



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:13 PM GMT

PDB ID : 4RGZ  
Title : Crystal structure of recombinant prolidase from *Thermococcus sibiricus* at P21221 spacegroup  
Authors : Timofeev, V.I.; Korgenevsky, D.A.; Gorbacheva, M.A.; Boyko, K.M.; Slutsky, E.; Rakitina, T.V.; Lipkin, A.V.; Popov, V.O.  
Deposited on : 2014-10-01  
Resolution : 2.60 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

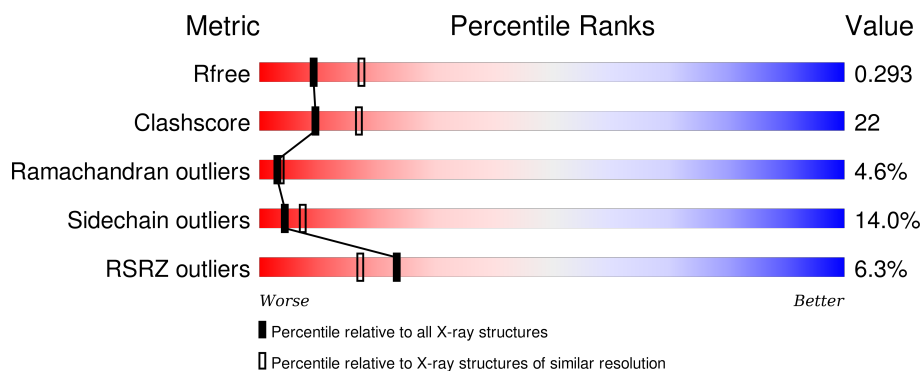
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	1	367	<div> <div>4%</div> <div>65%</div> <div>25%</div> <div>8%</div> <div>.</div> </div>
1	A	367	<div> <div>10%</div> <div>61%</div> <div>29%</div> <div>9%</div> <div>.</div> </div>
1	N	367	<div> <div>9%</div> <div>56%</div> <div>31%</div> <div>10%</div> <div>.</div> </div>
1	e	367	<div> <div>2%</div> <div>86%</div> <div>14%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	e	402	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11879 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 Xaa-Pro aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2919	1882	489	543	5			
1	N	367	Total	C	N	O	S	0	0	0
			2919	1882	489	543	5			
1	1	367	Total	C	N	O	S	0	0	0
			2919	1882	489	543	5			
1	e	367	Total	C	N	O	S	0	0	0
			2919	1882	489	543	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLY	-	EXPRESSION TAG	UNP C6A2N7
A	5	SER	-	EXPRESSION TAG	UNP C6A2N7
N	4	GLY	-	EXPRESSION TAG	UNP C6A2N7
N	5	SER	-	EXPRESSION TAG	UNP C6A2N7
1	4	GLY	-	EXPRESSION TAG	UNP C6A2N7
1	5	SER	-	EXPRESSION TAG	UNP C6A2N7
e	4	GLY	-	EXPRESSION TAG	UNP C6A2N7
e	5	SER	-	EXPRESSION TAG	UNP C6A2N7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	N	2	Total	Zn	0	0
			2	2		
2	e	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1	1	Total	O	P	0	0
			5	4	1		
3	1	1	Total	O	P	0	0
			5	4	1		
3	1	1	Total	O	P	0	0
			5	4	1		

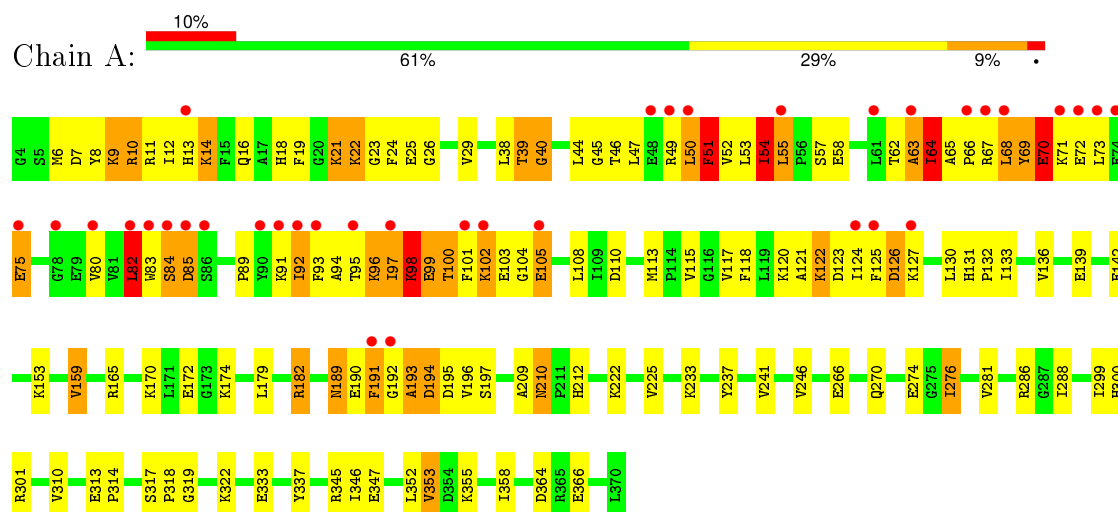
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	N	48	Total	O	0	0
			48	48		
4	1	47	Total	O	0	0
			47	47		
4	e	37	Total	O	0	0
			37	37		

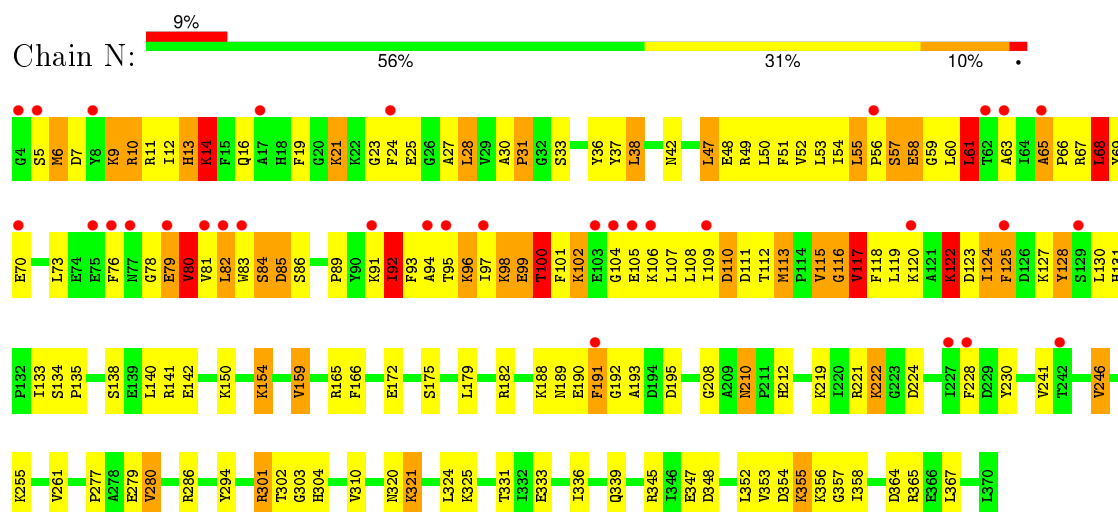
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Xaa-Pro aminopeptidase

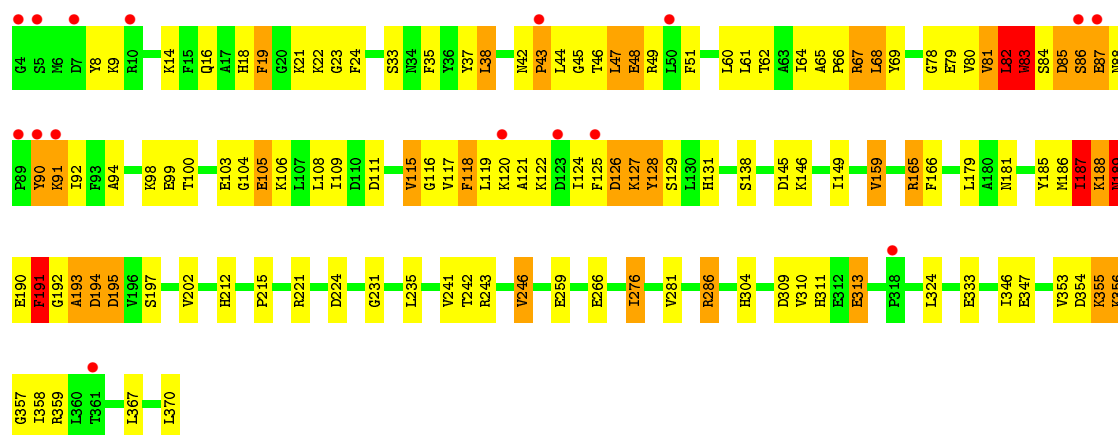


#### • Molecule 1: Xaa-Pro aminopeptidase

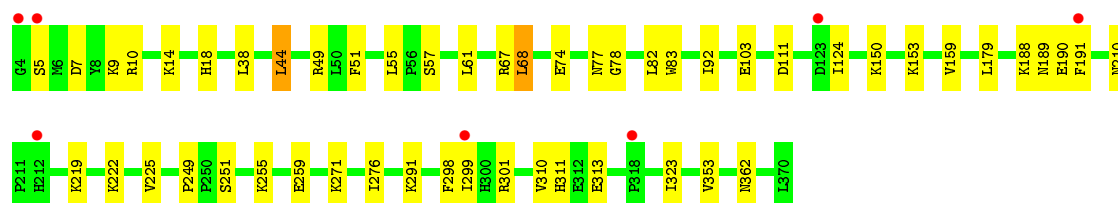
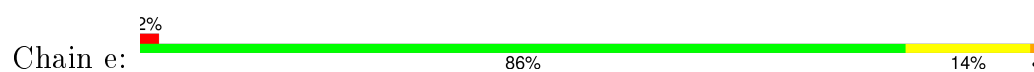


#### • Molecule 1: Xaa-Pro aminopeptidase





• Molecule 1: Xaa-Pro aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.60Å 123.72Å 136.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.60 29.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.48-2.60) 99.4 (29.48-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.221 , 0.296 0.224 , 0.293	Depositor DCC
$R_{free}$ test set	2598 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 51207 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: ZN, PO4

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	1	0.61	2/2984 (0.1%)	0.83	4/4021 (0.1%)
1	A	0.63	0/2984	0.88	5/4021 (0.1%)
1	N	0.60	1/2984 (0.0%)	0.85	3/4021 (0.1%)
1	e	0.60	1/2984 (0.0%)	0.79	4/4021 (0.1%)
All	All	0.61	4/11936 (0.0%)	0.84	16/16084 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	2
1	A	0	2
1	N	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	83	TRP	CD2-CE2	5.69	1.48	1.41
1	1	43	PRO	N-CD	5.42	1.55	1.47
1	e	83	TRP	CD2-CE2	5.30	1.47	1.41
1	N	14	LYS	CE-NZ	5.20	1.62	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	345	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	e	68	LEU	CA-CB-CG	8.99	135.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	345	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	N	345	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	e	78	GLY	N-CA-C	6.83	130.18	113.10
1	A	286	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	N	286	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	e	44	LEU	CA-CB-CG	5.78	128.59	115.30
1	1	42	ASN	C-N-CD	5.56	140.08	128.40
1	1	187	ILE	N-CA-C	5.41	125.59	111.00
1	e	61	LEU	CA-CB-CG	5.37	127.66	115.30
1	1	286	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	96	LYS	C-N-CA	5.13	134.52	121.70
1	A	82	LEU	CA-CB-CG	5.11	127.05	115.30
1	1	82	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	187	ILE	Peptide
1	1	189	ASN	Peptide
1	A	319	GLY	Peptide
1	A	63	ALA	Peptide
1	N	92	ILE	Peptide

## 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	1	2919	0	2942	127	0
1	A	2919	0	2942	168	0
1	N	2919	0	2942	154	0
1	e	2919	0	2942	0	0
2	1	2	0	0	0	0
2	A	2	0	0	0	0
2	N	2	0	0	0	0
2	e	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1	15	0	0	1	0
4	1	47	0	0	2	0
4	A	48	0	0	3	0
4	N	48	0	0	6	0
4	e	37	0	0	0	0
All	All	11879	0	11768	440	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 22.

All (440) 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)
1:1:116:GLY:C	1:1:118:PHE:HA	1.60	1.21
1:1:83:TRP:CB	1:1:84:SER:HA	1.72	1.19
1:A:123:ASP:HA	1:A:125:PHE:H	1.02	1.17
1:N:79:GLU:HB2	1:N:80:VAL:HG22	1.16	1.16
1:1:83:TRP:HB2	1:1:84:SER:CA	1.75	1.16
1:N:65:ALA:HB1	1:N:66:PRO:HA	1.15	1.13
1:A:126:ASP:CB	1:A:127:LYS:HA	1.78	1.12
1:1:86:SER:HB3	1:1:87:GLU:HB2	1.17	1.10
1:1:115:VAL:HG12	1:1:116:GLY:H	1.13	1.10
1:A:22:LYS:N	1:A:23:GLY:HA2	1.67	1.09
1:N:7:ASP:OD2	1:N:10:ARG:HG2	1.53	1.08
1:A:126:ASP:HB3	1:A:127:LYS:CA	1.82	1.08
1:1:118:PHE:HB2	1:1:119:LEU:CB	1.81	1.08
1:A:9:LYS:HA	1:A:10:ARG:C	1.70	1.08
1:1:118:PHE:CB	1:1:119:LEU:HB2	1.82	1.07
1:1:45:GLY:HA2	1:1:69:TYR:OH	1.53	1.07
1:1:192:GLY:HA2	1:1:193:ALA:HB2	1.11	1.07
1:A:96:LYS:H	1:A:97:ILE:HG12	0.98	1.05
1:A:54:ILE:HG23	1:A:55:LEU:N	1.71	1.05
1:A:22:LYS:H	1:A:23:GLY:HA2	0.92	1.05
1:A:11:ARG:HB3	1:A:14:LYS:HB2	1.39	1.04
1:A:96:LYS:N	1:A:97:ILE:HG12	1.73	1.04
1:A:54:ILE:HG23	1:A:55:LEU:H	0.88	1.03
1:A:69:TYR:HA	1:A:70:GLU:CB	1.88	1.03
1:1:104:GLY:HA3	1:1:105:GLU:HB2	1.41	1.03
1:A:54:ILE:CG2	1:A:55:LEU:H	1.71	1.03
1:A:69:TYR:CA	1:A:70:GLU:HB3	1.88	1.02
1:A:192:GLY:HA2	1:A:193:ALA:C	1.74	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:188:LYS:HG3	1:1:193:ALA:CB	1.90	1.02
1:A:123:ASP:HA	1:A:125:PHE:N	1.74	1.01
1:1:192:GLY:HA2	1:1:193:ALA:CB	1.90	1.01
1:1:86:SER:CB	1:1:87:GLU:HB2	1.90	1.01
1:A:66:PRO:HB2	1:A:67:ARG:O	1.60	0.98
1:A:96:LYS:H	1:A:97:ILE:CG1	1.76	0.98
1:A:126:ASP:HB3	1:A:127:LYS:HA	0.97	0.96
1:N:65:ALA:HB1	1:N:66:PRO:CA	1.95	0.96
1:N:116:GLY:C	1:N:118:PHE:H	1.67	0.95
1:N:246:VAL:HG22	1:N:367:LEU:HD11	1.47	0.93
1:N:16:GLN:NE2	1:N:59:GLY:H	1.66	0.93
1:A:22:LYS:H	1:A:23:GLY:CA	1.81	0.93
1:A:69:TYR:HA	1:A:70:GLU:HB3	0.94	0.92
1:A:118:PHE:HE1	1:A:124:ILE:HG21	1.34	0.91
1:A:11:ARG:HA	1:A:13:HIS:N	1.85	0.91
1:N:67:ARG:HA	1:N:82:LEU:HG	1.53	0.91
1:N:98:LYS:HA	1:N:99:GLU:C	1.89	0.90
1:A:193:ALA:HA	1:A:194:ASP:HB2	1.55	0.88
1:A:21:LYS:HA	1:A:21:LYS:HE2	1.54	0.88
1:1:194:ASP:HB2	4:1:539:HOH:O	1.73	0.88
1:N:190:GLU:HG2	4:N:530:HOH:O	1.73	0.86
1:1:115:VAL:HG12	1:1:116:GLY:N	1.92	0.84
1:A:11:ARG:HD3	1:A:13:HIS:HB2	1.60	0.84
1:N:65:ALA:CB	1:N:66:PRO:HA	2.04	0.84
1:1:189:ASN:N	1:1:189:ASN:HD22	1.76	0.83
1:A:11:ARG:HA	1:A:13:HIS:H	1.39	0.83
1:N:96:LYS:NZ	1:N:96:LYS:HB2	1.94	0.83
1:A:118:PHE:CE1	1:A:124:ILE:HG21	2.13	0.82
1:N:19:PHE:HB2	1:N:24:PHE:HB2	1.59	0.82
1:A:9:LYS:HA	1:A:10:ARG:O	1.80	0.81
1:A:67:ARG:HG3	1:A:84:SER:N	1.96	0.80
1:A:8:TYR:HD2	1:A:10:ARG:O	1.63	0.80
1:1:104:GLY:CA	1:1:105:GLU:HB2	2.11	0.80
1:1:116:GLY:O	1:1:118:PHE:HA	1.83	0.79
1:1:83:TRP:HB2	1:1:84:SER:HA	0.85	0.79
1:N:191:PHE:HD1	1:N:191:PHE:H	1.31	0.78
1:A:193:ALA:CA	1:A:194:ASP:HB2	2.13	0.78
1:1:122:LYS:H	1:1:125:PHE:H	1.27	0.78
1:1:117:VAL:N	1:1:118:PHE:HA	1.98	0.77
1:A:91:LYS:C	1:A:93:PHE:H	1.87	0.77
1:A:70:GLU:HG2	1:A:71:LYS:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:116:GLY:C	1:N:118:PHE:N	2.39	0.76
1:1:192:GLY:CA	1:1:193:ALA:HB2	2.05	0.76
1:A:353:VAL:HG13	1:A:358:ILE:HD13	1.66	0.75
1:N:79:GLU:HB2	1:N:80:VAL:CG2	2.07	0.74
1:1:188:LYS:CB	1:1:189:ASN:HB3	2.17	0.74
1:A:333:GLU:HB3	1:A:347:GLU:HG3	1.68	0.74
1:A:142:GLU:OE2	1:A:322:LYS:HE2	1.86	0.74
1:A:66:PRO:HA	1:A:67:ARG:HB2	1.70	0.74
1:N:124:ILE:O	1:N:125:PHE:HB2	1.88	0.73
1:1:120:LYS:N	1:1:121:ALA:HA	2.04	0.73
1:N:191:PHE:HB2	1:N:192:GLY:HA2	1.71	0.73
1:N:47:LEU:C	1:N:49:ARG:H	1.90	0.72
1:N:70:GLU:HB2	1:N:82:LEU:HD21	1.72	0.71
1:1:115:VAL:C	1:1:117:VAL:H	1.93	0.71
1:A:47:LEU:CD2	1:N:112:THR:HA	2.21	0.70
1:A:21:LYS:HA	1:A:21:LYS:CE	2.21	0.70
1:A:97:ILE:O	1:A:98:LYS:HB2	1.89	0.70
1:1:165:ARG:HD3	4:1:525:HOH:O	1.91	0.69
1:N:116:GLY:O	1:N:118:PHE:N	2.25	0.69
1:A:193:ALA:HA	1:A:194:ASP:CB	2.23	0.68
1:N:93:PHE:C	1:N:97:ILE:H	1.97	0.68
1:A:115:VAL:HG22	1:N:115:VAL:HA	1.74	0.68
1:A:47:LEU:HD23	1:N:112:THR:HA	1.75	0.68
1:N:28:LEU:HD23	1:N:54:ILE:HG12	1.75	0.68
1:1:266:GLU:OE2	1:1:359:ARG:NH2	2.27	0.67
1:1:188:LYS:HB3	1:1:189:ASN:HB3	1.77	0.67
1:1:188:LYS:HG3	1:1:193:ALA:HB1	1.74	0.67
1:1:190:GLU:O	1:1:191:PHE:HB2	1.93	0.67
1:A:71:LYS:HG2	1:A:72:GLU:HA	1.77	0.66
1:A:22:LYS:N	1:A:23:GLY:CA	2.48	0.66
1:1:86:SER:HB3	1:1:87:GLU:CB	2.11	0.66
1:A:98:LYS:O	1:A:102:LYS:HG3	1.96	0.66
1:N:96:LYS:HA	1:N:97:ILE:C	2.16	0.66
1:A:132:PRO:HG3	1:N:120:LYS:HG2	1.78	0.65
1:N:96:LYS:HD3	1:N:97:ILE:O	1.96	0.65
1:N:261:VAL:CG2	1:N:336:ILE:HG13	2.28	0.64
1:A:98:LYS:N	1:A:99:GLU:O	2.31	0.64
1:N:188:LYS:HE2	1:N:195:ASP:OD1	1.97	0.64
1:A:53:LEU:HA	1:A:64:ILE:HD12	1.79	0.63
1:A:233:LYS:HA	1:A:237:TYR:O	1.98	0.63
1:1:86:SER:CA	1:1:87:GLU:HB2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:192:GLY:CA	1:1:193:ALA:CB	2.70	0.63
1:1:354:ASP:O	1:1:355:LYS:HB2	1.99	0.62
1:1:119:LEU:C	1:1:121:ALA:HA	2.20	0.62
1:A:159:VAL:HG13	1:A:241:VAL:HG11	1.81	0.62
1:N:159:VAL:HG13	1:N:241:VAL:HG11	1.81	0.62
1:A:66:PRO:CB	1:A:67:ARG:O	2.41	0.62
1:1:115:VAL:CG1	1:1:116:GLY:H	1.95	0.62
1:A:51:PHE:HA	1:A:66:PRO:HD3	1.82	0.62
1:1:83:TRP:HE3	1:1:85:ASP:H	1.48	0.61
1:A:70:GLU:HG2	1:A:71:LYS:N	2.14	0.61
1:1:189:ASN:N	1:1:189:ASN:ND2	2.47	0.61
1:A:39:THR:OG1	1:A:40:GLY:N	2.33	0.61
1:1:118:PHE:HB2	1:1:119:LEU:HB2	0.86	0.61
1:A:63:ALA:HB3	1:A:80:VAL:HA	1.81	0.61
1:N:65:ALA:HB3	1:N:83:TRP:CD1	2.36	0.61
1:A:50:LEU:HA	1:A:117:VAL:HG13	1.81	0.61
1:A:49:ARG:O	1:A:51:PHE:N	2.33	0.60
1:N:294:TYR:CB	1:N:336:ILE:HD13	2.30	0.60
1:N:55:LEU:HG	1:N:61:LEU:HB3	1.83	0.60
1:1:125:PHE:O	1:1:126:ASP:HB3	2.01	0.60
1:N:49:ARG:HH21	1:N:85:ASP:CG	2.04	0.60
1:1:276:ILE:HD11	1:1:281:VAL:HG22	1.84	0.60
1:1:45:GLY:HA2	1:1:69:TYR:HH	1.66	0.59
1:N:19:PHE:CB	1:N:24:PHE:HB2	2.32	0.59
1:A:122:LYS:O	1:A:124:ILE:HB	2.01	0.59
1:N:210:ASN:HD22	1:N:210:ASN:C	2.05	0.59
1:N:59:GLY:HA2	4:N:522:HOH:O	2.02	0.59
1:N:96:LYS:HG3	1:N:97:ILE:HA	1.85	0.58
1:N:353:VAL:HG23	1:N:358:ILE:HD13	1.85	0.58
1:A:8:TYR:HA	1:A:9:LYS:O	2.03	0.58
1:A:96:LYS:CA	1:A:97:ILE:HG12	2.34	0.58
1:A:49:ARG:HD3	1:A:66:PRO:HB3	1.86	0.58
1:A:91:LYS:C	1:A:93:PHE:N	2.57	0.58
1:A:16:GLN:NE2	4:A:533:HOH:O	2.36	0.58
1:N:210:ASN:ND2	1:N:212:HIS:H	2.01	0.58
1:A:301:ARG:HB2	1:A:317:SER:HB3	1.86	0.58
1:N:65:ALA:HB2	1:N:82:LEU:HA	1.85	0.58
1:1:47:LEU:HD23	1:1:49:ARG:HE	1.67	0.58
1:N:50:LEU:HD13	1:N:89:PRO:HB2	1.85	0.58
1:N:166:PHE:HE2	1:N:228:PHE:CE1	2.22	0.58
1:1:60:LEU:HD23	1:1:78:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLY:HA2	1:A:194:ASP:N	2.17	0.57
1:A:93:PHE:HA	1:A:97:ILE:HD12	1.86	0.57
1:N:16:GLN:NE2	1:N:59:GLY:N	2.47	0.57
1:A:83:TRP:CB	1:A:84:SER:HB3	2.35	0.57
1:N:54:ILE:HD11	1:N:93:PHE:HE2	1.69	0.57
1:1:187:ILE:N	1:1:188:LYS:O	2.38	0.57
1:N:66:PRO:HB3	1:N:83:TRP:CE2	2.40	0.57
1:1:94:ALA:HB2	1:1:124:ILE:HG21	1.87	0.57
1:1:104:GLY:CA	1:1:105:GLU:CB	2.81	0.56
1:N:95:THR:N	1:N:96:LYS:O	2.37	0.56
1:1:188:LYS:HG3	1:1:193:ALA:HB2	1.81	0.56
1:A:193:ALA:N	1:A:194:ASP:HB2	2.20	0.56
1:N:159:VAL:HG22	1:N:230:TYR:CE2	2.40	0.56
1:A:16:GLN:NE2	1:A:58:GLU:HA	2.21	0.56
1:1:67:ARG:HH21	1:1:82:LEU:HD23	1.71	0.56
1:A:11:ARG:CD	1:A:13:HIS:HB2	2.33	0.56
1:A:66:PRO:HB2	1:A:67:ARG:C	2.27	0.56
1:N:96:LYS:HZ3	1:N:96:LYS:HB2	1.69	0.56
1:N:124:ILE:O	1:N:124:ILE:HG22	2.06	0.56
1:A:26:GLY:HA3	1:A:101:PHE:CZ	2.42	0.55
1:N:49:ARG:NH2	1:N:85:ASP:OD2	2.39	0.55
1:A:82:LEU:HD22	1:A:82:LEU:H	1.72	0.55
1:A:313:GLU:HG2	1:A:322:LYS:HE2	1.89	0.55
1:A:83:TRP:HA	1:A:84:SER:HB3	1.89	0.55
1:A:113:MET:O	1:N:115:VAL:HG23	2.07	0.55
1:A:9:LYS:C	1:A:9:LYS:HD3	2.28	0.54
1:1:67:ARG:N	1:1:84:SER:OG	2.38	0.54
1:N:67:ARG:O	1:N:69:TYR:N	2.41	0.54
1:1:333:GLU:HB3	1:1:347:GLU:HG3	1.88	0.54
1:N:94:ALA:N	1:N:96:LYS:O	2.41	0.54
1:A:49:ARG:HG3	1:A:51:PHE:HB2	1.90	0.54
1:N:89:PRO:O	1:N:91:LYS:N	2.39	0.54
1:1:116:GLY:O	1:1:118:PHE:CA	2.55	0.54
1:A:8:TYR:HB2	1:A:10:ARG:N	2.23	0.54
1:1:35:PHE:CD1	1:1:43:PRO:HD3	2.42	0.54
1:A:52:VAL:C	1:A:64:ILE:HG13	2.28	0.54
1:1:94:ALA:HB2	1:1:124:ILE:CG2	2.37	0.54
1:A:192:GLY:CA	1:A:193:ALA:C	2.63	0.54
1:N:47:LEU:C	1:N:49:ARG:N	2.59	0.54
1:1:24:PHE:CD1	1:1:106:LYS:HB3	2.43	0.54
1:N:84:SER:C	1:N:86:SER:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:CG	1:A:71:LYS:N	2.70	0.53
1:A:73:LEU:O	1:A:80:VAL:HG11	2.08	0.53
1:N:115:VAL:O	1:N:117:VAL:N	2.41	0.53
1:N:210:ASN:ND2	1:N:210:ASN:C	2.62	0.53
1:1:242:THR:H	1:1:347:GLU:HB3	1.73	0.53
1:N:13:HIS:HA	1:N:16:GLN:OE1	2.08	0.53
1:1:281:VAL:HG21	1:1:324:LEU:HD11	1.91	0.53
1:N:96:LYS:HZ2	1:N:96:LYS:HB2	1.72	0.53
1:A:126:ASP:CB	1:A:127:LYS:CA	2.62	0.53
1:N:191:PHE:HA	1:N:193:ALA:H	1.72	0.53
1:A:131:HIS:CE1	1:N:122:LYS:HE2	2.43	0.53
1:1:243:ARG:NH1	1:1:347:GLU:O	2.42	0.53
1:N:36:TYR:CD2	1:N:42:ASN:HB2	2.45	0.52
1:1:16:GLN:HA	1:1:19:PHE:CE2	2.44	0.52
1:A:16:GLN:HA	1:A:19:PHE:CE2	2.44	0.52
1:1:166:PHE:HB2	1:1:186:MET:CE	2.39	0.52
1:N:301:ARG:HG3	1:N:301:ARG:HH11	1.74	0.52
1:N:98:LYS:HA	1:N:100:THR:N	2.24	0.52
1:1:181:ASN:N	1:1:181:ASN:HD22	2.07	0.52
1:1:90:TYR:O	1:1:92:ILE:N	2.43	0.52
1:A:94:ALA:HA	1:A:98:LYS:HB2	1.91	0.52
1:N:191:PHE:CB	1:N:192:GLY:HA2	2.31	0.52
1:1:24:PHE:HE1	1:1:131:HIS:HD2	1.57	0.52
1:1:187:ILE:O	1:1:187:ILE:CG2	2.59	0.52
1:1:333:GLU:O	1:1:333:GLU:HG3	2.10	0.52
1:1:246:VAL:HG22	1:1:367:LEU:HD11	1.92	0.52
1:1:33:SER:OG	1:1:309:ASP:OD1	2.28	0.52
1:1:304:HIS:HD2	3:1:402:PO4:O3	1.92	0.52
1:1:193:ALA:O	1:1:194:ASP:CB	2.57	0.51
1:N:54:ILE:HD11	1:N:93:PHE:CE2	2.44	0.51
1:A:68:LEU:HD12	1:A:69:TYR:N	2.25	0.51
1:A:83:TRP:CA	1:A:84:SER:HB3	2.39	0.51
1:A:24:PHE:CZ	1:A:131:HIS:HB2	2.46	0.51
1:A:72:GLU:O	1:A:75:GLU:HB2	2.11	0.51
1:N:94:ALA:O	1:N:95:THR:HG23	2.11	0.51
1:N:19:PHE:C	1:N:21:LYS:H	2.14	0.51
1:A:97:ILE:O	1:A:98:LYS:HD3	2.11	0.51
1:A:51:PHE:CD2	1:A:66:PRO:HG3	2.46	0.51
1:A:46:THR:HB	1:A:49:ARG:HH11	1.75	0.51
1:N:166:PHE:HE2	1:N:228:PHE:CZ	2.29	0.51
1:A:92:ILE:CG2	1:A:92:ILE:O	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ASN:HD22	1:A:210:ASN:C	2.13	0.51
1:1:115:VAL:CG1	1:1:116:GLY:N	2.64	0.51
1:A:192:GLY:HA2	1:A:193:ALA:O	2.08	0.51
1:N:97:ILE:O	1:N:100:THR:HG23	2.11	0.51
1:1:120:LYS:N	1:1:121:ALA:CA	2.74	0.51
1:N:94:ALA:N	1:N:97:ILE:H	2.09	0.51
1:N:84:SER:O	1:N:86:SER:N	2.38	0.50
1:A:29:VAL:HA	1:A:110:ASP:HB2	1.94	0.50
1:1:188:LYS:HZ1	1:1:195:ASP:HB2	1.77	0.50
1:A:102:LYS:HA	1:A:103:GLU:HG3	1.92	0.50
1:A:64:ILE:N	1:A:64:ILE:HD13	2.27	0.50
1:N:134:SER:N	1:N:135:PRO:HD2	2.26	0.50
1:1:185:TYR:O	1:1:188:LYS:O	2.29	0.50
1:A:54:ILE:CG2	1:A:55:LEU:N	2.44	0.50
1:A:8:TYR:HA	1:A:9:LYS:C	2.32	0.50
1:N:277:PRO:HB2	1:N:280:VAL:HG12	1.94	0.50
1:N:279:GLU:HB3	1:N:320:ASN:O	2.12	0.50
1:A:53:LEU:HA	1:A:64:ILE:HG21	1.94	0.49
1:N:25:GLU:HG3	1:N:25:GLU:O	2.11	0.49
1:A:8:TYR:CD2	1:A:10:ARG:O	2.54	0.49
1:N:102:LYS:O	1:N:105:GLU:HG2	2.13	0.49
1:A:190:GLU:O	1:A:191:PHE:CB	2.60	0.49
1:N:33:SER:HB3	1:N:141:ARG:HH12	1.76	0.49
1:N:150:LYS:O	1:N:154:LYS:HB2	2.13	0.49
1:A:67:ARG:HG3	1:A:84:SER:H	1.75	0.49
1:N:12:ILE:HG23	1:N:55:LEU:HD21	1.94	0.49
1:N:95:THR:N	1:N:96:LYS:C	2.65	0.49
1:1:115:VAL:O	1:1:118:PHE:CD2	2.66	0.49
1:N:28:LEU:CD2	1:N:54:ILE:HG12	2.43	0.49
1:N:356:LYS:HG3	1:N:357:GLY:N	2.28	0.49
1:A:191:PHE:O	1:A:193:ALA:O	2.31	0.48
1:A:67:ARG:NH2	1:A:89:PRO:CG	2.76	0.48
1:1:356:LYS:HD3	1:1:357:GLY:O	2.12	0.48
1:N:66:PRO:HB3	1:N:83:TRP:CZ2	2.48	0.48
1:1:115:VAL:C	1:1:117:VAL:N	2.62	0.48
1:N:93:PHE:C	1:N:97:ILE:N	2.66	0.48
1:A:313:GLU:HG3	1:A:314:PRO:HA	1.96	0.48
1:N:16:GLN:HE21	1:N:59:GLY:H	1.55	0.48
1:A:29:VAL:O	1:A:53:LEU:N	2.39	0.48
1:A:115:VAL:CG2	1:N:115:VAL:HA	2.43	0.48
1:1:126:ASP:H	1:1:127:LYS:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:HD2	1:A:14:LYS:N	2.29	0.48
1:A:313:GLU:CG	1:A:322:LYS:HE2	2.43	0.48
1:N:358:ILE:HD12	1:N:358:ILE:N	2.28	0.48
1:N:208:GLY:HA3	4:N:515:HOH:O	2.13	0.48
1:N:221:ARG:HG2	1:N:224:ASP:OD2	2.13	0.48
1:A:364:ASP:HB3	1:A:366:GLU:OE2	2.14	0.47
1:1:103:GLU:HA	1:1:128:TYR:CE1	2.48	0.47
1:A:212:HIS:NE2	1:N:68:LEU:HB2	2.29	0.47
1:A:120:LYS:HA	1:A:121:ALA:HA	1.56	0.47
1:A:96:LYS:HB2	1:A:97:ILE:HG12	1.96	0.47
1:N:6:MET:HB2	1:N:11:ARG:HH12	1.79	0.47
1:N:222:LYS:HE3	4:N:535:HOH:O	2.13	0.47
1:1:127:LYS:HA	1:1:127:LYS:HD2	1.77	0.47
1:1:66:PRO:HG3	1:1:83:TRP:CZ2	2.50	0.47
1:1:242:THR:N	1:1:347:GLU:HB3	2.29	0.47
1:N:108:LEU:HA	1:N:131:HIS:O	2.14	0.47
1:N:304:HIS:CE1	1:N:310:VAL:O	2.68	0.47
1:1:121:ALA:HB3	1:1:122:LYS:HB3	1.96	0.47
1:1:194:ASP:O	1:1:195:ASP:OD1	2.31	0.47
1:A:195:ASP:HB3	1:A:233:LYS:HD2	1.97	0.47
1:1:159:VAL:HG13	1:1:241:VAL:HG11	1.96	0.47
1:1:64:ILE:HA	1:1:81:VAL:O	2.14	0.47
1:A:67:ARG:CZ	1:A:89:PRO:HG2	2.45	0.47
1:N:111:ASP:HB2	4:N:523:HOH:O	2.14	0.47
1:N:348:ASP:OD2	1:N:365:ARG:HD3	2.14	0.47
1:A:91:LYS:O	1:A:93:PHE:N	2.48	0.47
1:N:56:PRO:O	1:N:57:SER:C	2.53	0.47
1:1:189:ASN:H	1:1:189:ASN:HD22	1.61	0.46
1:N:190:GLU:O	1:N:193:ALA:HB3	2.15	0.46
1:A:299:ILE:O	1:N:68:LEU:HD22	2.14	0.46
1:1:145:ASP:O	1:1:149:ILE:HD12	2.15	0.46
1:1:125:PHE:O	1:1:126:ASP:CB	2.63	0.46
1:N:108:LEU:HD22	1:N:133:ILE:HA	1.96	0.46
1:N:30:ALA:O	1:N:31:PRO:C	2.53	0.46
1:A:124:ILE:HG23	1:A:130:LEU:HD21	1.97	0.46
1:A:63:ALA:HA	1:A:64:ILE:HD13	1.98	0.46
1:N:191:PHE:CD1	1:N:191:PHE:N	2.75	0.46
1:1:19:PHE:HB2	1:1:108:LEU:HD11	1.97	0.46
1:N:133:ILE:C	1:N:135:PRO:HD2	2.36	0.46
1:A:122:LYS:NZ	1:A:122:LYS:HB2	2.31	0.46
1:N:67:ARG:C	1:N:69:TYR:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:188:LYS:CA	1:1:189:ASN:HB3	2.45	0.46
1:A:99:GLU:HA	1:A:100:THR:HA	1.59	0.46
1:N:37:TYR:HD2	1:N:38:LEU:HD13	1.81	0.46
1:A:136:VAL:O	1:A:139:GLU:HB2	2.16	0.46
1:1:185:TYR:C	1:1:188:LYS:O	2.53	0.46
1:A:26:GLY:HA3	1:A:101:PHE:CE1	2.51	0.46
1:1:24:PHE:CE1	1:1:131:HIS:HD2	2.34	0.46
1:A:172:GLU:OE1	1:A:222:LYS:HE3	2.15	0.46
1:A:9:LYS:HE2	1:A:10:ARG:HA	1.98	0.46
1:A:266:GLU:OE2	1:A:270:GLN:NE2	2.49	0.46
1:A:276:ILE:HD11	1:A:281:VAL:HG23	1.98	0.46
1:1:65:ALA:O	1:1:82:LEU:HA	2.15	0.46
1:1:193:ALA:O	1:1:194:ASP:HB3	2.17	0.45
1:N:333:GLU:HB3	1:N:347:GLU:HB2	1.99	0.45
1:N:106:LYS:O	1:N:107:LEU:HD23	2.17	0.45
1:A:123:ASP:N	1:A:123:ASP:OD1	2.50	0.45
1:1:188:LYS:CD	1:1:188:LYS:N	2.79	0.45
1:A:108:LEU:HD22	1:A:133:ILE:HA	1.99	0.45
1:A:45:GLY:HA3	4:A:532:HOH:O	2.16	0.45
1:1:62:THR:HG23	1:1:79:GLU:HG2	1.99	0.45
1:1:126:ASP:H	1:1:127:LYS:CA	2.30	0.45
1:A:24:PHE:CE1	1:A:131:HIS:HB2	2.51	0.45
1:N:354:ASP:O	1:N:355:LYS:HB2	2.17	0.45
1:N:123:ASP:HB2	1:N:124:ILE:HB	1.99	0.45
1:N:124:ILE:O	1:N:125:PHE:CB	2.63	0.44
1:N:96:LYS:CD	1:N:97:ILE:O	2.64	0.44
1:A:83:TRP:HB3	1:A:84:SER:HB3	1.99	0.44
1:A:7:ASP:HB3	1:A:8:TYR:HA	1.98	0.44
1:N:100:THR:HB	1:N:101:PHE:H	1.71	0.44
1:A:189:ASN:OD1	1:A:189:ASN:N	2.51	0.44
1:A:209:ALA:O	1:A:337:TYR:HB3	2.17	0.44
1:A:68:LEU:HD12	1:A:69:TYR:H	1.82	0.44
1:N:191:PHE:HA	1:N:193:ALA:N	2.33	0.44
1:N:27:ALA:HA	1:N:108:LEU:O	2.18	0.44
1:1:21:LYS:C	1:1:23:GLY:H	2.21	0.44
1:1:188:LYS:HG3	1:1:193:ALA:HB3	1.92	0.43
1:N:98:LYS:CA	1:N:99:GLU:C	2.75	0.43
1:N:110:ASP:HB3	1:N:113:MET:HB3	2.00	0.43
1:1:126:ASP:OD1	1:1:127:LYS:HB2	2.18	0.43
1:1:187:ILE:HG23	1:1:187:ILE:O	2.19	0.43
1:N:6:MET:H	1:N:6:MET:HG2	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:16:GLN:HB3	1:N:58:GLU:HB2	2.00	0.43
1:N:134:SER:O	1:N:138:SER:HB3	2.17	0.43
1:N:16:GLN:NE2	1:N:59:GLY:O	2.51	0.43
1:N:96:LYS:HD3	1:N:100:THR:H	1.83	0.43
1:1:45:GLY:CA	1:1:69:TYR:OH	2.45	0.43
1:N:78:GLY:O	1:N:79:GLU:O	2.36	0.43
1:N:191:PHE:HB2	1:N:192:GLY:CA	2.47	0.43
1:1:117:VAL:N	1:1:118:PHE:CA	2.76	0.43
1:N:70:GLU:HA	1:N:73:LEU:HB2	2.01	0.43
1:A:83:TRP:HB3	1:A:84:SER:CB	2.49	0.43
1:1:159:VAL:HG21	1:1:231:GLY:HA2	2.01	0.43
1:N:302:THR:O	1:N:333:GLU:N	2.44	0.43
1:1:202:VAL:H	1:1:215:PRO:HG3	1.84	0.43
1:A:44:LEU:HA	1:A:45:GLY:HA2	1.74	0.43
1:A:174:LYS:HE2	1:A:182:ARG:HH12	1.83	0.43
1:A:55:LEU:HG	1:A:55:LEU:O	2.19	0.43
1:N:100:THR:HG21	1:N:128:TYR:OH	2.18	0.43
1:A:274:GLU:HB3	1:A:355:LYS:HG3	2.00	0.43
1:N:294:TYR:HB3	1:N:336:ILE:HD13	2.00	0.42
1:A:16:GLN:HA	1:A:19:PHE:CD2	2.53	0.42
1:A:153:LYS:HE3	4:A:536:HOH:O	2.19	0.42
1:1:188:LYS:HA	1:1:189:ASN:HA	1.81	0.42
1:A:142:GLU:OE2	1:A:322:LYS:CE	2.60	0.42
1:A:317:SER:HB2	1:A:318:PRO:HD2	2.00	0.42
1:N:25:GLU:HG2	1:N:105:GLU:CD	2.39	0.42
1:N:11:ARG:HD3	1:N:37:TYR:CE2	2.54	0.42
1:A:276:ILE:HD11	1:A:281:VAL:CG2	2.50	0.42
1:1:221:ARG:HG2	1:1:224:ASP:OD2	2.20	0.42
1:A:170:LYS:HB3	1:A:174:LYS:NZ	2.34	0.42
1:1:83:TRP:CB	1:1:84:SER:CA	2.59	0.42
1:A:125:PHE:O	1:A:125:PHE:CD1	2.72	0.42
1:N:303:GLY:HA3	1:N:331:THR:O	2.19	0.42
1:1:126:ASP:N	1:1:127:LYS:HB2	2.34	0.42
1:N:36:TYR:HD2	1:N:42:ASN:HB2	1.84	0.42
1:1:83:TRP:HE3	1:1:85:ASP:N	2.15	0.42
1:A:18:HIS:O	1:A:22:LYS:HB2	2.20	0.42
1:1:353:VAL:HB	1:1:358:ILE:HD12	2.02	0.42
1:A:82:LEU:O	1:A:83:TRP:HB2	2.20	0.42
1:1:121:ALA:N	1:1:122:LYS:O	2.53	0.41
1:1:138:SER:HB2	1:1:313:GLU:HG3	2.01	0.41
1:N:356:LYS:O	1:N:358:ILE:HD12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:166:PHE:HB2	1:1:186:MET:HE3	2.02	0.41
1:1:37:TYR:HD2	1:1:38:LEU:HD13	1.85	0.41
1:N:76:PHE:HD2	1:N:79:GLU:H	1.68	0.41
1:N:70:GLU:O	1:N:73:LEU:N	2.54	0.41
1:N:59:GLY:CA	4:N:522:HOH:O	2.65	0.41
1:N:96:LYS:HE3	1:N:99:GLU:HG2	2.02	0.41
1:N:53:LEU:HD12	1:N:63:ALA:HA	2.03	0.41
1:1:88:ASN:OD1	1:1:91:LYS:HB2	2.20	0.41
1:A:125:PHE:HA	1:A:126:ASP:HA	1.78	0.41
1:A:68:LEU:HG	1:A:68:LEU:H	1.70	0.41
1:A:333:GLU:HA	1:A:346:ILE:O	2.20	0.41
1:N:175:SER:HA	1:N:219:LYS:HA	2.01	0.41
1:1:61:LEU:N	1:1:61:LEU:HD23	2.35	0.41
1:1:121:ALA:HB3	1:1:122:LYS:CB	2.51	0.41
1:1:120:LYS:C	1:1:122:LYS:O	2.59	0.41
1:N:14:LYS:HA	1:N:14:LYS:HD2	1.84	0.41
1:N:98:LYS:HG2	1:N:98:LYS:O	2.19	0.41
1:A:300:HIS:HE1	1:A:333:GLU:O	2.03	0.41
1:A:210:ASN:ND2	1:A:212:HIS:H	2.19	0.41
1:A:25:GLU:HB2	1:A:105:GLU:HB2	2.03	0.41
1:1:103:GLU:HB3	1:1:127:LYS:HZ3	1.86	0.41
1:N:89:PRO:C	1:N:91:LYS:N	2.74	0.41
1:1:119:LEU:HA	1:1:120:LYS:HA	1.28	0.41
1:1:67:ARG:O	1:1:69:TYR:N	2.54	0.41
1:A:124:ILE:O	1:A:126:ASP:HA	2.21	0.41
1:N:9:LYS:HA	1:N:12:ILE:HD12	2.02	0.41
1:N:23:GLY:O	1:N:106:LYS:HD2	2.21	0.41
1:A:96:LYS:CB	1:A:97:ILE:HG23	2.51	0.41
1:N:100:THR:O	1:N:101:PHE:CG	2.73	0.41
1:1:129:SER:OG	1:1:131:HIS:NE2	2.54	0.41
1:N:321:LYS:HE2	1:N:321:LYS:HB3	1.84	0.41
1:N:104:GLY:N	1:N:127:LYS:O	2.54	0.41
1:A:9:LYS:CE	1:A:10:ARG:HA	2.51	0.41
1:A:70:GLU:OE1	1:A:73:LEU:HD13	2.20	0.41
1:1:86:SER:CA	1:1:87:GLU:CB	2.99	0.40
1:A:51:PHE:HA	1:A:65:ALA:HB3	2.03	0.40
1:A:14:LYS:HD3	1:A:18:HIS:CD2	2.56	0.40
1:N:16:GLN:HE22	1:N:59:GLY:H	1.56	0.40
1:1:19:PHE:CD1	1:1:19:PHE:C	2.95	0.40
1:1:333:GLU:HA	1:1:346:ILE:O	2.21	0.40
1:N:134:SER:N	1:N:135:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:8:TYR:O	1:1:9:LYS:C	2.59	0.40
1:N:101:PHE:O	1:N:102:LYS:C	2.60	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	1	365/367 (100%)	317 (87%)	31 (8%)	17 (5%)	3	3
1	A	365/367 (100%)	293 (80%)	48 (13%)	24 (7%)	1	1
1	N	365/367 (100%)	310 (85%)	32 (9%)	23 (6%)	2	2
1	e	365/367 (100%)	335 (92%)	27 (7%)	3 (1%)	24	46
All	All	1460/1468 (100%)	1255 (86%)	138 (10%)	67 (5%)	3	3

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	54	ILE
1	A	57	SER
1	A	69	TYR
1	A	70	GLU
1	A	92	ILE
1	A	97	ILE
1	A	98	LYS
1	A	99	GLU
1	N	47	LEU
1	N	79	GLU
1	N	81	VAL
1	N	85	ASP

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Mol	Chain	Res	Type
1	N	92	ILE
1	N	115	VAL
1	N	116	GLY
1	N	117	VAL
1	N	125	PHE
1	1	87	GLU
1	1	105	GLU
1	1	126	ASP
1	1	191	PHE
1	1	193	ALA
1	1	194	ASP
1	e	74	GLU
1	A	193	ALA
1	N	21	LYS
1	N	48	GLU
1	N	57	SER
1	N	61	LEU
1	N	65	ALA
1	N	99	GLU
1	N	100	THR
1	N	102	LYS
1	N	122	LYS
1	N	124	ILE
1	1	47	LEU
1	1	86	SER
1	1	91	LYS
1	1	115	VAL
1	1	128	TYR
1	e	77	ASN
1	A	9	LYS
1	A	12	ILE
1	A	51	PHE
1	A	104	GLY
1	A	105	GLU
1	A	194	ASP
1	N	364	ASP
1	1	68	LEU
1	1	85	ASP
1	1	90	TYR
1	1	235	LEU
1	A	10	ARG
1	A	39	THR

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Mol	Chain	Res	Type
1	A	40	GLY
1	A	85	ASP
1	A	191	PHE
1	N	31	PRO
1	N	68	LEU
1	N	80	VAL
1	A	50	LEU
1	1	22	LYS
1	1	48	GLU
1	e	190	GLU
1	A	84	SER
1	A	64	ILE

### 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	1	311/311 (100%)	270 (87%)	41 (13%)	5	9
1	A	311/311 (100%)	276 (89%)	35 (11%)	7	13
1	N	311/311 (100%)	259 (83%)	52 (17%)	3	4
1	e	311/311 (100%)	265 (85%)	46 (15%)	4	6
All	All	1244/1244 (100%)	1070 (86%)	174 (14%)	4	7

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	21	LYS
1	A	22	LYS
1	A	38	LEU
1	A	51	PHE
1	A	54	ILE
1	A	55	LEU
1	A	62	THR
1	A	64	ILE

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Mol	Chain	Res	Type
1	A	68	LEU
1	A	70	GLU
1	A	75	GLU
1	A	82	LEU
1	A	85	ASP
1	A	95	THR
1	A	98	LYS
1	A	100	THR
1	A	102	LYS
1	A	122	LYS
1	A	126	ASP
1	A	159	VAL
1	A	165	ARG
1	A	179	LEU
1	A	182	ARG
1	A	189	ASN
1	A	196	VAL
1	A	197	SER
1	A	210	ASN
1	A	225	VAL
1	A	246	VAL
1	A	276	ILE
1	A	288	ILE
1	A	310	VAL
1	A	352	LEU
1	A	353	VAL
1	N	5	SER
1	N	6	MET
1	N	9	LYS
1	N	10	ARG
1	N	13	HIS
1	N	14	LYS
1	N	28	LEU
1	N	38	LEU
1	N	51	PHE
1	N	52	VAL
1	N	55	LEU
1	N	58	GLU
1	N	60	LEU
1	N	61	LEU
1	N	68	LEU
1	N	80	VAL

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Mol	Chain	Res	Type
1	N	82	LEU
1	N	84	SER
1	N	92	ILE
1	N	96	LYS
1	N	98	LYS
1	N	100	THR
1	N	109	ILE
1	N	110	ASP
1	N	113	MET
1	N	117	VAL
1	N	119	LEU
1	N	122	LYS
1	N	128	TYR
1	N	130	LEU
1	N	140	LEU
1	N	142	GLU
1	N	154	LYS
1	N	159	VAL
1	N	165	ARG
1	N	172	GLU
1	N	179	LEU
1	N	182	ARG
1	N	189	ASN
1	N	191	PHE
1	N	210	ASN
1	N	222	LYS
1	N	246	VAL
1	N	255	LYS
1	N	280	VAL
1	N	301	ARG
1	N	321	LYS
1	N	324	LEU
1	N	325	LYS
1	N	339	GLN
1	N	352	LEU
1	N	355	LYS
1	1	14	LYS
1	1	18	HIS
1	1	19	PHE
1	1	38	LEU
1	1	44	LEU
1	1	46	THR

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Mol	Chain	Res	Type
1	1	48	GLU
1	1	51	PHE
1	1	67	ARG
1	1	68	LEU
1	1	80	VAL
1	1	81	VAL
1	1	82	LEU
1	1	83	TRP
1	1	98	LYS
1	1	99	GLU
1	1	100	THR
1	1	109	ILE
1	1	111	ASP
1	1	118	PHE
1	1	127	LYS
1	1	146	LYS
1	1	159	VAL
1	1	165	ARG
1	1	179	LEU
1	1	188	LYS
1	1	189	ASN
1	1	191	PHE
1	1	195	ASP
1	1	197	SER
1	1	212	HIS
1	1	246	VAL
1	1	259	GLU
1	1	276	ILE
1	1	286	ARG
1	1	310	VAL
1	1	311	HIS
1	1	313	GLU
1	1	355	LYS
1	1	356	LYS
1	1	370	LEU
1	e	5	SER
1	e	7	ASP
1	e	9	LYS
1	e	10	ARG
1	e	14	LYS
1	e	18	HIS
1	e	38	LEU

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Mol	Chain	Res	Type
1	e	44	LEU
1	e	49	ARG
1	e	51	PHE
1	e	55	LEU
1	e	57	SER
1	e	67	ARG
1	e	68	LEU
1	e	82	LEU
1	e	92	ILE
1	e	103	GLU
1	e	111	ASP
1	e	124	ILE
1	e	150	LYS
1	e	153	LYS
1	e	159	VAL
1	e	179	LEU
1	e	188	LYS
1	e	189	ASN
1	e	191	PHE
1	e	210	ASN
1	e	219	LYS
1	e	222	LYS
1	e	225	VAL
1	e	249	PRO
1	e	251	SER
1	e	255	LYS
1	e	259	GLU
1	e	271	LYS
1	e	276	ILE
1	e	291	LYS
1	e	298	PHE
1	e	299	ILE
1	e	301	ARG
1	e	310	VAL
1	e	311	HIS
1	e	313	GLU
1	e	323	ILE
1	e	353	VAL
1	e	362	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	210	ASN
1	N	13	HIS
1	N	16	GLN
1	N	189	ASN
1	N	210	ASN
1	N	311	HIS
1	1	181	ASN
1	1	189	ASN
1	1	207	ASN
1	1	210	ASN
1	1	212	HIS
1	1	217	HIS
1	1	304	HIS
1	1	311	HIS
1	e	181	ASN
1	e	207	ASN
1	e	217	HIS

### 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](#)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	PO4	1	402	2	4,4,4	0.62	0	6,6,6	0.25	0
3	PO4	1	403	-	4,4,4	0.69	0	6,6,6	0.24	0
3	PO4	1	405	-	4,4,4	0.51	0	6,6,6	0.23	0

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	PO4	1	402	2	-	0/0/0/0	0/0/0/0
3	PO4	1	403	-	-	0/0/0/0	0/0/0/0
3	PO4	1	405	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1	402	PO4	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	1	367/367 (100%)	-0.01	16 (4%) 38 30	28, 54, 128, 163	0
1	A	367/367 (100%)	0.22	36 (9%) 10 6	24, 50, 181, 211	0
1	N	367/367 (100%)	0.34	33 (8%) 12 8	27, 61, 180, 242	0
1	e	367/367 (100%)	-0.16	7 (1%) 70 64	31, 54, 82, 136	0
All	All	1468/1468 (100%)	0.10	92 (6%) 23 17	24, 55, 159, 242	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	95	THR	8.9
1	1	5	SER	7.3
1	N	4	GLY	7.3
1	1	4	GLY	6.9
1	A	127	LYS	6.7
1	e	4	GLY	6.4
1	e	5	SER	6.3
1	A	83	TRP	5.5
1	N	63	ALA	5.5
1	N	94	ALA	5.1
1	A	192	GLY	5.1
1	A	82	LEU	5.0
1	A	63	ALA	4.6
1	A	191	PHE	4.5
1	e	123	ASP	4.5
1	A	90	TYR	4.4
1	N	191	PHE	4.4
1	A	84	SER	4.2
1	1	125	PHE	4.2
1	A	49	ARG	4.1
1	A	95	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	e	191	PHE	4.0
1	1	90	TYR	4.0
1	A	102	LYS	3.9
1	A	48	GLU	3.7
1	N	106	LYS	3.7
1	1	86	SER	3.7
1	1	123	ASP	3.5
1	A	124	ILE	3.5
1	N	103	GLU	3.4
1	A	75	GLU	3.4
1	A	50	LEU	3.3
1	A	67	ARG	3.2
1	N	82	LEU	3.2
1	N	24	PHE	3.1
1	A	66	PRO	3.0
1	N	91	LYS	3.0
1	N	125	PHE	2.9
1	N	70	GLU	2.9
1	A	105	GLU	2.9
1	1	89	PRO	2.9
1	N	227	ILE	2.9
1	N	56	PRO	2.9
1	A	93	PHE	2.8
1	N	97	ILE	2.8
1	N	79	GLU	2.8
1	N	104	GLY	2.7
1	e	299	ILE	2.7
1	A	78	GLY	2.6
1	A	61	LEU	2.6
1	A	92	ILE	2.6
1	N	65	ALA	2.6
1	1	10	ARG	2.6
1	A	72	GLU	2.6
1	A	80	VAL	2.6
1	N	77	ASN	2.6
1	N	17	ALA	2.5
1	1	7	ASP	2.5
1	N	81	VAL	2.5
1	A	85	ASP	2.5
1	1	318	PRO	2.5
1	1	50	LEU	2.5
1	N	5	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	75	GLU	2.5
1	A	74	GLU	2.5
1	A	86	SER	2.5
1	N	8	TYR	2.4
1	N	120	LYS	2.4
1	1	120	LYS	2.4
1	N	129	SER	2.4
1	1	43	PRO	2.4
1	A	71	LYS	2.3
1	A	97	ILE	2.3
1	A	91	LYS	2.3
1	N	62	THR	2.3
1	N	76	PHE	2.2
1	A	55	LEU	2.2
1	N	228	PHE	2.2
1	1	87	GLU	2.2
1	1	91	LYS	2.2
1	A	73	LEU	2.2
1	N	83	TRP	2.2
1	N	105	GLU	2.2
1	e	318	PRO	2.2
1	1	361	THR	2.1
1	A	68	LEU	2.1
1	A	125	PHE	2.1
1	N	242	THR	2.1
1	A	13	HIS	2.0
1	A	101	PHE	2.0
1	N	109	ILE	2.0
1	e	212	HIS	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	e	402	1/1	0.97	0.28	3.69	121,121,121,121	0
2	ZN	N	401	1/1	0.96	0.23	1.80	77,77,77,77	0
2	ZN	1	404	1/1	0.94	0.20	1.02	131,131,131,131	0
3	PO4	1	403	5/5	0.94	0.20	0.18	111,112,114,116	0
3	PO4	1	402	5/5	0.98	0.15	0.00	49,49,52,54	0
3	PO4	1	405	5/5	0.95	0.12	-0.60	74,78,79,81	0
2	ZN	1	401	1/1	0.98	0.16	-0.61	58,58,58,58	0
2	ZN	A	401	1/1	0.98	0.12	-1.08	50,50,50,50	0
2	ZN	e	401	1/1	0.98	0.17	-1.09	70,70,70,70	0
2	ZN	N	402	1/1	0.96	0.09	-1.96	91,91,91,91	0
2	ZN	A	402	1/1	0.95	0.27	-	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.