

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	GAI	A	1001	-	-	0/0/0/0	0/0/0/0
3	GAI	A	1004	-	-	0/0/0/0	0/0/0/0
4	LYS	A	3001	1,4	-	0/5/9/9	0/0/0/0
3	GAI	B	1006	-	-	0/0/0/0	0/0/0/0
4	LYS	B	3006	-	-	0/5/9/9	0/0/0/0
3	GAI	D	1002	-	-	0/0/0/0	0/0/0/0
4	LYS	D	3002	-	-	0/5/9/9	0/0/0/0
3	GAI	E	1003	-	-	0/0/0/0	0/0/0/0
4	LYS	E	3003	4	-	0/5/9/9	0/0/0/0
4	LYS	F	3004	4	-	0/5/9/9	0/0/0/0
3	GAI	G	1005	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LYS	G	3005	4	-	0/5/9/9	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3003	LYS	CD-CG	-3.28	1.32	1.51
4	E	3003	LYS	CG-CB	2.40	1.62	1.52
4	G	3005	LYS	CE-NZ	2.56	1.66	1.46
4	F	3004	LYS	CD-CE	2.79	1.64	1.51
4	A	3001	LYS	CE-NZ	2.93	1.69	1.46
4	G	3005	LYS	CD-CG	3.05	1.68	1.51
4	D	3002	LYS	CG-CB	3.30	1.66	1.52
4	A	3001	LYS	CG-CB	3.50	1.67	1.52
4	G	3005	LYS	CD-CE	3.62	1.68	1.51
4	A	3001	LYS	CD-CE	3.71	1.69	1.51
4	E	3003	LYS	CE-NZ	4.47	1.81	1.46
4	E	3003	LYS	CD-CE	4.62	1.73	1.51
4	G	3005	LYS	CG-CB	4.75	1.72	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3006	LYS	CD-CG-CB	-5.31	95.02	113.59
4	D	3002	LYS	CD-CG-CB	-5.15	95.57	113.59
4	E	3003	LYS	CD-CG-CB	-3.09	102.78	113.59
4	F	3004	LYS	CD-CG-CB	-2.52	104.79	113.59
4	E	3003	LYS	CG-CD-CE	2.24	129.82	113.60
4	A	3001	LYS	CD-CE-NZ	2.62	130.55	112.64
4	G	3005	LYS	CD-CE-NZ	3.63	137.42	112.64
4	A	3001	LYS	CD-CG-CB	3.90	127.23	113.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	LYS	16	0
4	B	3006	LYS	3	0
4	D	3002	LYS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3003	LYS	9	0
4	F	3004	LYS	12	2
4	G	3005	LYS	11	2

## 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	273/290 (94%)	0.04	3 (1%) 80 79	15, 27, 42, 52	0
1	B	273/290 (94%)	0.17	18 (6%) 18 18	12, 25, 43, 53	0
1	D	273/290 (94%)	0.24	17 (6%) 20 20	14, 28, 46, 55	0
1	E	273/290 (94%)	0.13	12 (4%) 34 33	12, 22, 40, 53	0
1	F	273/290 (94%)	0.54	24 (8%) 10 9	17, 31, 47, 54	0
1	G	273/290 (94%)	0.14	15 (5%) 25 25	13, 24, 41, 53	0
All	All	1638/1740 (94%)	0.21	89 (5%) 26 25	12, 26, 44, 55	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	64	LEU	7.6
1	B	65	ALA	6.9
1	G	291	PHE	6.7
1	F	52	SER	6.5
1	F	69	GLU	5.3
1	B	111	ARG	5.1
1	B	52	SER	5.0
1	F	66	TYR	5.0
1	D	52	SER	4.6
1	E	110	GLY	4.5
1	F	128	GLU	4.5
1	F	2	GLU	4.2
1	F	134	ASN	4.0
1	D	65	ALA	3.9
1	D	231	GLY	3.8
1	D	64	LEU	3.8
1	E	111	ARG	3.7
1	F	154	VAL	3.6
1	F	73	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	65	ALA	3.4
1	E	52	SER	3.3
1	E	209	GLN	3.3
1	E	2	GLU	3.3
1	D	232	THR	3.2
1	F	111	ARG	3.2
1	D	2	GLU	3.2
1	D	111	ARG	3.1
1	F	156	ARG	3.1
1	B	130	SER	3.1
1	E	64	LEU	3.1
1	B	79	GLU	3.1
1	D	136	HIS	3.0
1	F	173	PRO	3.0
1	F	132	SER	3.0
1	B	291	PHE	2.9
1	B	2	GLU	2.9
1	G	132	SER	2.9
1	A	64	LEU	2.9
1	B	64	LEU	2.9
1	B	231	GLY	2.9
1	G	156	ARG	2.9
1	B	128	GLU	2.8
1	G	86	GLU	2.8
1	D	225	THR	2.8
1	F	136	HIS	2.8
1	F	74	ALA	2.8
1	D	177	ARG	2.7
1	G	82	ALA	2.7
1	G	231	GLY	2.7
1	B	232	THR	2.6
1	G	111	ARG	2.6
1	G	109	ARG	2.5
1	F	82	ALA	2.5
1	E	109	ARG	2.5
1	D	148	HIS	2.5
1	G	52	SER	2.5
1	G	33	LEU	2.5
1	F	231	GLY	2.5
1	B	132	SER	2.5
1	E	66	TYR	2.4
1	B	136	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	51	VAL	2.4
1	F	65	ALA	2.3
1	B	75	LEU	2.3
1	G	66	TYR	2.3
1	D	149	PRO	2.3
1	D	109	ARG	2.2
1	A	29	TYR	2.2
1	F	109	ARG	2.2
1	B	148	HIS	2.2
1	G	64	LEU	2.2
1	D	66	TYR	2.2
1	E	130	SER	2.2
1	F	95	GLY	2.1
1	B	86	GLU	2.1
1	D	126	THR	2.1
1	G	161	LYS	2.1
1	A	65	ALA	2.1
1	G	232	THR	2.1
1	E	86	GLU	2.1
1	D	51	VAL	2.1
1	G	289	ARG	2.1
1	B	177	ARG	2.0
1	B	156	ARG	2.0
1	F	79	GLU	2.0
1	D	135	VAL	2.0
1	E	271	ARG	2.0
1	F	150	ARG	2.0
1	F	87	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LYS	B	3006	10/10	0.31	0.73	54,56,57,57	0
4	LYS	F	3004	10/10	0.37	0.99	57,58,59,61	0
4	LYS	G	3005	10/10	0.40	0.93	56,57,59,59	0
4	LYS	D	3002	10/10	0.56	0.78	55,56,58,60	0
4	LYS	E	3003	10/10	0.57	1.02	56,58,58,58	0
4	LYS	A	3001	10/10	0.60	0.72	54,55,57,57	0
2	MN	E	1301	1/1	0.95	0.05	30,30,30,30	0
3	GAI	A	1001	4/4	0.95	0.09	20,20,21,21	0
3	GAI	A	1004	4/4	0.95	0.12	20,20,21,22	0
2	MN	D	1201	1/1	0.95	0.05	43,43,43,43	0
3	GAI	E	1003	4/4	0.97	0.14	12,13,13,15	0
2	MN	A	1101	1/1	0.97	0.09	42,42,42,42	0
3	GAI	G	1005	4/4	0.97	0.12	14,16,16,16	0
2	MN	A	1102	1/1	0.97	0.06	28,28,28,28	0
2	MN	F	1401	1/1	0.97	0.09	47,47,47,47	0
2	MN	B	1601	1/1	0.97	0.06	38,38,38,38	0
3	GAI	B	1006	4/4	0.97	0.11	14,15,15,16	0
2	MN	D	1202	1/1	0.98	0.07	30,30,30,30	0
3	GAI	D	1002	4/4	0.98	0.10	19,20,20,21	0
2	MN	B	1602	1/1	0.99	0.18	32,32,32,32	0
2	MN	E	1302	1/1	0.99	0.03	16,16,16,16	0
2	MN	G	1501	1/1	0.99	0.06	40,40,40,40	0
2	MN	F	1402	1/1	0.99	0.07	31,31,31,31	0
2	MN	G	1502	1/1	0.99	0.20	36,36,36,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.