



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:46 PM GMT

PDB ID : 4ADS  
Title : Crystal structure of plasmodial PLP synthase complex  
Authors : Guedez, G.; Sinning, I.; Tews, I.  
Deposited on : 2012-01-03  
Resolution : 3.61 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

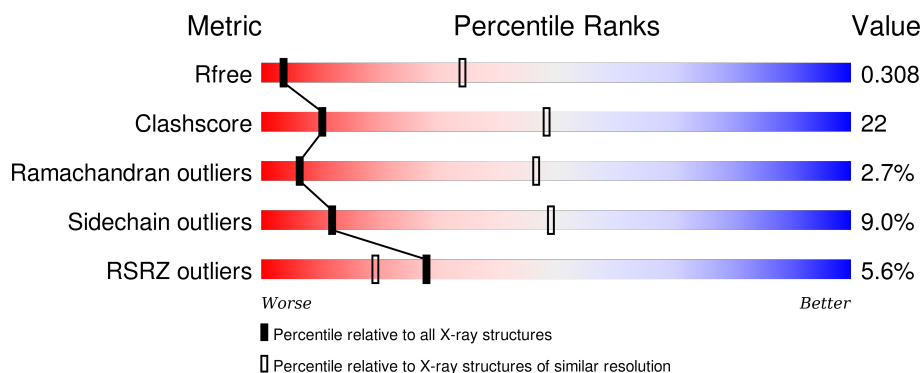
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.61 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	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)

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	282	<div> <div>2%</div> <div>81% 17% ..</div> </div>
1	B	282	<div> <div>2%</div> <div>81% 16% ..</div> </div>
1	C	282	<div> <div>2%</div> <div>84% 13% ..</div> </div>
1	D	282	<div> <div>2%</div> <div>83% 15% ..</div> </div>
1	E	282	<div> <div>%</div> <div>80% 17% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	282	<div><div></div><div>2%</div><div>82%</div><div>16%</div><div></div></div>
2	G	217	<div><div></div><div>7%</div><div>63%</div><div>24%</div><div>13%</div><div></div></div>
2	H	217	<div><div></div><div>6%</div><div>64%</div><div>24%</div><div>11%</div><div></div></div>
2	I	217	<div><div></div><div>16%</div><div>61%</div><div>26%</div><div>12%</div><div></div></div>
2	J	217	<div><div></div><div>%</div><div>61%</div><div>28%</div><div>10%</div><div></div></div>
2	K	217	<div><div></div><div>8%</div><div>63%</div><div>26%</div><div>10%</div><div></div></div>
2	L	217	<div><div></div><div>23%</div><div>59%</div><div>27%</div><div>13%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23152 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 PYRIDOXINE BIOSYNTHETIC ENZYME PDX1 HOMOLOGUE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2148	1353	373	404	18			
1	B	282	Total	C	N	O	S	0	0	0
			2148	1353	373	404	18			
1	C	282	Total	C	N	O	S	0	0	0
			2148	1353	373	404	18			
1	D	282	Total	C	N	O	S	0	0	0
			2148	1353	373	404	18			
1	E	282	Total	C	N	O	S	0	0	0
			2148	1353	373	404	18			
1	F	282	Total	C	N	O	S	0	0	0
			2148	1353	373	404	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
A	284	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
B	283	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
B	284	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
C	283	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
C	284	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
D	283	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
D	284	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
E	283	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
E	284	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
F	283	ALA	-	EXPRESSION TAG	UNP Q4Z0E8
F	284	ALA	-	EXPRESSION TAG	UNP Q4Z0E8

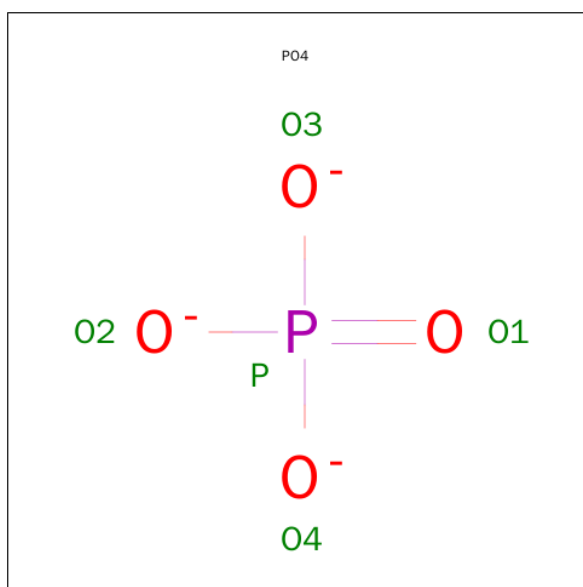
- Molecule 2 is a protein called PDX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	217	Total	C	N	O	S	0	0	0
			1700	1092	285	314	9			
2	H	217	Total	C	N	O	S	0	0	0
			1700	1092	285	314	9			
2	I	217	Total	C	N	O	S	0	0	0
			1700	1092	285	314	9			
2	J	217	Total	C	N	O	S	0	0	0
			1700	1092	285	314	9			
2	K	217	Total	C	N	O	S	0	0	0
			1700	1092	285	314	9			
2	L	217	Total	C	N	O	S	0	0	0
			1700	1092	285	314	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	196	ASN	HIS	ENGINEERED MUTATION	UNP Q5ND68
H	196	ASN	HIS	ENGINEERED MUTATION	UNP Q5ND68
I	196	ASN	HIS	ENGINEERED MUTATION	UNP Q5ND68
J	196	ASN	HIS	ENGINEERED MUTATION	UNP Q5ND68
K	196	ASN	HIS	ENGINEERED MUTATION	UNP Q5ND68
L	196	ASN	HIS	ENGINEERED MUTATION	UNP Q5ND68

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

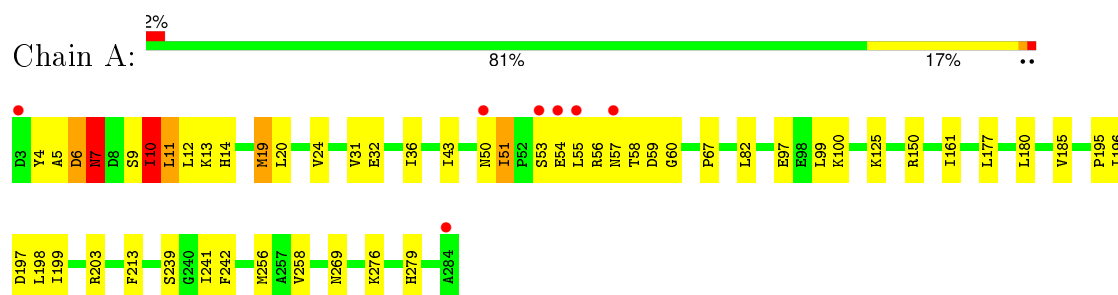
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O 1 1	0	0
4	H	3	Total O 3 3	0	0

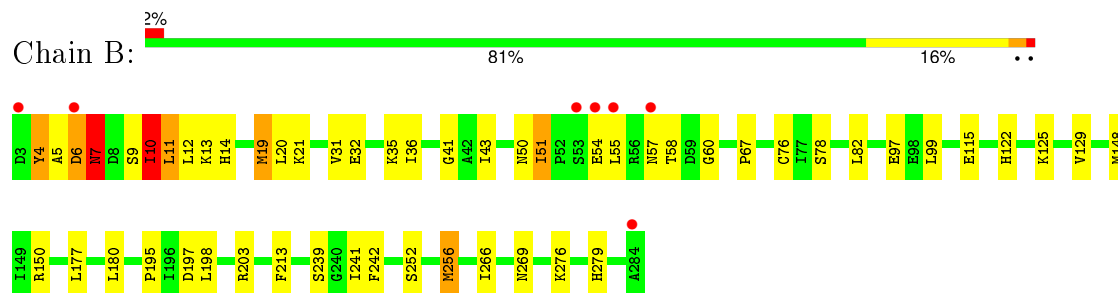
### 3 Residue-property plots [i](#)

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

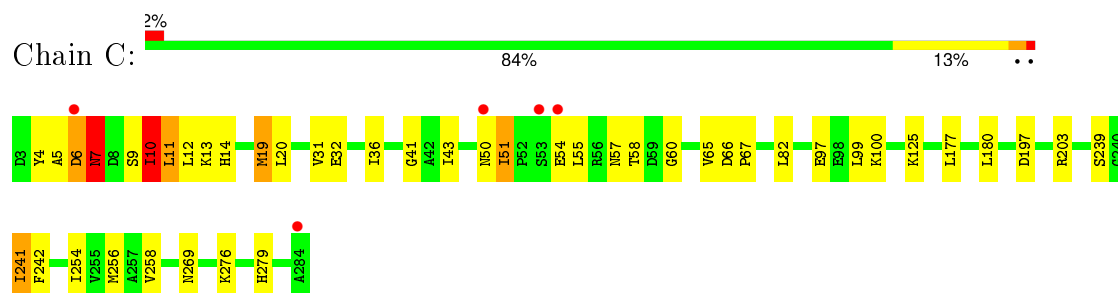
- Molecule 1: PYRIDOXINE BIOSYNTHETIC ENZYME PDX1 HOMOLOGUE, PUTATIVE



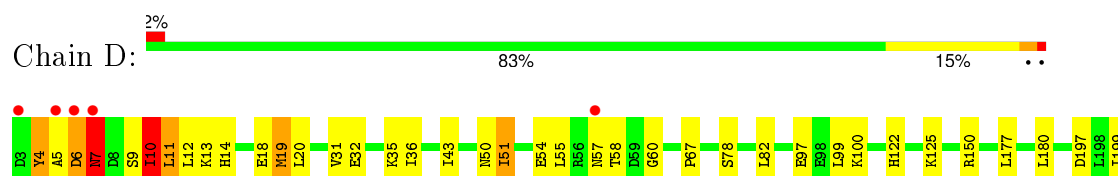
- Molecule 1: PYRIDOXINE BIOSYNTHETIC ENZYME PDX1 HOMOLOGUE, PUTATIVE



- Molecule 1: PYRIDOXINE BIOSYNTHETIC ENZYME PDX1 HOMOLOGUE, PUTATIVE

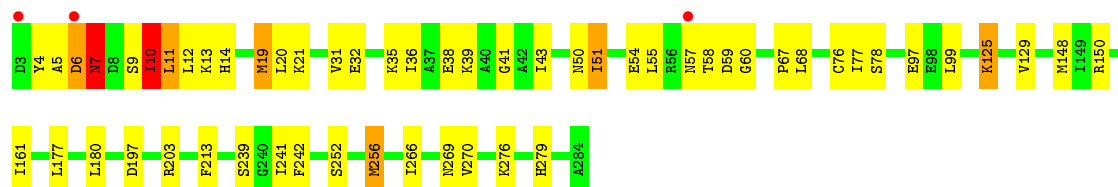
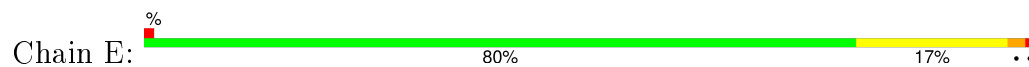


- Molecule 1: PYRIDOXINE BIOSYNTHETIC ENZYME PDX1 HOMOLOGUE, PUTATIVE

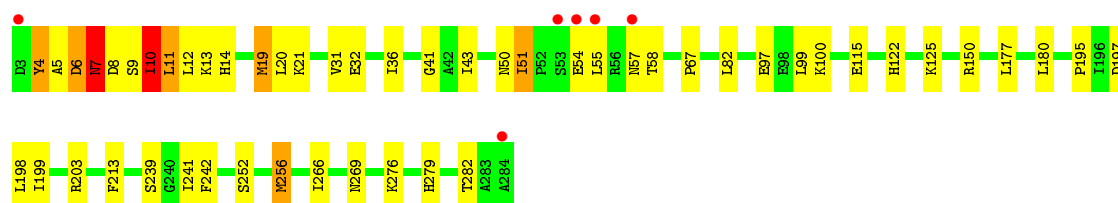
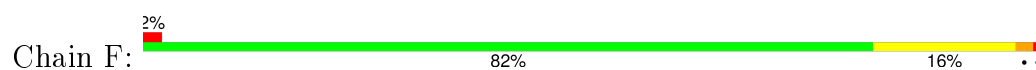




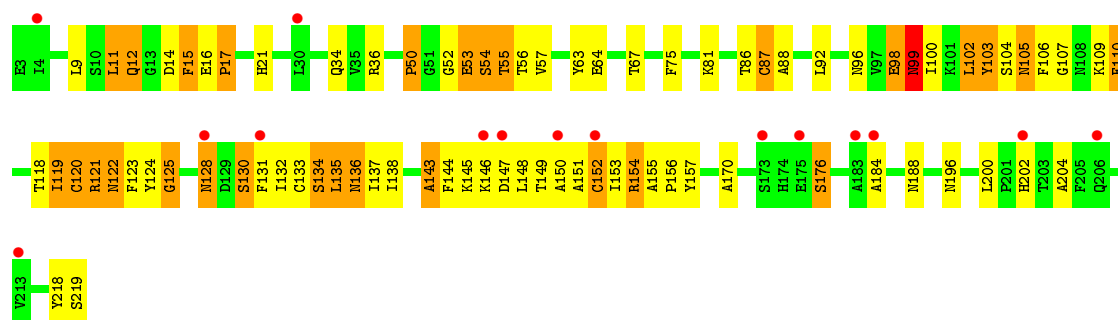
• Molecule 1: PYRIDOXINE BIOSYNTHETIC ENZYME PDX1 HOMOLOGUE, PUTATIVE



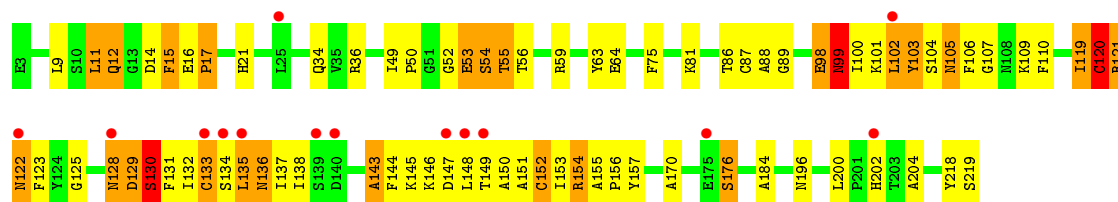
• Molecule 1: PYRIDOXINE BIOSYNTHETIC ENZYME PDX1 HOMOLOGUE, PUTATIVE



• Molecule 2: PDX2 PROTEIN



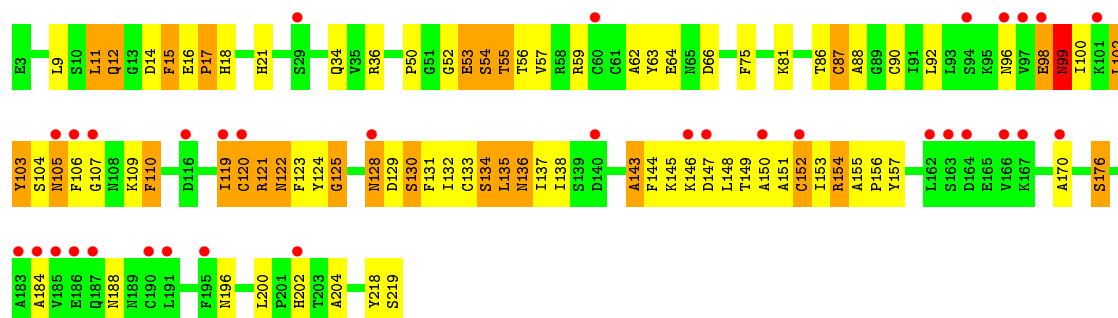
• Molecule 2: PDX2 PROTEIN



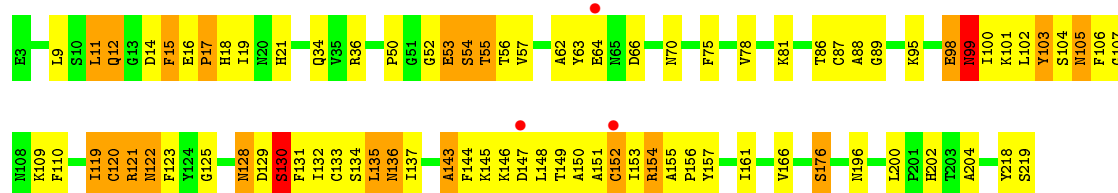
• Molecule 2: PDX2 PROTEIN



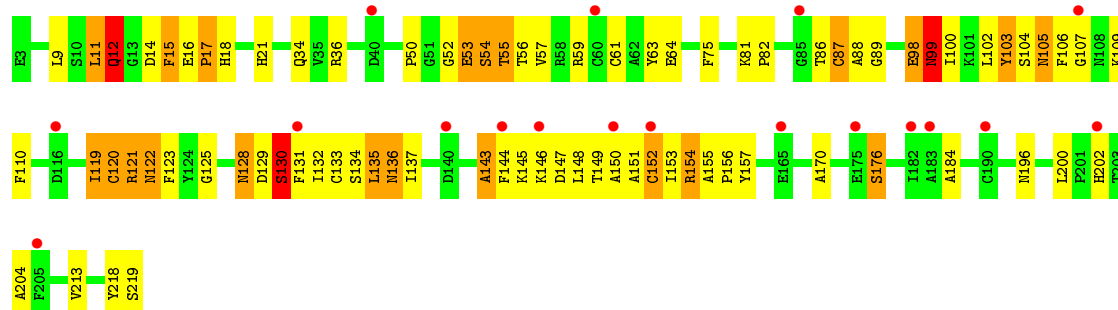




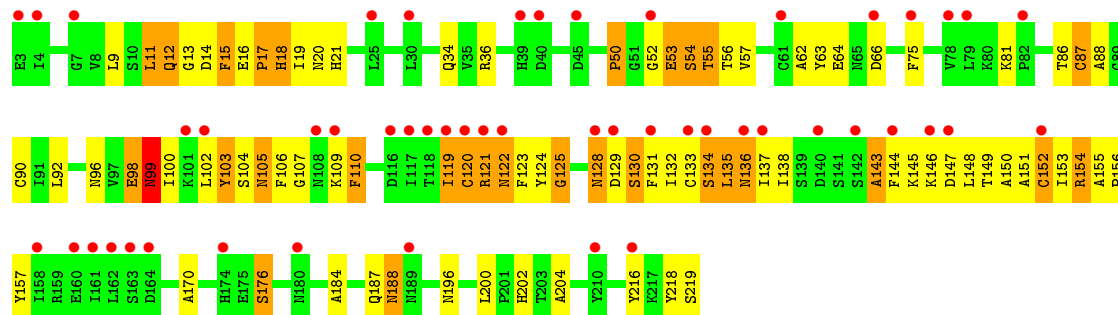
• Molecule 2: PDX2 PROTEIN



• Molecule 2: PDX2 PROTEIN



• Molecule 2: PDX2 PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.01Å 160.01Å 583.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.61 49.52 – 3.61	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-3.61) 96.8 (49.52-3.61)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.293 , 0.314 0.289 , 0.308	Depositor DCC
$R_{free}$ test set	2560 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 63.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 50227 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	23152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.52	0/2175	0.67	2/2928 (0.1%)
1	B	0.51	0/2175	0.67	3/2928 (0.1%)
1	C	0.54	0/2175	0.67	2/2928 (0.1%)
1	D	0.53	0/2175	0.66	2/2928 (0.1%)
1	E	0.55	0/2175	0.68	3/2928 (0.1%)
1	F	0.53	0/2175	0.67	3/2928 (0.1%)
2	G	0.47	0/1738	0.60	0/2358
2	H	0.59	1/1738 (0.1%)	0.66	0/2358
2	I	0.49	0/1738	0.60	0/2358
2	J	0.60	1/1738 (0.1%)	0.67	0/2358
2	K	0.53	1/1738 (0.1%)	0.64	0/2358
2	L	0.35	0/1738	0.54	0/2358
All	All	0.52	3/23478 (0.0%)	0.65	15/31716 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
2	G	0	2
2	H	0	2
2	I	0	2
2	J	0	2
2	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	2
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	120	CYS	CB-SG	-5.37	1.73	1.81
2	J	120	CYS	CB-SG	-5.22	1.73	1.81
2	K	61	CYS	CB-SG	-5.13	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	ASN	N-CA-C	-5.92	95.01	111.00
1	A	7	ASN	N-CA-C	-5.82	95.28	111.00
1	E	7	ASN	N-CA-C	-5.82	95.29	111.00
1	D	7	ASN	N-CA-C	-5.79	95.36	111.00
1	F	7	ASN	N-CA-C	-5.70	95.62	111.00
1	A	10	ILE	CB-CA-C	-5.69	100.22	111.60
1	B	7	ASN	N-CA-C	-5.65	95.74	111.00
1	D	10	ILE	CB-CA-C	-5.63	100.35	111.60
1	E	10	ILE	CB-CA-C	-5.62	100.35	111.60
1	C	10	ILE	CB-CA-C	-5.55	100.49	111.60
1	B	10	ILE	CB-CA-C	-5.50	100.61	111.60
1	F	256	MET	CG-SD-CE	-5.31	91.70	100.20
1	F	10	ILE	CB-CA-C	-5.31	100.99	111.60
1	E	256	MET	CG-SD-CE	-5.11	92.03	100.20
1	B	256	MET	CG-SD-CE	-5.09	92.06	100.20

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	ASP	Peptide
1	B	6	ASP	Peptide
1	C	6	ASP	Peptide
1	D	6	ASP	Peptide
1	E	6	ASP	Peptide
1	F	6	ASP	Peptide
2	G	98	GLU	Peptide
2	G	99	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	H	98	GLU	Peptide
2	H	99	ASN	Peptide
2	I	98	GLU	Peptide
2	I	99	ASN	Peptide
2	J	98	GLU	Peptide
2	J	99	ASN	Peptide
2	K	98	GLU	Peptide
2	K	99	ASN	Peptide
2	L	98	GLU	Peptide
2	L	99	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2148	0	2214	66	0
1	B	2148	0	2214	73	0
1	C	2148	0	2214	59	0
1	D	2148	0	2214	58	0
1	E	2148	0	2214	101	3
1	F	2148	0	2214	85	0
2	G	1700	0	1678	109	1
2	H	1700	0	1678	139	3
2	I	1700	0	1678	136	0
2	J	1700	0	1678	101	7
2	K	1700	0	1678	118	0
2	L	1700	0	1678	151	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	E	1	0	0	2	0
4	H	3	0	0	3	0
All	All	23152	0	23352	1006	7

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 (1006) 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:E:35:LYS:HE2	2:H:102:LEU:CD2	1.40	1.51
1:F:256:MET:HE3	2:K:63:TYR:CG	1.56	1.41
1:E:256:MET:CE	2:H:63:TYR:HB2	1.55	1.34
2:L:133:CYS:SG	2:L:150:ALA:HB3	1.69	1.32
1:F:256:MET:CE	2:K:63:TYR:CD1	2.11	1.31
1:E:256:MET:HE1	2:H:63:TYR:CG	1.73	1.24
2:I:133:CYS:SG	2:I:150:ALA:HB3	1.78	1.24
1:E:256:MET:CE	2:H:63:TYR:CB	2.17	1.23
2:L:98:GLU:HG2	2:L:120:CYS:SG	1.79	1.23
1:E:256:MET:CE	2:H:63:TYR:CG	2.21	1.22
2:L:123:PHE:CE2	2:L:157:TYR:HB2	1.74	1.22
2:G:133:CYS:SG	2:G:150:ALA:HB3	1.79	1.21
1:F:256:MET:CE	2:K:63:TYR:CG	2.29	1.15
1:C:100:LYS:HD2	2:J:128:ASN:HD21	1.10	1.13
1:B:256:MET:CE	2:I:63:TYR:CD1	2.33	1.12
1:E:256:MET:CE	2:H:63:TYR:CD1	2.33	1.12
1:F:100:LYS:HD2	2:K:128:ASN:HD21	1.05	1.11
2:G:98:GLU:HG2	2:G:120:CYS:SG	1.90	1.10
1:E:256:MET:HE2	2:H:63:TYR:CB	1.78	1.10
2:I:98:GLU:HG2	2:I:120:CYS:SG	1.92	1.09
1:F:266:ILE:HG12	2:K:63:TYR:HE2	1.18	1.09
1:E:35:LYS:CE	2:H:102:LEU:CD2	2.31	1.08
2:L:123:PHE:CD2	2:L:157:TYR:HB2	1.88	1.08
1:E:256:MET:HE1	2:H:63:TYR:CB	1.81	1.08
2:G:123:PHE:CE1	2:G:157:TYR:HB2	1.87	1.08
1:E:35:LYS:HE2	2:H:102:LEU:HD21	1.32	1.07
1:E:35:LYS:HE2	2:H:102:LEU:HD22	1.12	1.07
2:I:123:PHE:CE1	2:I:157:TYR:HB2	1.88	1.07
1:A:100:LYS:HD2	2:L:128:ASN:ND2	1.70	1.07
2:J:123:PHE:CE1	2:J:157:TYR:HB2	1.88	1.06
2:L:34:GLN:OE1	2:L:36:ARG:NH1	1.87	1.05
2:K:123:PHE:CE1	2:K:157:TYR:HB2	1.90	1.05
1:B:256:MET:CE	2:I:63:TYR:HB2	1.87	1.03
1:B:256:MET:HE3	2:I:63:TYR:CG	1.92	1.03
1:E:256:MET:HE1	2:H:63:TYR:HB2	1.38	1.03
2:H:123:PHE:CE1	2:H:157:TYR:HB2	1.93	1.02
1:F:256:MET:CE	2:K:63:TYR:HB2	1.89	1.02
1:A:100:LYS:CD	2:L:128:ASN:HD21	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ALA:HB2	1:A:13:LYS:NZ	1.74	1.02
1:F:256:MET:HE3	2:K:63:TYR:CB	1.90	1.01
1:E:269:ASN:HB3	2:H:63:TYR:OH	1.59	1.01
1:E:35:LYS:CE	2:H:102:LEU:HD22	1.92	1.00
1:F:256:MET:CE	2:K:63:TYR:CB	2.38	1.00
1:F:256:MET:HE3	2:K:63:TYR:CD1	1.85	1.00
1:B:5:ALA:HB2	1:B:13:LYS:NZ	1.78	0.99
1:C:269:ASN:ND2	2:J:63:TYR:OH	1.94	0.99
1:E:5:ALA:HB2	1:E:13:LYS:NZ	1.77	0.99
1:F:266:ILE:HG12	2:K:63:TYR:CE2	1.96	0.98
2:G:123:PHE:CD1	2:G:157:TYR:HB2	1.97	0.98
2:H:149:THR:HB	4:H:2002:HOH:O	1.62	0.98
2:I:123:PHE:CD1	2:I:157:TYR:HB2	1.98	0.98
1:C:5:ALA:HB2	1:C:13:LYS:NZ	1.79	0.98
2:L:137:ILE:HG21	2:L:144:PHE:CD2	1.99	0.97
1:A:100:LYS:HD2	2:L:128:ASN:HD21	0.84	0.97
1:B:256:MET:HE1	2:I:63:TYR:CB	1.94	0.97
2:L:100:ILE:HG22	2:L:104:SER:N	1.80	0.97
1:D:279:HIS:CE1	1:E:58:THR:HG1	1.82	0.97
1:E:252:SER:HB3	2:H:59:ARG:HH21	1.27	0.97
2:I:34:GLN:OE1	2:I:36:ARG:NH1	1.96	0.96
2:K:133:CYS:SG	2:K:150:ALA:HB3	2.04	0.96
1:C:9:SER:O	1:C:12:LEU:HB3	1.66	0.96
1:F:9:SER:O	1:F:12:LEU:HB3	1.65	0.96
2:G:34:GLN:OE1	2:G:36:ARG:NH1	1.97	0.95
2:H:98:GLU:HG2	2:H:120:CYS:SG	2.06	0.95
2:J:133:CYS:SG	2:J:150:ALA:HB3	2.07	0.94
2:K:63:TYR:CE2	2:K:64:GLU:HG3	2.02	0.94
2:J:123:PHE:CD1	2:J:157:TYR:HB2	2.03	0.94
1:E:9:SER:O	1:E:12:LEU:HB3	1.67	0.94
1:B:256:MET:CE	2:I:63:TYR:CG	2.48	0.94
2:L:119:ILE:HD11	2:L:156:PRO:HB2	1.50	0.94
1:A:9:SER:O	1:A:12:LEU:HB3	1.67	0.94
1:F:9:SER:C	1:F:12:LEU:HB3	1.89	0.93
2:K:123:PHE:CD1	2:K:157:TYR:HB2	2.03	0.93
1:A:9:SER:C	1:A:12:LEU:HB3	1.89	0.93
1:E:256:MET:HE2	2:H:63:TYR:HB2	1.35	0.92
1:C:9:SER:C	1:C:12:LEU:HB3	1.89	0.92
1:B:266:ILE:HG12	2:I:63:TYR:CE2	2.04	0.92
2:I:137:ILE:HG21	2:I:144:PHE:CD2	2.05	0.92
2:L:9:LEU:HD11	2:L:11:LEU:HD11	1.47	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:SER:C	1:E:12:LEU:HB3	1.91	0.92
1:D:5:ALA:HB2	1:D:13:LYS:NZ	1.85	0.92
2:G:137:ILE:HG21	2:G:144:PHE:CD2	2.04	0.92
2:J:34:GLN:OE1	2:J:36:ARG:NH1	2.03	0.91
2:H:34:GLN:OE1	2:H:36:ARG:NH1	2.02	0.91
1:F:5:ALA:HB2	1:F:13:LYS:NZ	1.84	0.91
1:D:9:SER:O	1:D:12:LEU:HB3	1.70	0.91
1:A:269:ASN:ND2	2:L:63:TYR:OH	2.03	0.91
2:I:100:ILE:HG22	2:I:104:SER:N	1.86	0.91
2:H:123:PHE:CD1	2:H:157:TYR:HB2	2.05	0.91
1:B:256:MET:CE	2:I:63:TYR:CB	2.47	0.90
2:H:63:TYR:CE2	2:H:64:GLU:HG3	2.05	0.90
2:K:34:GLN:OE1	2:K:36:ARG:NH1	2.02	0.90
1:D:269:ASN:ND2	2:G:63:TYR:OH	2.03	0.90
2:H:100:ILE:HG22	2:H:104:SER:N	1.86	0.90
1:F:256:MET:HE2	2:K:63:TYR:CD1	2.04	0.90
1:D:279:HIS:NE2	1:E:58:THR:OG1	2.05	0.90
2:L:133:CYS:SG	2:L:150:ALA:CB	2.60	0.90
1:B:256:MET:HE1	2:I:63:TYR:HB2	1.49	0.90
1:B:9:SER:O	1:B:12:LEU:HB3	1.72	0.90
1:E:35:LYS:CE	2:H:102:LEU:HD21	1.98	0.90
2:J:63:TYR:CE2	2:J:64:GLU:HG3	2.06	0.90
2:G:9:LEU:HD11	2:G:11:LEU:HD11	1.53	0.89
1:A:256:MET:HE1	2:L:63:TYR:CG	2.07	0.89
1:B:9:SER:C	1:B:12:LEU:HB3	1.92	0.89
1:A:256:MET:CE	2:L:63:TYR:CD1	2.55	0.89
2:L:63:TYR:CE2	2:L:64:GLU:HG3	2.08	0.89
1:B:5:ALA:HB2	1:B:13:LYS:HZ1	1.35	0.88
1:A:256:MET:CE	2:L:63:TYR:CG	2.56	0.88
2:H:133:CYS:SG	2:H:150:ALA:HB3	2.13	0.88
1:C:100:LYS:CD	2:J:128:ASN:HD21	1.86	0.88
2:I:63:TYR:CE2	2:I:64:GLU:HG3	2.09	0.88
2:L:107:GLY:O	2:L:110:PHE:HB3	1.73	0.87
2:L:107:GLY:O	2:L:110:PHE:CB	2.23	0.87
1:C:5:ALA:HB2	1:C:13:LYS:HZ2	1.40	0.87
2:K:100:ILE:HG22	2:K:104:SER:N	1.89	0.87
2:G:100:ILE:HG22	2:G:104:SER:N	1.89	0.87
1:A:256:MET:HE2	2:L:63:TYR:CD1	2.10	0.87
1:F:100:LYS:HD2	2:K:128:ASN:ND2	1.89	0.86
2:J:100:ILE:HG22	2:J:104:SER:N	1.89	0.86
2:J:98:GLU:HG2	2:J:120:CYS:SG	2.14	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:135:LEU:HD21	2:I:150:ALA:HB2	1.57	0.86
1:A:5:ALA:HB2	1:A:13:LYS:HZ1	1.36	0.86
1:E:252:SER:CB	2:H:59:ARG:HH21	1.88	0.86
2:L:135:LEU:HD21	2:L:150:ALA:HB2	1.57	0.86
2:L:100:ILE:HG23	2:L:103:TYR:HB2	1.56	0.86
1:D:9:SER:C	1:D:12:LEU:HB3	1.94	0.86
2:H:100:ILE:HB	4:H:2001:HOH:O	1.73	0.86
1:E:78:SER:HB3	2:H:103:TYR:CE2	2.11	0.85
2:L:98:GLU:CG	2:L:120:CYS:SG	2.64	0.85
1:F:256:MET:CE	2:K:63:TYR:HD1	1.85	0.85
2:L:63:TYR:CD2	2:L:64:GLU:HG3	2.12	0.85
1:E:256:MET:HE3	2:H:63:TYR:CD1	2.08	0.85
2:K:98:GLU:HG2	2:K:120:CYS:SG	2.16	0.85
1:F:100:LYS:CD	2:K:128:ASN:HD21	1.90	0.85
2:K:137:ILE:HG21	2:K:144:PHE:CD2	2.12	0.85
2:H:135:LEU:HD21	2:H:150:ALA:HB2	1.57	0.84
2:K:135:LEU:HD21	2:K:150:ALA:HB2	1.57	0.84
1:F:256:MET:HE1	2:K:63:TYR:CD1	2.13	0.84
2:I:119:ILE:HD11	2:I:156:PRO:HB2	1.58	0.84
2:H:63:TYR:CD2	2:H:64:GLU:HG3	2.13	0.84
1:B:266:ILE:HG12	2:I:63:TYR:HE2	1.40	0.84
2:K:63:TYR:CD2	2:K:64:GLU:HG3	2.12	0.84
2:G:135:LEU:HD21	2:G:150:ALA:HB2	1.59	0.83
1:E:252:SER:HB3	2:H:59:ARG:NH2	1.92	0.83
1:C:256:MET:CE	2:J:63:TYR:HB2	2.09	0.83
1:B:78:SER:HB3	2:I:103:TYR:CE2	2.15	0.82
2:H:137:ILE:HG21	2:H:144:PHE:CD2	2.14	0.82
1:B:256:MET:HE3	2:I:63:TYR:CD1	2.08	0.82
1:E:269:ASN:ND2	2:H:63:TYR:OH	2.12	0.81
2:I:63:TYR:CD2	2:I:64:GLU:HG3	2.15	0.81
2:L:123:PHE:HE2	2:L:157:TYR:HB2	1.42	0.81
2:L:103:TYR:N	2:L:103:TYR:CD1	2.46	0.81
2:J:137:ILE:HG21	2:J:144:PHE:CD2	2.16	0.81
2:G:119:ILE:HD11	2:G:156:PRO:HB2	1.61	0.81
1:E:180:LEU:O	1:E:203:ARG:NH2	2.11	0.80
2:L:100:ILE:CG2	2:L:104:SER:N	2.43	0.80
1:C:256:MET:HE1	2:J:63:TYR:CG	2.16	0.80
2:K:9:LEU:HD11	2:K:11:LEU:HD11	1.63	0.80
1:C:100:LYS:HD2	2:J:128:ASN:ND2	1.93	0.80
1:F:19:MET:HG3	2:K:52:GLY:HA2	1.64	0.80
1:F:269:ASN:HB3	2:K:63:TYR:OH	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ALA:HB2	1:E:13:LYS:HZ1	1.45	0.79
2:J:135:LEU:HD21	2:J:150:ALA:HB2	1.63	0.79
1:D:279:HIS:CE1	1:E:58:THR:OG1	2.36	0.78
1:B:269:ASN:HB3	2:I:63:TYR:OH	1.82	0.78
1:C:256:MET:CE	2:J:63:TYR:CD1	2.67	0.78
2:I:9:LEU:HD11	2:I:11:LEU:HD11	1.66	0.78
1:F:256:MET:HE1	2:K:63:TYR:CB	2.13	0.78
2:I:107:GLY:O	2:I:110:PHE:HB3	1.83	0.78
2:L:98:GLU:HG2	2:L:120:CYS:HG	1.47	0.78
1:A:256:MET:CE	2:L:63:TYR:HB2	2.13	0.78
2:L:98:GLU:HA	2:L:99:ASN:ND2	1.99	0.77
2:J:63:TYR:CD2	2:J:64:GLU:HG3	2.18	0.77
1:E:256:MET:HE2	2:H:63:TYR:CD1	2.19	0.77
2:I:133:CYS:SG	2:I:150:ALA:CB	2.69	0.77
2:K:119:ILE:HD11	2:K:156:PRO:HB2	1.66	0.77
1:B:252:SER:HB3	2:I:59:ARG:HH21	1.48	0.77
2:I:100:ILE:HG23	2:I:103:TYR:HB2	1.65	0.76
2:G:133:CYS:HG	2:G:150:ALA:HB3	1.46	0.76
2:G:63:TYR:CE2	2:G:64:GLU:HG3	2.20	0.76
2:I:107:GLY:O	2:I:110:PHE:CB	2.33	0.76
2:L:150:ALA:N	2:L:200:LEU:HD11	2.01	0.76
2:G:100:ILE:HG23	2:G:103:TYR:HB2	1.68	0.76
2:G:107:GLY:O	2:G:110:PHE:HB3	1.84	0.76
1:C:256:MET:CE	2:J:63:TYR:CG	2.68	0.76
2:G:107:GLY:O	2:G:110:PHE:CB	2.34	0.76
2:L:54:SER:C	2:L:56:THR:H	1.85	0.76
2:G:98:GLU:HG2	2:G:120:CYS:HG	1.48	0.76
2:J:107:GLY:O	2:J:110:PHE:CB	2.34	0.75
2:I:133:CYS:HG	2:I:150:ALA:HB3	1.50	0.75
1:F:180:LEU:O	1:F:203:ARG:NH2	2.16	0.75
1:A:58:THR:HG1	1:F:279:HIS:CE1	2.03	0.75
2:H:100:ILE:HG23	2:H:103:TYR:HB2	1.67	0.75
1:B:279:HIS:CE1	1:C:58:THR:OG1	2.40	0.75
1:A:5:ALA:HB2	1:A:13:LYS:HZ2	1.50	0.74
2:L:143:ALA:O	2:L:145:LYS:HG3	1.87	0.74
2:I:103:TYR:CD1	2:I:103:TYR:N	2.55	0.74
2:I:100:ILE:CG2	2:I:104:SER:N	2.50	0.74
2:J:100:ILE:HG23	2:J:103:TYR:HB2	1.69	0.74
1:E:5:ALA:HB2	1:E:13:LYS:HZ2	1.49	0.74
1:C:180:LEU:O	1:C:203:ARG:NH2	2.16	0.74
1:E:269:ASN:CB	2:H:63:TYR:OH	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:107:GLY:O	2:J:110:PHE:HB3	1.87	0.74
2:G:63:TYR:CD2	2:G:64:GLU:HG3	2.23	0.74
1:A:58:THR:OG1	1:F:279:HIS:NE2	2.20	0.74
2:G:103:TYR:N	2:G:103:TYR:CD1	2.55	0.73
2:J:119:ILE:HD11	2:J:156:PRO:HB2	1.69	0.73
2:K:107:GLY:O	2:K:110:PHE:CB	2.36	0.73
2:L:123:PHE:CD2	2:L:157:TYR:CB	2.69	0.73
2:H:98:GLU:HB3	2:H:120:CYS:HA	1.69	0.73
1:E:10:ILE:HG22	1:E:11:LEU:N	2.03	0.73
2:J:143:ALA:O	2:J:145:LYS:HG3	1.89	0.73
1:B:180:LEU:O	1:B:203:ARG:NH2	2.16	0.73
2:I:143:ALA:O	2:I:145:LYS:HG3	1.89	0.73
2:H:107:GLY:O	2:H:110:PHE:CB	2.37	0.73
1:E:76:CYS:HB3	2:H:102:LEU:HD13	1.71	0.73
2:K:100:ILE:HG23	2:K:103:TYR:HB2	1.70	0.73
2:G:143:ALA:O	2:G:145:LYS:HG3	1.89	0.72
1:F:5:ALA:HB2	1:F:13:LYS:HZ1	1.52	0.72
1:A:279:HIS:CE1	1:B:58:THR:OG1	2.43	0.72
1:D:5:ALA:HB2	1:D:13:LYS:HZ2	1.55	0.72
2:L:54:SER:C	2:L:56:THR:N	2.43	0.72
2:H:143:ALA:O	2:H:145:LYS:HG3	1.90	0.72
2:L:123:PHE:CE2	2:L:157:TYR:CB	2.66	0.72
1:D:5:ALA:HB2	1:D:13:LYS:HZ1	1.54	0.72
2:I:98:GLU:HA	2:I:99:ASN:ND2	2.05	0.72
1:A:10:ILE:HG22	1:A:11:LEU:N	2.04	0.71
2:L:98:GLU:HB3	2:L:120:CYS:HA	1.70	0.71
2:G:100:ILE:CG2	2:G:104:SER:N	2.53	0.71
1:C:10:ILE:HG22	1:C:11:LEU:N	2.06	0.71
2:L:130:SER:HB3	2:L:153:ILE:HA	1.73	0.71
2:I:98:GLU:HB3	2:I:120:CYS:HA	1.71	0.71
1:F:5:ALA:HB2	1:F:13:LYS:HZ2	1.55	0.71
1:A:180:LEU:O	1:A:203:ARG:NH2	2.16	0.71
2:G:98:GLU:HB3	2:G:120:CYS:HA	1.72	0.71
1:F:256:MET:HE3	2:K:63:TYR:HB2	1.59	0.71
2:L:131:PHE:HD1	2:L:132:ILE:N	1.89	0.71
2:L:153:ILE:O	2:L:154:ARG:HG3	1.89	0.71
1:B:10:ILE:HG22	1:B:11:LEU:N	2.04	0.71
2:G:54:SER:C	2:G:56:THR:H	1.94	0.71
1:C:5:ALA:CB	1:C:13:LYS:HZ2	2.03	0.70
2:L:132:ILE:HG22	2:L:133:CYS:N	2.06	0.70
2:H:119:ILE:HD11	2:H:156:PRO:HB2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:LEU:HD12	2:K:153:ILE:HD11	1.73	0.70
1:C:51:ILE:HG22	1:C:55:LEU:HD23	1.73	0.70
2:L:107:GLY:HA2	2:L:110:PHE:HB2	1.73	0.70
2:K:143:ALA:O	2:K:145:LYS:HG3	1.91	0.70
1:B:21:LYS:O	2:I:12:GLN:HG2	1.92	0.70
2:K:107:GLY:O	2:K:110:PHE:HB3	1.90	0.70
2:L:149:THR:OG1	2:L:200:LEU:HD13	1.91	0.70
2:L:105:ASN:O	2:L:106:PHE:CD1	2.45	0.70
1:B:256:MET:HE1	2:I:63:TYR:CD1	2.27	0.70
2:I:150:ALA:N	2:I:200:LEU:HD11	2.07	0.70
2:H:130:SER:HB3	2:H:153:ILE:HA	1.74	0.70
1:F:9:SER:CA	1:F:12:LEU:HB3	2.22	0.69
2:J:150:ALA:N	2:J:200:LEU:HD11	2.07	0.69
2:L:131:PHE:CE1	2:L:152:CYS:HB2	2.27	0.69
2:H:107:GLY:O	2:H:110:PHE:HB3	1.90	0.69
1:F:51:ILE:HG22	1:F:55:LEU:HD23	1.74	0.69
2:I:130:SER:HB3	2:I:153:ILE:HA	1.74	0.69
2:H:100:ILE:CG2	2:H:104:SER:N	2.55	0.69
2:H:50:PRO:HA	2:H:86:THR:HG22	1.74	0.69
2:L:105:ASN:O	2:L:106:PHE:CG	2.45	0.69
2:G:150:ALA:N	2:G:200:LEU:HD11	2.07	0.69
2:J:50:PRO:HA	2:J:86:THR:HG22	1.75	0.69
2:L:149:THR:C	2:L:200:LEU:CD1	2.60	0.69
1:B:256:MET:HE2	2:I:63:TYR:CD1	2.26	0.69
1:F:10:ILE:HG22	1:F:11:LEU:N	2.08	0.69
1:D:10:ILE:HG22	1:D:11:LEU:N	2.06	0.69
2:G:98:GLU:CG	2:G:120:CYS:SG	2.76	0.69
1:E:9:SER:CA	1:E:12:LEU:HB3	2.23	0.69
2:L:11:LEU:O	2:L:12:GLN:HB2	1.92	0.69
1:C:279:HIS:CE1	1:D:58:THR:OG1	2.45	0.69
1:E:51:ILE:HG22	1:E:55:LEU:HD23	1.74	0.69
2:K:98:GLU:HB3	2:K:120:CYS:HA	1.73	0.69
2:I:54:SER:C	2:I:56:THR:H	1.95	0.68
2:G:133:CYS:SG	2:G:150:ALA:CB	2.70	0.68
1:A:9:SER:CA	1:A:12:LEU:HB3	2.23	0.68
2:K:103:TYR:CD1	2:K:103:TYR:N	2.60	0.68
2:L:53:GLU:O	2:L:57:VAL:HG23	1.92	0.68
2:K:50:PRO:HA	2:K:86:THR:HG22	1.74	0.68
1:C:5:ALA:HB2	1:C:13:LYS:HZ1	1.57	0.68
1:C:9:SER:CA	1:C:12:LEU:HB3	2.23	0.68
2:G:131:PHE:CE1	2:G:152:CYS:HB2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:GLU:HA	2:G:99:ASN:ND2	2.09	0.68
2:J:100:ILE:CG2	2:J:104:SER:N	2.57	0.68
2:K:98:GLU:HA	2:K:99:ASN:ND2	2.09	0.68
1:B:51:ILE:HG22	1:B:55:LEU:HD23	1.76	0.68
1:D:180:LEU:O	1:D:203:ARG:NH2	2.16	0.68
2:L:119:ILE:HG13	2:L:120:CYS:N	2.08	0.68
1:B:256:MET:CE	2:I:63:TYR:HD1	2.06	0.67
2:H:103:TYR:N	2:H:103:TYR:CD1	2.60	0.67
2:I:123:PHE:HE1	2:I:157:TYR:HB2	1.59	0.67
2:L:131:PHE:CD1	2:L:132:ILE:N	2.63	0.67
1:B:9:SER:CA	1:B:12:LEU:HB3	2.24	0.67
2:J:98:GLU:HB3	2:J:120:CYS:HA	1.75	0.67
1:B:35:LYS:HE2	2:I:102:LEU:CD2	2.24	0.67
1:E:78:SER:OG	2:H:121:ARG:NH1	2.28	0.67
1:E:51:ILE:CG2	1:E:55:LEU:HD23	2.24	0.67
2:L:150:ALA:CA	2:L:200:LEU:HD11	2.25	0.67
2:K:150:ALA:N	2:K:200:LEU:HD11	2.09	0.67
1:B:256:MET:HE3	2:I:63:TYR:HB2	1.78	0.66
1:D:9:SER:CA	1:D:12:LEU:HB3	2.25	0.66
1:F:21:LYS:O	2:K:12:GLN:HG2	1.95	0.66
1:C:256:MET:HE2	2:J:63:TYR:HB2	1.76	0.66
2:I:149:THR:OG1	2:I:200:LEU:HD13	1.96	0.66
2:L:9:LEU:HD11	2:L:11:LEU:CD1	2.24	0.66
2:G:54:SER:C	2:G:56:THR:N	2.49	0.66
1:E:35:LYS:HE2	2:H:102:LEU:CG	2.21	0.66
2:K:123:PHE:HE1	2:K:157:TYR:HB2	1.58	0.66
2:J:103:TYR:CD1	2:J:103:TYR:N	2.61	0.66
2:G:149:THR:OG1	2:G:200:LEU:HD13	1.96	0.66
2:G:123:PHE:HE1	2:G:157:TYR:HB2	1.57	0.66
2:J:131:PHE:CE1	2:J:152:CYS:HB2	2.31	0.66
2:G:107:GLY:HA2	2:G:110:PHE:HB2	1.77	0.66
2:K:100:ILE:CG2	2:K:104:SER:N	2.58	0.65
2:G:130:SER:HB3	2:G:153:ILE:HA	1.77	0.65
2:J:54:SER:C	2:J:56:THR:H	1.97	0.65
2:J:98:GLU:HA	2:J:99:ASN:ND2	2.11	0.65
2:J:149:THR:OG1	2:J:200:LEU:HD13	1.97	0.65
1:A:51:ILE:HG22	1:A:55:LEU:HD23	1.78	0.65
1:D:43:ILE:HA	2:G:53:GLU:HG2	1.77	0.65
1:F:252:SER:HB3	2:K:59:ARG:HH21	1.61	0.65
2:I:131:PHE:CE1	2:I:152:CYS:HB2	2.31	0.65
2:I:98:GLU:CG	2:I:120:CYS:SG	2.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ILE:HG22	2:I:133:CYS:N	2.12	0.64
2:J:123:PHE:HE1	2:J:157:TYR:HB2	1.55	0.64
2:K:153:ILE:O	2:K:154:ARG:HG3	1.97	0.64
2:J:153:ILE:O	2:J:154:ARG:HG3	1.96	0.64
1:C:256:MET:CE	2:J:63:TYR:CB	2.75	0.64
2:G:153:ILE:O	2:G:154:ARG:HG3	1.96	0.64
1:A:5:ALA:CB	1:A:13:LYS:NZ	2.58	0.64
2:I:53:GLU:O	2:I:57:VAL:HG23	1.95	0.64
2:L:100:ILE:CG2	2:L:103:TYR:C	2.66	0.64
2:L:14:ASP:OD1	2:L:14:ASP:O	2.14	0.64
1:B:256:MET:HE3	2:I:63:TYR:CB	2.22	0.64
2:I:11:LEU:O	2:I:12:GLN:HB2	1.96	0.64
2:H:131:PHE:CE1	2:H:152:CYS:HB2	2.32	0.64
2:K:131:PHE:CE1	2:K:152:CYS:HB2	2.32	0.64
1:A:256:MET:CE	2:L:63:TYR:CB	2.75	0.64
1:D:35:LYS:HE2	2:G:102:LEU:HD13	1.79	0.64
2:J:9:LEU:HD11	2:J:11:LEU:HD11	1.79	0.64
2:H:150:ALA:N	2:H:200:LEU:HD11	2.12	0.64
2:I:107:GLY:HA2	2:I:110:PHE:HB2	1.78	0.64
1:A:58:THR:OG1	1:F:279:HIS:CE1	2.51	0.64
1:C:51:ILE:CG2	1:C:55:LEU:HD23	2.27	0.64
2:G:53:GLU:O	2:G:57:VAL:HG23	1.98	0.64
2:K:130:SER:HB3	2:K:153:ILE:HA	1.79	0.64
2:I:153:ILE:O	2:I:154:ARG:HG3	1.98	0.63
1:B:35:LYS:HE2	2:I:102:LEU:HD22	1.79	0.63
2:G:132:ILE:HG22	2:G:133:CYS:N	2.14	0.63
2:G:11:LEU:O	2:G:12:GLN:HB2	1.98	0.63
2:J:11:LEU:O	2:J:12:GLN:HB2	1.98	0.63
2:H:9:LEU:HD11	2:H:11:LEU:HD11	1.79	0.63
1:D:51:ILE:HG22	1:D:55:LEU:HD23	1.80	0.63
1:B:5:ALA:HB2	1:B:13:LYS:HZ2	1.59	0.63
1:C:256:MET:HE2	2:J:63:TYR:CD1	2.32	0.63
2:H:98:GLU:HA	2:H:99:ASN:ND2	2.13	0.63
1:B:279:HIS:NE2	1:C:58:THR:OG1	2.31	0.63
2:H:54:SER:C	2:H:56:THR:H	2.01	0.63
2:J:54:SER:C	2:J:56:THR:N	2.52	0.63
2:L:50:PRO:HA	2:L:86:THR:HG22	1.80	0.63
2:K:149:THR:OG1	2:K:200:LEU:HD13	1.98	0.63
1:A:5:ALA:CB	1:A:13:LYS:HZ2	2.11	0.63
2:J:150:ALA:CA	2:J:200:LEU:HD11	2.29	0.63
2:G:50:PRO:HA	2:G:86:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:54:SER:C	2:I:56:THR:N	2.52	0.63
1:E:256:MET:HE2	2:H:63:TYR:CA	2.28	0.62
1:C:256:MET:HE1	2:J:63:TYR:HB2	1.81	0.62
1:E:41:GLY:HA3	2:H:59:ARG:HG2	1.81	0.62
2:L:122:ASN:HA	2:L:155:ALA:O	2.00	0.62
2:J:149:THR:C	2:J:200:LEU:CD1	2.68	0.62
1:F:51:ILE:CG2	1:F:55:LEU:HD23	2.30	0.62
1:B:51:ILE:CG2	1:B:55:LEU:HD23	2.29	0.62
2:I:150:ALA:CA	2:I:200:LEU:HD11	2.29	0.62
2:L:92:LEU:HD23	2:L:110:PHE:CE1	2.34	0.62
2:J:130:SER:HB3	2:J:153:ILE:HA	1.80	0.62
1:E:5:ALA:CB	1:E:13:LYS:HZ2	2.12	0.62
2:L:150:ALA:N	2:L:200:LEU:CD1	2.62	0.61
2:I:132:ILE:HG23	2:I:150:ALA:O	1.99	0.61
2:G:9:LEU:HD11	2:G:11:LEU:CD1	2.28	0.61
2:L:132:ILE:HG23	2:L:150:ALA:O	2.00	0.61
2:H:98:GLU:CG	2:H:120:CYS:SG	2.86	0.61
1:E:35:LYS:CD	2:H:102:LEU:HD22	2.31	0.61
1:E:256:MET:HE2	2:H:63:TYR:CG	2.14	0.61
2:G:92:LEU:HD23	2:G:110:PHE:CE1	2.36	0.61
2:G:131:PHE:HD1	2:G:132:ILE:N	1.99	0.61
2:L:107:GLY:O	2:L:110:PHE:N	2.32	0.60
2:H:123:PHE:HE1	2:H:157:TYR:HB2	1.62	0.60
2:H:54:SER:C	2:H:56:THR:N	2.53	0.60
2:L:86:THR:O	2:L:90:CYS:N	2.29	0.60
2:I:149:THR:C	2:I:200:LEU:CD1	2.70	0.60
1:C:6:ASP:H	1:C:10:ILE:HG13	1.66	0.60
2:I:50:PRO:HA	2:I:86:THR:HG22	1.83	0.60
2:G:149:THR:C	2:G:200:LEU:CD1	2.69	0.60
2:H:153:ILE:O	2:H:154:ARG:HG3	2.01	0.60
2:K:54:SER:C	2:K:56:THR:H	2.03	0.60
2:I:131:PHE:HD1	2:I:132:ILE:N	2.00	0.60
2:G:119:ILE:HG13	2:G:120:CYS:N	2.17	0.60
2:J:119:ILE:HG13	2:J:120:CYS:N	2.16	0.60
2:K:11:LEU:O	2:K:12:GLN:HB2	2.02	0.60
1:A:51:ILE:CG2	1:A:55:LEU:HD23	2.31	0.60
1:D:6:ASP:H	1:D:10:ILE:HG13	1.67	0.60
2:I:119:ILE:HG13	2:I:120:CYS:N	2.15	0.60
2:I:105:ASN:O	2:I:106:PHE:CG	2.54	0.59
1:A:256:MET:HE1	2:L:63:TYR:CB	2.30	0.59
2:J:153:ILE:O	2:J:153:ILE:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:105:ASN:O	2:I:106:PHE:CD1	2.55	0.59
1:E:279:HIS:CE1	1:F:58:THR:OG1	2.55	0.59
2:G:150:ALA:CA	2:G:200:LEU:HD11	2.32	0.59
1:E:6:ASP:H	1:E:10:ILE:HG13	1.68	0.59
1:A:9:SER:HB3	1:A:12:LEU:HD23	1.85	0.59
1:A:256:MET:HE1	2:L:63:TYR:HB2	1.84	0.59
1:A:6:ASP:H	1:A:10:ILE:HG13	1.67	0.59
2:K:149:THR:C	2:K:200:LEU:CD1	2.71	0.59
1:F:6:ASP:H	1:F:10:ILE:HG13	1.66	0.59
2:L:15:PHE:CD1	2:L:15:PHE:N	2.71	0.59
2:L:121:ARG:O	2:L:122:ASN:C	2.40	0.59
1:C:256:MET:HE2	2:J:63:TYR:CB	2.33	0.58
1:E:256:MET:SD	2:H:63:TYR:HB2	2.43	0.58
1:B:20:LEU:HD23	1:B:43:ILE:HD12	1.85	0.58
2:K:150:ALA:CA	2:K:200:LEU:HD11	2.33	0.58
2:L:92:LEU:HD23	2:L:110:PHE:HE1	1.68	0.58
1:D:51:ILE:CG2	1:D:55:LEU:HD23	2.34	0.58
2:G:121:ARG:O	2:G:122:ASN:C	2.42	0.58
2:G:14:ASP:O	2:G:14:ASP:OD1	2.22	0.58
1:B:256:MET:HE1	2:I:63:TYR:CA	2.33	0.58
2:L:149:THR:CB	2:L:200:LEU:HD13	2.33	0.58
2:L:150:ALA:C	2:L:200:LEU:HD11	2.24	0.58
2:H:150:ALA:O	2:H:200:LEU:HD11	2.04	0.58
2:H:150:ALA:CA	2:H:200:LEU:HD11	2.34	0.58
2:K:119:ILE:HG13	2:K:120:CYS:N	2.18	0.58
2:G:122:ASN:HA	2:G:155:ALA:O	2.04	0.58
2:H:121:ARG:O	2:H:122:ASN:C	2.42	0.58
2:J:98:GLU:CG	2:J:120:CYS:SG	2.91	0.58
1:E:20:LEU:HD23	1:E:43:ILE:HD12	1.84	0.58
1:F:266:ILE:HG23	2:K:63:TYR:CZ	2.39	0.58
1:E:266:ILE:HG12	2:H:63:TYR:HE2	1.69	0.58
1:E:76:CYS:HB3	2:H:102:LEU:CD1	2.33	0.58
2:L:100:ILE:CG2	2:L:103:TYR:HB2	2.30	0.58
2:G:123:PHE:CD1	2:G:157:TYR:CB	2.81	0.58
1:F:20:LEU:HD23	1:F:43:ILE:HD12	1.85	0.58
2:K:54:SER:C	2:K:56:THR:N	2.57	0.58
1:C:256:MET:HE1	2:J:63:TYR:CB	2.34	0.58
2:G:105:ASN:O	2:G:106:PHE:CD1	2.57	0.58
2:L:100:ILE:HG22	2:L:104:SER:H	1.64	0.57
1:F:10:ILE:HG23	1:F:14:HIS:CD2	2.39	0.57
1:F:9:SER:HB3	1:F:12:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:105:ASN:O	2:G:106:PHE:CG	2.57	0.57
2:J:149:THR:O	2:J:202:HIS:HE1	1.86	0.57
1:B:6:ASP:H	1:B:10:ILE:HG13	1.68	0.57
1:E:20:LEU:CD2	1:E:43:ILE:HD12	2.35	0.57
2:I:52:GLY:O	2:I:88:ALA:HB2	2.05	0.57
1:E:35:LYS:NZ	2:H:102:LEU:HD21	2.18	0.57
2:J:132:ILE:HG23	2:J:150:ALA:O	2.04	0.57
2:H:11:LEU:O	2:H:12:GLN:HB2	2.04	0.57
2:L:131:PHE:HD1	2:L:132:ILE:O	1.88	0.57
1:E:51:ILE:HG22	1:E:55:LEU:CD2	2.34	0.57
2:K:150:ALA:O	2:K:200:LEU:HD11	2.04	0.57
2:J:107:GLY:HA2	2:J:110:PHE:HB2	1.86	0.57
1:F:5:ALA:CB	1:F:13:LYS:HZ2	2.17	0.57
2:L:11:LEU:O	2:L:12:GLN:CB	2.53	0.57
2:H:100:ILE:CG2	2:H:103:TYR:C	2.73	0.57
1:A:19:MET:SD	2:L:14:ASP:OD2	2.63	0.57
1:E:266:ILE:HG12	2:H:63:TYR:CE2	2.40	0.57
2:L:110:PHE:C	2:L:110:PHE:CD1	2.78	0.57
1:D:20:LEU:HD23	1:D:43:ILE:HD12	1.87	0.57
1:F:266:ILE:HG23	2:K:63:TYR:CE2	2.39	0.57
2:H:132:ILE:HG23	2:H:150:ALA:O	2.04	0.57
2:H:149:THR:OG1	2:H:200:LEU:HD13	2.04	0.57
1:C:9:SER:HB3	1:C:12:LEU:HD23	1.85	0.57
2:L:54:SER:O	2:L:56:THR:N	2.37	0.56
1:F:256:MET:HE1	2:K:63:TYR:HD1	1.59	0.56
2:I:92:LEU:HD23	2:I:110:PHE:CE1	2.40	0.56
1:A:10:ILE:HG23	1:A:14:HIS:CD2	2.40	0.56
2:G:52:GLY:O	2:G:88:ALA:HB2	2.06	0.56
2:J:121:ARG:O	2:J:122:ASN:C	2.44	0.56
1:E:9:SER:HB3	1:E:12:LEU:HD23	1.87	0.56
1:D:9:SER:HB3	1:D:12:LEU:HD23	1.87	0.56
2:I:100:ILE:CG2	2:I:103:TYR:C	2.73	0.56
2:I:121:ARG:O	2:I:122:ASN:C	2.43	0.56
1:D:5:ALA:CB	1:D:13:LYS:HZ2	2.17	0.56
1:A:279:HIS:NE2	1:B:58:THR:OG1	2.38	0.56
2:G:15:PHE:N	2:G:15:PHE:CD1	2.74	0.56
1:C:20:LEU:HD23	1:C:43:ILE:HD12	1.88	0.56
2:J:100:ILE:CG2	2:J:103:TYR:C	2.74	0.56
2:L:202:HIS:HD2	2:L:204:ALA:H	1.54	0.56
2:K:123:PHE:CD1	2:K:157:TYR:CB	2.86	0.56
2:L:52:GLY:O	2:L:88:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:LYS:O	2:H:12:GLN:HG2	2.06	0.56
2:K:132:ILE:HG23	2:K:150:ALA:O	2.05	0.55
1:B:9:SER:HA	1:B:12:LEU:HB3	1.87	0.55
1:B:9:SER:HB3	1:B:12:LEU:HD23	1.86	0.55
2:H:14:ASP:OD1	2:H:14:ASP:O	2.24	0.55
2:H:150:ALA:C	2:H:200:LEU:HD11	2.27	0.55
2:H:149:THR:C	2:H:200:LEU:CD1	2.75	0.55
1:F:10:ILE:CG2	1:F:14:HIS:CD2	2.90	0.55
1:E:10:ILE:HG23	1:E:14:HIS:CD2	2.40	0.55
1:E:9:SER:HA	1:E:12:LEU:HB3	1.88	0.55
2:K:150:ALA:C	2:K:200:LEU:HD11	2.27	0.55
1:F:9:SER:HA	1:F:12:LEU:HB3	1.88	0.55
2:I:122:ASN:HA	2:I:155:ALA:O	2.06	0.55
1:B:32:GLU:O	1:B:36:ILE:HG13	2.07	0.55
2:I:123:PHE:CD1	2:I:157:TYR:CB	2.82	0.55
2:K:100:ILE:CG2	2:K:103:TYR:C	2.75	0.55
1:F:256:MET:HE1	2:K:63:TYR:HA	1.89	0.55
1:C:10:ILE:HG23	1:C:14:HIS:CD2	2.42	0.55
1:B:20:LEU:CD2	1:B:43:ILE:HD12	2.37	0.55
1:F:20:LEU:CD2	1:F:43:ILE:HD12	2.37	0.55
2:G:131:PHE:CD1	2:G:132:ILE:N	2.75	0.54
1:B:269:ASN:CB	2:I:63:TYR:OH	2.55	0.54
2:J:11:LEU:O	2:J:12:GLN:CB	2.55	0.54
2:J:123:PHE:CE1	2:J:157:TYR:CB	2.79	0.54
2:K:14:ASP:OD1	2:K:14:ASP:O	2.25	0.54
1:F:256:MET:HE1	2:K:63:TYR:CA	2.37	0.54
2:K:50:PRO:HA	2:K:86:THR:CG2	2.38	0.54
1:F:256:MET:SD	2:K:63:TYR:HB2	2.47	0.54
2:I:131:PHE:CD1	2:I:132:ILE:N	2.75	0.54
2:H:119:ILE:HG13	2:H:120:CYS:N	2.23	0.54
1:A:256:MET:HE2	2:L:63:TYR:CB	2.38	0.54
1:E:35:LYS:HE2	2:H:102:LEU:CD1	2.37	0.54
1:B:19:MET:HG3	2:I:52:GLY:HA2	1.88	0.54
2:I:15:PHE:N	2:I:15:PHE:CD1	2.76	0.54
2:L:149:THR:O	2:L:202:HIS:HE1	1.91	0.54
2:G:132:ILE:HG23	2:G:150:ALA:O	2.07	0.54
2:K:150:ALA:N	2:K:200:LEU:CD1	2.70	0.54
1:A:256:MET:HE2	2:L:63:TYR:HB2	1.86	0.54
2:L:92:LEU:CD2	2:L:110:PHE:CE1	2.91	0.54
1:B:252:SER:HB3	2:I:59:ARG:NH2	2.22	0.54
2:G:110:PHE:CD1	2:G:110:PHE:C	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:MET:SD	2:J:14:ASP:OD2	2.66	0.54
1:D:241:ILE:HG22	1:D:242:PHE:N	2.22	0.54
2:L:131:PHE:CD1	2:L:132:ILE:O	2.61	0.54
2:K:149:THR:O	2:K:202:HIS:HE1	1.91	0.54
2:K:63:TYR:CE2	2:K:64:GLU:CG	2.85	0.53
2:L:150:ALA:CA	2:L:200:LEU:CD1	2.87	0.53
1:E:10:ILE:CG2	1:E:14:HIS:CD2	2.91	0.53
1:D:10:ILE:HG23	1:D:14:HIS:CD2	2.42	0.53
2:I:150:ALA:N	2:I:200:LEU:CD1	2.71	0.53
1:E:252:SER:CB	2:H:59:ARG:NH2	2.61	0.53
2:J:132:ILE:HG22	2:J:133:CYS:N	2.23	0.53
2:G:54:SER:O	2:G:56:THR:N	2.42	0.53
2:L:86:THR:O	2:L:87:CYS:C	2.47	0.53
2:L:16:GLU:N	2:L:17:PRO:CD	2.72	0.53
2:I:100:ILE:CG2	2:I:103:TYR:HB2	2.37	0.53
2:K:121:ARG:O	2:K:122:ASN:C	2.47	0.53
2:G:123:PHE:CZ	2:G:124:TYR:CE2	2.96	0.53
2:H:131:PHE:HD1	2:H:132:ILE:N	2.07	0.53
2:H:100:ILE:HG22	2:H:103:TYR:C	2.28	0.53
2:H:122:ASN:HA	2:H:155:ALA:O	2.08	0.53
2:L:153:ILE:O	2:L:153:ILE:HG22	2.06	0.53
1:D:51:ILE:HD12	1:D:51:ILE:H	1.74	0.53
1:D:32:GLU:O	1:D:36:ILE:HG13	2.08	0.53
2:I:150:ALA:C	2:I:200:LEU:HD11	2.28	0.53
1:C:9:SER:HA	1:C:12:LEU:HB3	1.90	0.53
1:D:9:SER:HA	1:D:12:LEU:HB3	1.89	0.53
1:B:78:SER:HB3	2:I:103:TYR:CZ	2.43	0.53
1:C:241:ILE:HG22	1:C:242:PHE:N	2.22	0.53
2:K:100:ILE:HG22	2:K:103:TYR:C	2.29	0.53
1:A:9:SER:HA	1:A:12:LEU:HB3	1.89	0.53
1:A:256:MET:HE2	2:L:63:TYR:CG	2.33	0.53
2:I:100:ILE:HG22	2:I:104:SER:H	1.72	0.53
2:G:100:ILE:CG2	2:G:103:TYR:C	2.77	0.53
2:J:100:ILE:CG2	2:J:103:TYR:HB2	2.38	0.53
2:J:150:ALA:N	2:J:200:LEU:CD1	2.71	0.53
2:G:100:ILE:CG2	2:G:103:TYR:HB2	2.37	0.53
2:H:50:PRO:HA	2:H:86:THR:CG2	2.39	0.53
2:L:218:TYR:O	2:L:219:SER:C	2.47	0.53
2:G:123:PHE:CE1	2:G:157:TYR:CB	2.78	0.53
2:L:137:ILE:HD12	2:L:144:PHE:HB3	1.91	0.53
2:K:107:GLY:HA2	2:K:110:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ILE:HG22	1:C:55:LEU:CD2	2.39	0.53
2:H:63:TYR:CE2	2:H:64:GLU:CG	2.87	0.53
2:I:123:PHE:CZ	2:I:124:TYR:CE2	2.96	0.53
1:C:20:LEU:CD2	1:C:43:ILE:HD12	2.39	0.53
1:E:19:MET:HG3	2:H:52:GLY:HA2	1.90	0.53
2:L:148:LEU:HD13	2:L:202:HIS:NE2	2.24	0.52
2:J:150:ALA:C	2:J:200:LEU:HD11	2.30	0.52
2:H:100:ILE:CG2	2:H:103:TYR:HB2	2.36	0.52
1:B:10:ILE:HG23	1:B:14:HIS:CD2	2.43	0.52
2:L:131:PHE:O	2:L:132:ILE:HG12	2.08	0.52
2:L:150:ALA:O	2:L:200:LEU:HD11	2.09	0.52
2:H:123:PHE:CD1	2:H:157:TYR:CB	2.88	0.52
2:L:63:TYR:CE2	2:L:64:GLU:CG	2.88	0.52
2:H:107:GLY:HA2	2:H:110:PHE:HB2	1.91	0.52
1:F:266:ILE:CG1	2:K:63:TYR:CE2	2.83	0.52
2:L:123:PHE:CZ	2:L:124:TYR:CE2	2.97	0.52
2:K:148:LEU:HD13	2:K:202:HIS:NE2	2.24	0.52
2:K:100:ILE:CG2	2:K:103:TYR:HB2	2.38	0.52
2:G:92:LEU:HD23	2:G:110:PHE:HE1	1.75	0.52
1:A:10:ILE:CG2	1:A:14:HIS:CD2	2.92	0.52
2:J:50:PRO:HA	2:J:86:THR:CG2	2.39	0.52
2:I:14:ASP:OD1	2:I:14:ASP:O	2.26	0.52
2:G:123:PHE:CZ	2:G:124:TYR:CZ	2.97	0.52
2:G:11:LEU:O	2:G:12:GLN:CB	2.57	0.52
1:F:41:GLY:HA3	2:K:59:ARG:HG2	1.91	0.52
2:L:16:GLU:N	2:L:17:PRO:HD2	2.25	0.52
1:E:39:LYS:HD3	2:H:105:ASN:OD1	2.10	0.52
2:L:132:ILE:HG22	2:L:133:CYS:H	1.75	0.52
1:B:5:ALA:CB	1:B:13:LYS:HZ2	2.23	0.52
1:D:10:ILE:CG2	1:D:14:HIS:CD2	2.93	0.52
1:E:51:ILE:HD12	1:E:51:ILE:H	1.73	0.52
2:K:132:ILE:HG22	2:K:133:CYS:N	2.25	0.52
1:E:241:ILE:HG22	1:E:242:PHE:N	2.25	0.52
2:H:15:PHE:CD1	2:H:15:PHE:N	2.78	0.52
2:I:149:THR:CB	2:I:200:LEU:HD13	2.40	0.52
2:L:136:ASN:OD1	2:L:136:ASN:N	2.42	0.52
2:L:134:SER:HA	2:L:148:LEU:O	2.10	0.51
2:H:150:ALA:N	2:H:200:LEU:CD1	2.73	0.51
1:B:9:SER:HA	1:B:12:LEU:CB	2.40	0.51
2:G:107:GLY:O	2:G:110:PHE:N	2.38	0.51
1:C:10:ILE:CG2	1:C:14:HIS:CD2	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:149:THR:O	2:I:202:HIS:HE1	1.93	0.51
2:G:202:HIS:HD2	2:G:204:ALA:H	1.57	0.51
2:J:131:PHE:HD1	2:J:132:ILE:N	2.08	0.51
2:J:100:ILE:HG22	2:J:103:TYR:C	2.30	0.51
2:L:50:PRO:HA	2:L:86:THR:CG2	2.39	0.51
2:J:14:ASP:O	2:J:14:ASP:OD1	2.28	0.51
2:G:134:SER:HA	2:G:148:LEU:O	2.10	0.51
2:L:151:ALA:HB3	2:L:196:ASN:HB2	1.93	0.51
1:D:20:LEU:CD2	1:D:43:ILE:HD12	2.41	0.51
1:E:76:CYS:O	2:H:102:LEU:HD13	2.10	0.51
1:E:9:SER:HA	1:E:12:LEU:CB	2.40	0.51
1:D:100:LYS:HD2	2:G:128:ASN:HD21	1.76	0.51
2:L:100:ILE:HG22	2:L:103:TYR:C	2.29	0.51
2:G:150:ALA:N	2:G:200:LEU:CD1	2.73	0.51
2:K:86:THR:O	2:K:87:CYS:C	2.48	0.51
2:L:132:ILE:CG2	2:L:133:CYS:N	2.71	0.51
2:I:202:HIS:HD2	2:I:204:ALA:H	1.57	0.51
2:J:148:LEU:HD13	2:J:202:HIS:NE2	2.26	0.51
2:I:110:PHE:CD1	2:I:110:PHE:C	2.84	0.51
2:G:153:ILE:O	2:G:153:ILE:HG22	2.09	0.51
1:A:32:GLU:O	1:A:36:ILE:HG13	2.11	0.51
2:G:148:LEU:HD13	2:G:202:HIS:NE2	2.26	0.51
1:E:5:ALA:CB	1:E:13:LYS:NZ	2.62	0.51
1:C:5:ALA:CB	1:C:13:LYS:NZ	2.62	0.51
2:I:123:PHE:CZ	2:I:124:TYR:CZ	2.99	0.50
2:K:98:GLU:HG2	2:K:120:CYS:HG	1.76	0.50
2:I:11:LEU:O	2:I:12:GLN:CB	2.59	0.50
1:A:20:LEU:HD23	1:A:43:ILE:HD12	1.92	0.50
2:H:132:ILE:HG22	2:H:133:CYS:N	2.25	0.50
1:B:51:ILE:H	1:B:51:ILE:HD12	1.76	0.50
2:I:75:PHE:CE2	2:I:81:LYS:HD2	2.47	0.50
2:I:123:PHE:CE1	2:I:157:TYR:CB	2.80	0.50
1:C:256:MET:HE2	2:J:63:TYR:CG	2.46	0.50
1:F:5:ALA:CB	1:F:13:LYS:NZ	2.68	0.50
2:K:153:ILE:O	2:K:153:ILE:HG22	2.10	0.50
1:A:9:SER:HA	1:A:12:LEU:CB	2.41	0.50
1:B:51:ILE:HG22	1:B:55:LEU:CD2	2.41	0.50
1:E:43:ILE:HG22	2:H:53:GLU:HB2	1.92	0.50
1:A:20:LEU:CD2	1:A:43:ILE:HD12	2.41	0.50
2:L:123:PHE:CZ	2:L:124:TYR:CZ	2.99	0.50
1:F:9:SER:HA	1:F:12:LEU:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:149:THR:O	2:G:202:HIS:HE1	1.94	0.50
2:I:98:GLU:HG2	2:I:120:CYS:HG	1.70	0.50
1:B:10:ILE:CG2	1:B:14:HIS:CD2	2.94	0.50
2:I:54:SER:O	2:I:56:THR:N	2.44	0.50
1:D:282:THR:HG23	1:E:59:ASP:O	2.12	0.50
2:K:15:PHE:N	2:K:15:PHE:CD1	2.79	0.50
1:E:32:GLU:O	1:E:36:ILE:HG13	2.11	0.50
2:I:63:TYR:CE2	2:I:64:GLU:CG	2.90	0.50
2:L:128:ASN:O	2:L:128:ASN:CG	2.49	0.50
2:L:107:GLY:O	2:L:110:PHE:HB2	2.09	0.50
1:F:51:ILE:HG22	1:F:55:LEU:CD2	2.41	0.50
2:G:16:GLU:N	2:G:17:PRO:CD	2.74	0.50
2:L:124:TYR:O	2:L:125:GLY:C	2.49	0.50
1:A:51:ILE:HD12	1:A:51:ILE:H	1.76	0.50
2:J:122:ASN:HA	2:J:155:ALA:O	2.11	0.50
2:G:16:GLU:N	2:G:17:PRO:HD2	2.27	0.50
2:I:16:GLU:N	2:I:17:PRO:CD	2.75	0.50
1:C:32:GLU:O	1:C:36:ILE:HG13	2.12	0.50
2:K:123:PHE:CE1	2:K:157:TYR:CB	2.81	0.50
1:D:177:LEU:O	1:D:203:ARG:NH1	2.45	0.50
1:C:177:LEU:O	1:C:203:ARG:NH1	2.45	0.50
1:D:78:SER:OG	2:G:121:ARG:NH2	2.43	0.50
1:B:241:ILE:HG22	1:B:242:PHE:N	2.26	0.50
2:G:170:ALA:HB3	2:G:184:ALA:HB3	1.94	0.50
2:K:86:THR:O	2:K:89:GLY:N	2.45	0.49
1:A:241:ILE:HG22	1:A:242:PHE:N	2.26	0.49
2:K:98:GLU:CG	2:K:120:CYS:SG	2.97	0.49
2:L:153:ILE:O	2:L:154:ARG:CG	2.60	0.49
1:B:76:CYS:O	2:I:102:LEU:HD13	2.13	0.49
2:K:122:ASN:HA	2:K:155:ALA:O	2.12	0.49
1:F:241:ILE:HG22	1:F:242:PHE:N	2.27	0.49
1:C:9:SER:HA	1:C:12:LEU:CB	2.41	0.49
2:K:11:LEU:O	2:K:12:GLN:CB	2.61	0.49
1:D:100:LYS:CD	2:G:128:ASN:HD21	2.26	0.49
2:L:75:PHE:CE2	2:L:81:LYS:HD2	2.47	0.49
1:F:51:ILE:HD12	1:F:51:ILE:H	1.76	0.49
2:H:52:GLY:O	2:H:88:ALA:HB2	2.13	0.49
2:K:105:ASN:O	2:K:106:PHE:CD1	2.66	0.49
2:I:100:ILE:HG22	2:I:103:TYR:C	2.33	0.49
2:L:131:PHE:CE1	2:L:152:CYS:CB	2.96	0.49
2:I:148:LEU:HD13	2:I:202:HIS:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:103:TYR:HD1	2:L:103:TYR:N	2.09	0.49
2:L:106:PHE:O	2:L:106:PHE:HD1	1.95	0.49
2:G:149:THR:CB	2:G:200:LEU:HD13	2.43	0.49
1:D:279:HIS:NE2	1:E:58:THR:CB	2.76	0.49
1:D:5:ALA:CB	1:D:13:LYS:NZ	2.68	0.49
2:L:53:GLU:HB3	2:L:56:THR:OG1	2.13	0.49
2:I:16:GLU:N	2:I:17:PRO:HD2	2.27	0.49
2:H:149:THR:O	2:H:202:HIS:HE1	1.95	0.49
2:K:131:PHE:HD1	2:K:132:ILE:N	2.11	0.49
2:G:131:PHE:CE1	2:G:152:CYS:CB	2.96	0.49
2:H:131:PHE:CD1	2:H:132:ILE:N	2.81	0.49
2:J:150:ALA:CA	2:J:200:LEU:CD1	2.91	0.49
2:I:137:ILE:HD12	2:I:144:PHE:HB3	1.95	0.49
1:D:9:SER:HA	1:D:12:LEU:CB	2.42	0.49
2:J:107:GLY:O	2:J:110:PHE:HB2	2.13	0.49
2:L:170:ALA:HB3	2:L:184:ALA:HB3	1.95	0.49
2:J:123:PHE:CD1	2:J:157:TYR:CB	2.86	0.49
1:D:100:LYS:HA	2:G:128:ASN:ND2	2.28	0.49
2:K:105:ASN:O	2:K:106:PHE:CG	2.66	0.49
1:F:256:MET:HE1	2:K:63:TYR:HB2	1.81	0.48
2:I:150:ALA:O	2:I:200:LEU:HD11	2.13	0.48
1:A:51:ILE:HG22	1:A:55:LEU:CD2	2.42	0.48
2:I:132:ILE:CG2	2:I:133:CYS:N	2.76	0.48
1:C:9:SER:HA	1:C:12:LEU:CD2	2.43	0.48
1:C:43:ILE:HA	2:J:53:GLU:HG2	1.94	0.48
2:I:136:ASN:N	2:I:136:ASN:OD1	2.46	0.48
1:E:11:LEU:HB3	4:E:2001:HOH:O	2.13	0.48
1:C:51:ILE:H	1:C:51:ILE:HD12	1.78	0.48
2:I:153:ILE:O	2:I:153:ILE:HG22	2.13	0.48
2:I:86:THR:O	2:I:87:CYS:C	2.52	0.48
2:H:148:LEU:HD13	2:H:202:HIS:NE2	2.28	0.48
2:K:150:ALA:CA	2:K:200:LEU:CD1	2.92	0.48
2:K:149:THR:CB	2:K:200:LEU:HD13	2.43	0.48
1:E:32:GLU:N	1:E:32:GLU:OE1	2.46	0.48
2:J:131:PHE:CD1	2:J:132:ILE:N	2.82	0.48
2:I:9:LEU:HD11	2:I:11:LEU:CD1	2.41	0.48
2:G:132:ILE:CG2	2:G:133:CYS:N	2.77	0.48
2:G:150:ALA:C	2:G:200:LEU:HD11	2.34	0.48
1:B:269:ASN:ND2	2:I:63:TYR:OH	2.47	0.48
2:G:137:ILE:HD12	2:G:144:PHE:HB3	1.95	0.48
1:B:43:ILE:HG22	2:I:53:GLU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLU:OE1	1:D:32:GLU:N	2.45	0.48
1:F:32:GLU:O	1:F:36:ILE:HG13	2.14	0.47
1:D:203:ARG:HG3	1:D:203:ARG:HH11	1.79	0.47
2:H:133:CYS:HG	2:H:152:CYS:HG	1.61	0.47
2:H:107:GLY:O	2:H:110:PHE:HB2	2.15	0.47
2:J:53:GLU:O	2:J:57:VAL:HG23	2.14	0.47
2:J:52:GLY:O	2:J:88:ALA:HB2	2.14	0.47
2:G:136:ASN:N	2:G:136:ASN:OD1	2.48	0.47
1:E:12:LEU:N	4:E:2001:HOH:O	2.48	0.47
2:L:17:PRO:O	2:L:20:ASN:N	2.47	0.47
1:B:5:ALA:CB	1:B:13:LYS:NZ	2.64	0.47
2:G:92:LEU:CD2	2:G:110:PHE:CE1	2.97	0.47
2:G:151:ALA:HB3	2:G:196:ASN:HB2	1.97	0.47
2:I:107:GLY:O	2:I:110:PHE:N	2.40	0.47
2:I:92:LEU:HD23	2:I:110:PHE:HE1	1.78	0.47
2:J:110:PHE:CD1	2:J:110:PHE:C	2.87	0.47
1:F:9:SER:HA	1:F:12:LEU:CD2	2.45	0.47
2:H:11:LEU:O	2:H:12:GLN:CB	2.62	0.47
2:K:53:GLU:O	2:K:57:VAL:HG23	2.14	0.47
2:I:128:ASN:CG	2:I:128:ASN:O	2.53	0.47
2:J:15:PHE:N	2:J:15:PHE:CD1	2.82	0.47
2:L:103:TYR:HD2	2:L:121:ARG:NH1	2.13	0.47
1:E:9:SER:HA	1:E:12:LEU:CD2	2.44	0.47
2:G:100:ILE:HG22	2:G:104:SER:H	1.73	0.47
1:E:177:LEU:O	1:E:203:ARG:NH1	2.48	0.47
1:D:51:ILE:HG22	1:D:55:LEU:CD2	2.45	0.47
2:L:138:ILE:N	2:L:138:ILE:HD12	2.30	0.47
2:I:131:PHE:CE1	2:I:152:CYS:CB	2.98	0.47
1:B:78:SER:CB	2:I:103:TYR:CE2	2.93	0.47
2:L:100:ILE:HG21	2:L:104:SER:N	2.29	0.46
1:B:177:LEU:O	1:B:203:ARG:NH1	2.48	0.46
2:H:110:PHE:C	2:H:110:PHE:CD1	2.88	0.46
2:J:86:THR:O	2:J:89:GLY:N	2.48	0.46
2:J:54:SER:O	2:J:56:THR:N	2.47	0.46
1:D:282:THR:OG1	1:E:59:ASP:HB3	2.15	0.46
1:C:32:GLU:N	1:C:32:GLU:OE1	2.47	0.46
1:E:77:ILE:HA	2:H:103:TYR:CE1	2.51	0.46
2:I:150:ALA:CA	2:I:200:LEU:CD1	2.93	0.46
2:J:149:THR:CB	2:J:200:LEU:HD13	2.44	0.46
2:H:150:ALA:CA	2:H:200:LEU:CD1	2.93	0.46
1:A:9:SER:HA	1:A:12:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:HIS:HE1	1:F:58:THR:OG1	1.99	0.46
2:H:123:PHE:CE1	2:H:157:TYR:CB	2.83	0.46
2:J:131:PHE:CE1	2:J:152:CYS:CB	2.98	0.46
1:F:177:LEU:O	1:F:203:ARG:NH1	2.48	0.46
2:K:107:GLY:O	2:K:110:PHE:N	2.43	0.46
1:A:59:ASP:O	1:F:282:THR:HG23	2.16	0.46
2:G:75:PHE:CE2	2:G:81:LYS:HD2	2.51	0.46
2:H:149:THR:CB	2:H:200:LEU:HD13	2.46	0.46
1:A:177:LEU:O	1:A:203:ARG:NH1	2.49	0.46
1:B:9:SER:HA	1:B:12:LEU:CD2	2.46	0.46
2:L:154:ARG:O	2:L:154:ARG:HG3	2.16	0.46
1:A:203:ARG:HH11	1:A:203:ARG:HG3	1.81	0.46
2:J:150:ALA:O	2:J:200:LEU:HD11	2.16	0.46
2:H:86:THR:O	2:H:89:GLY:N	2.49	0.46
2:J:136:ASN:OD1	2:J:136:ASN:N	2.49	0.46
2:I:218:TYR:O	2:I:219:SER:C	2.54	0.46
1:E:11:LEU:HA	1:E:11:LEU:HD12	1.85	0.46
1:D:256:MET:CE	2:G:63:TYR:CD1	2.99	0.46
1:B:256:MET:HE1	2:I:63:TYR:HA	1.99	0.45
2:K:107:GLY:O	2:K:110:PHE:HB2	2.15	0.45
2:K:151:ALA:HB3	2:K:196:ASN:HB2	1.98	0.45
2:L:100:ILE:HG23	2:L:103:TYR:CB	2.38	0.45
2:K:131:PHE:CD1	2:K:132:ILE:N	2.84	0.45
2:H:63:TYR:CG	2:H:64:GLU:N	2.85	0.45
2:H:100:ILE:HG22	2:H:104:SER:H	1.78	0.45
1:C:203:ARG:HH11	1:C:203:ARG:HG3	1.81	0.45
2:H:136:ASN:OD1	2:H:136:ASN:N	2.49	0.45
2:K:136:ASN:OD1	2:K:136:ASN:N	2.50	0.45
2:I:151:ALA:HB3	2:I:196:ASN:HB2	1.97	0.45
2:J:63:TYR:CE2	2:J:64:GLU:CG	2.90	0.45
1:D:279:HIS:CE1	1:E:55:LEU:HG	2.51	0.45
2:H:105:ASN:O	2:H:106:PHE:CG	2.70	0.45
1:C:279:HIS:HE1	1:D:58:THR:OG1	1.96	0.45
2:H:105:ASN:O	2:H:106:PHE:CD1	2.70	0.45
2:G:128:ASN:CG	2:G:128:ASN:O	2.54	0.45
1:E:161:ILE:HD11	1:F:115:GLU:HB3	1.97	0.45
2:J:16:GLU:N	2:J:17:PRO:CD	2.80	0.45
1:F:67:PRO:HB3	1:F:99:LEU:HD22	1.98	0.45
2:I:96:ASN:O	2:I:119:ILE:HG22	2.16	0.45
2:L:105:ASN:C	2:L:106:PHE:CG	2.89	0.45
2:G:133:CYS:O	2:G:149:THR:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:O	1:A:12:LEU:CB	2.54	0.45
2:K:110:PHE:C	2:K:110:PHE:CD1	2.89	0.45
1:B:203:ARG:HG3	1:B:203:ARG:HH11	1.82	0.45
2:I:134:SER:HA	2:I:148:LEU:O	2.17	0.45
2:K:148:LEU:HD13	2:K:202:HIS:CD2	2.52	0.45
1:D:9:SER:HA	1:D:12:LEU:CD2	2.46	0.45
1:F:177:LEU:HD11	1:F:199:ILE:HG23	1.98	0.45
2:H:16:GLU:N	2:H:17:PRO:HD2	2.32	0.45
2:K:75:PHE:CE2	2:K:81:LYS:HD2	2.52	0.45
1:E:269:ASN:HB3	2:H:63:TYR:HH	1.75	0.45
2:L:100:ILE:HB	2:L:104:SER:OG	2.17	0.45
1:B:11:LEU:HA	1:B:11:LEU:HD12	1.82	0.45
2:I:50:PRO:HA	2:I:86:THR:CG2	2.45	0.44
1:F:7:ASN:ND2	1:F:7:ASN:N	2.65	0.44
2:K:63:TYR:CG	2:K:64:GLU:N	2.85	0.44
1:D:256:MET:HE2	2:G:63:TYR:CD1	2.52	0.44
2:I:86:THR:O	2:I:90:CYS:N	2.37	0.44
2:K:218:TYR:O	2:K:219:SER:C	2.55	0.44
2:I:138:ILE:HD12	2:I:138:ILE:N	2.33	0.44
2:J:63:TYR:CG	2:J:64:GLU:N	2.85	0.44
2:I:92:LEU:CD2	2:I:110:PHE:CE1	3.00	0.44
2:J:107:GLY:O	2:J:110:PHE:N	2.43	0.44
1:F:203:ARG:HG3	1:F:203:ARG:HH11	1.81	0.44
1:C:11:LEU:HD12	1:C:11:LEU:HA	1.80	0.44
2:L:15:PHE:O	2:L:19:ILE:N	2.39	0.44
2:H:16:GLU:N	2:H:17:PRO:CD	2.80	0.44
2:I:170:ALA:HB3	2:I:184:ALA:HB3	1.99	0.44
1:C:269:ASN:HB3	2:J:63:TYR:OH	2.18	0.44
2:H:131:PHE:CE1	2:H:152:CYS:CB	3.00	0.44
1:A:82:LEU:N	1:A:82:LEU:HD12	2.32	0.44
1:D:67:PRO:HB3	1:D:99:LEU:HD22	1.98	0.44
2:I:124:TYR:O	2:I:125:GLY:C	2.56	0.44
1:F:9:SER:O	1:F:12:LEU:CB	2.52	0.44
2:H:75:PHE:CE2	2:H:81:LYS:HD2	2.53	0.44
2:J:151:ALA:HB3	2:J:196:ASN:HB2	1.99	0.44
2:I:131:PHE:HD1	2:I:132:ILE:O	1.99	0.44
1:C:41:GLY:O	2:J:56:THR:HG23	2.18	0.44
2:G:50:PRO:HA	2:G:86:THR:CG2	2.45	0.44
2:L:13:GLY:O	2:L:15:PHE:CE1	2.71	0.44
2:G:96:ASN:O	2:G:119:ILE:HG22	2.18	0.44
1:E:78:SER:HG	2:H:121:ARG:HH12	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:PRO:HB3	1:E:99:LEU:HD22	1.99	0.44
1:F:150:ARG:HA	1:F:213:PHE:O	2.17	0.44
2:J:105:ASN:O	2:J:106:PHE:CD1	2.70	0.44
2:L:120:CYS:O	2:L:121:ARG:C	2.55	0.44
2:L:17:PRO:O	2:L:18:HIS:C	2.56	0.44
1:F:32:GLU:N	1:F:32:GLU:OE1	2.50	0.44
1:F:10:ILE:O	1:F:13:LYS:N	2.51	0.43
1:F:252:SER:HB3	2:K:59:ARG:NH2	2.31	0.43
2:G:86:THR:O	2:G:87:CYS:C	2.57	0.43
2:J:105:ASN:O	2:J:106:PHE:CG	2.70	0.43
2:G:150:ALA:CA	2:G:200:LEU:CD1	2.96	0.43
1:E:38:GLU:OE2	2:H:103:TYR:HB3	2.18	0.43
2:L:133:CYS:O	2:L:149:THR:HA	2.17	0.43
2:K:202:HIS:HD2	2:K:204:ALA:H	1.66	0.43
1:B:7:ASN:N	1:B:7:ASN:ND2	2.67	0.43
1:E:203:ARG:HH11	1:E:203:ARG:HG3	1.82	0.43
1:A:177:LEU:HD11	1:A:199:ILE:HG23	1.99	0.43
2:I:132:ILE:HG22	2:I:133:CYS:H	1.84	0.43
1:E:43:ILE:HB	2:H:53:GLU:HG2	2.00	0.43
2:G:218:TYR:O	2:G:219:SER:C	2.57	0.43
2:J:148:LEU:HD13	2:J:202:HIS:CD2	2.53	0.43
1:B:241:ILE:HG22	1:B:242:PHE:CG	2.54	0.43
2:J:161:ILE:HD12	2:J:166:VAL:HG11	2.01	0.43
1:A:67:PRO:HB3	1:A:99:LEU:HD22	2.00	0.43
2:L:132:ILE:CG2	2:L:133:CYS:H	2.32	0.43
2:H:202:HIS:HD2	2:H:204:ALA:H	1.67	0.43
2:H:54:SER:O	2:H:56:THR:N	2.52	0.43
1:C:82:LEU:N	1:C:82:LEU:HD12	2.33	0.43
2:L:143:ALA:O	2:L:144:PHE:C	2.57	0.43
2:J:202:HIS:HD2	2:J:204:ALA:H	1.67	0.43
2:G:138:ILE:HD12	2:G:138:ILE:N	2.33	0.43
1:A:7:ASN:N	1:A:7:ASN:ND2	2.67	0.43
2:L:98:GLU:CA	2:L:99:ASN:ND2	2.71	0.43
2:G:131:PHE:HD1	2:G:132:ILE:O	2.02	0.43
2:K:131:PHE:CE1	2:K:152:CYS:CB	3.00	0.43
1:D:35:LYS:HE2	2:G:102:LEU:CD1	2.47	0.43
1:B:82:LEU:HD12	1:B:82:LEU:N	2.34	0.43
2:H:128:ASN:CG	2:H:128:ASN:O	2.57	0.43
2:L:96:ASN:O	2:L:119:ILE:HG22	2.18	0.43
2:H:151:ALA:HB3	2:H:196:ASN:HB2	2.00	0.43
1:B:129:VAL:HG23	1:B:148:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:104:SER:O	2:L:105:ASN:ND2	2.39	0.42
1:D:11:LEU:HD12	1:D:11:LEU:HA	1.86	0.42
1:C:241:ILE:HG22	1:C:242:PHE:CG	2.53	0.42
1:B:4:TYR:HB2	1:B:122:HIS:O	2.19	0.42
1:B:67:PRO:HB3	1:B:99:LEU:HD22	2.00	0.42
1:E:51:ILE:HG21	1:E:55:LEU:HD23	2.01	0.42
1:F:11:LEU:HD12	1:F:11:LEU:HA	1.81	0.42
1:F:9:SER:O	1:F:13:LYS:N	2.51	0.42
1:A:185:VAL:HG12	1:A:196:ILE:HD11	2.01	0.42
1:F:82:LEU:HD12	1:F:82:LEU:N	2.35	0.42
1:A:32:GLU:N	1:A:32:GLU:OE1	2.51	0.42
2:J:16:GLU:N	2:J:17:PRO:HD2	2.34	0.42
1:F:7:ASN:HB2	1:F:8:ASP:H	1.72	0.42
2:J:75:PHE:CE2	2:J:81:LYS:HD2	2.54	0.42
1:D:82:LEU:N	1:D:82:LEU:HD12	2.34	0.42
2:I:62:ALA:HA	2:I:66:ASP:OD1	2.19	0.42
1:D:177:LEU:HD11	1:D:199:ILE:HG23	2.01	0.42
2:J:15:PHE:O	2:J:19:ILE:N	2.35	0.42
2:K:16:GLU:N	2:K:17:PRO:HD2	2.35	0.42
1:A:161:ILE:HD11	1:B:115:GLU:HB3	2.02	0.42
1:F:269:ASN:CB	2:K:63:TYR:OH	2.62	0.42
2:G:148:LEU:HD13	2:G:202:HIS:CD2	2.55	0.42
1:C:279:HIS:NE2	1:D:58:THR:OG1	2.53	0.42
2:K:82:PRO:HG2	2:K:213:VAL:HA	2.02	0.42
2:L:130:SER:HB3	2:L:153:ILE:CA	2.46	0.42
2:G:154:ARG:O	2:G:154:ARG:HG3	2.18	0.42
1:E:39:LYS:HG3	2:H:105:ASN:OD1	2.20	0.42
2:L:187:GLN:O	2:L:188:ASN:HB2	2.20	0.42
2:I:148:LEU:HD13	2:I:202:HIS:CD2	2.55	0.42
2:L:137:ILE:CG2	2:L:144:PHE:CD2	2.88	0.42
1:A:55:LEU:HG	1:F:279:HIS:CE1	2.54	0.42
1:A:241:ILE:HG22	1:A:242:PHE:CG	2.55	0.42
1:E:125:LYS:HD3	2:H:128:ASN:HB2	2.01	0.42
2:K:16:GLU:N	2:K:17:PRO:CD	2.82	0.42
2:G:150:ALA:O	2:G:200:LEU:HD11	2.19	0.42
2:G:124:TYR:O	2:G:125:GLY:C	2.58	0.42
2:L:137:ILE:HG21	2:L:144:PHE:CE2	2.51	0.42
2:L:110:PHE:C	2:L:110:PHE:HD1	2.23	0.42
1:D:19:MET:CE	2:G:196:ASN:HD21	2.33	0.42
2:L:62:ALA:HA	2:L:66:ASP:OD1	2.20	0.42
1:A:11:LEU:HD12	1:A:11:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:131:PHE:HD1	2:L:132:ILE:H	1.62	0.41
2:L:106:PHE:C	2:L:106:PHE:CD1	2.93	0.41
2:H:132:ILE:CG2	4:H:2002:HOH:O	2.68	0.41
2:I:100:ILE:HB	2:I:104:SER:OG	2.20	0.41
2:J:218:TYR:O	2:J:219:SER:C	2.59	0.41
2:L:148:LEU:HD13	2:L:202:HIS:CD2	2.54	0.41
1:F:195:PRO:HG2	1:F:198:LEU:HD12	2.01	0.41
1:F:4:TYR:HB2	1:F:122:HIS:O	2.20	0.41
2:H:170:ALA:HB3	2:H:184:ALA:HB3	2.02	0.41
1:E:7:ASN:ND2	1:E:7:ASN:N	2.69	0.41
2:G:100:ILE:HG22	2:G:103:TYR:C	2.37	0.41
2:H:218:TYR:O	2:H:219:SER:C	2.59	0.41
1:E:35:LYS:CE	2:H:102:LEU:CD1	2.99	0.41
2:K:135:LEU:CD2	2:K:150:ALA:HB2	2.41	0.41
1:A:269:ASN:HB3	2:L:63:TYR:OH	2.21	0.41
2:H:138:ILE:N	2:H:138:ILE:HD12	2.35	0.41
2:L:106:PHE:O	2:L:106:PHE:CD1	2.73	0.41
1:F:10:ILE:HG22	1:F:14:HIS:HD2	1.85	0.41
1:A:53:SER:O	1:A:56:ARG:HB3	2.21	0.41
1:A:24:VAL:HG22	1:A:258:VAL:HG21	2.01	0.41
2:L:149:THR:O	2:L:200:LEU:HD12	2.21	0.41
2:H:131:PHE:HD1	2:H:132:ILE:O	2.04	0.41
2:H:148:LEU:HD13	2:H:202:HIS:CD2	2.56	0.41
1:E:9:SER:O	1:E:12:LEU:CB	2.54	0.41
2:H:129:ASP:O	2:H:130:SER:C	2.58	0.41
1:F:43:ILE:CG2	2:K:56:THR:HG21	2.51	0.41
1:E:150:ARG:HA	1:E:213:PHE:O	2.20	0.41
1:C:7:ASN:ND2	1:C:7:ASN:N	2.69	0.41
2:J:128:ASN:O	2:J:128:ASN:CG	2.59	0.41
1:E:78:SER:OG	2:H:121:ARG:NH2	2.53	0.41
1:B:41:GLY:HA3	2:I:59:ARG:HG2	2.03	0.41
2:G:107:GLY:O	2:G:110:PHE:HB2	2.18	0.41
2:L:216:TYR:O	2:L:219:SER:HB2	2.20	0.41
2:I:17:PRO:O	2:I:18:HIS:C	2.59	0.41
1:E:129:VAL:HG23	1:E:148:MET:HG2	2.03	0.41
1:E:270:VAL:HG12	2:H:63:TYR:CE1	2.56	0.41
2:L:155:ALA:HB1	2:L:156:PRO:HD2	2.03	0.41
1:F:19:MET:SD	2:K:14:ASP:OD2	2.79	0.41
2:L:151:ALA:O	2:L:153:ILE:N	2.54	0.41
2:H:49:ILE:O	2:H:89:GLY:HA3	2.21	0.41
1:D:4:TYR:HB2	1:D:122:HIS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:105:ASN:C	2:I:106:PHE:CG	2.94	0.40
2:J:62:ALA:HA	2:J:66:ASP:OD1	2.21	0.40
2:K:52:GLY:O	2:K:88:ALA:HB2	2.20	0.40
2:K:121:ARG:H	2:K:121:ARG:HG2	1.78	0.40
1:A:150:ARG:HA	1:A:213:PHE:O	2.21	0.40
1:A:195:PRO:HG2	1:A:198:LEU:HD12	2.03	0.40
1:C:254:ILE:O	1:C:258:VAL:HG23	2.20	0.40
2:L:135:LEU:CD2	2:L:150:ALA:HB2	2.39	0.40
2:I:131:PHE:CD1	2:I:132:ILE:O	2.74	0.40
2:L:154:ARG:CG	2:L:154:ARG:O	2.69	0.40
1:D:241:ILE:HG22	1:D:242:PHE:CG	2.57	0.40
1:A:185:VAL:HG12	1:A:196:ILE:CD1	2.52	0.40
1:C:67:PRO:HB3	1:C:99:LEU:HD22	2.02	0.40
2:K:170:ALA:HB3	2:K:184:ALA:HB3	2.03	0.40
2:I:131:PHE:O	2:I:132:ILE:HG12	2.20	0.40
1:F:10:ILE:C	1:F:12:LEU:N	2.70	0.40
2:I:137:ILE:HG21	2:I:144:PHE:CE2	2.55	0.40
1:B:195:PRO:HG2	1:B:198:LEU:HD12	2.03	0.40
1:D:7:ASN:N	1:D:7:ASN:ND2	2.69	0.40
1:B:150:ARG:HA	1:B:213:PHE:O	2.21	0.40
2:G:96:ASN:HB3	2:G:118:THR:HG23	2.04	0.40
1:E:10:ILE:CG2	1:E:14:HIS:HD2	2.35	0.40
1:D:14:HIS:O	1:D:18:GLU:HG2	2.21	0.40
1:D:150:ARG:HA	1:D:213:PHE:O	2.22	0.40
1:C:65:VAL:HG12	1:C:66:ASP:N	2.36	0.40

All (7) 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)
2:H:101:LYS:CE	2:J:70:ASN:O[8_445]	1.34	0.86
1:E:35:LYS:NZ	2:J:78:VAL:CG2[8_445]	1.49	0.71
1:E:68:LEU:CD2	2:J:95:LYS:NZ[8_445]	1.96	0.24
2:H:101:LYS:CE	2:J:70:ASN:C[8_445]	2.03	0.17
2:H:101:LYS:CD	2:J:70:ASN:O[8_445]	2.04	0.16
1:E:68:LEU:CD2	2:J:95:LYS:CE[8_445]	2.12	0.08
2:G:67:THR:OG1	2:J:101:LYS:CE[8_445]	2.14	0.06

## 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	280/282 (99%)	269 (96%)	9 (3%)	2 (1%)	26	72
1	B	280/282 (99%)	270 (96%)	8 (3%)	2 (1%)	26	72
1	C	280/282 (99%)	269 (96%)	9 (3%)	2 (1%)	26	72
1	D	280/282 (99%)	269 (96%)	9 (3%)	2 (1%)	26	72
1	E	280/282 (99%)	269 (96%)	9 (3%)	2 (1%)	26	72
1	F	280/282 (99%)	270 (96%)	9 (3%)	1 (0%)	39	79
2	G	215/217 (99%)	186 (86%)	17 (8%)	12 (6%)	2	26
2	H	215/217 (99%)	189 (88%)	15 (7%)	11 (5%)	2	28
2	I	215/217 (99%)	186 (86%)	18 (8%)	11 (5%)	2	28
2	J	215/217 (99%)	188 (87%)	16 (7%)	11 (5%)	2	28
2	K	215/217 (99%)	188 (87%)	16 (7%)	11 (5%)	2	28
2	L	215/217 (99%)	185 (86%)	18 (8%)	12 (6%)	2	26
All	All	2970/2994 (99%)	2738 (92%)	153 (5%)	79 (3%)	6	46

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	TYR
1	B	4	TYR
1	C	4	TYR
1	D	4	TYR
1	E	4	TYR
1	F	4	TYR
2	G	87	CYS
2	G	143	ALA
2	H	87	CYS
2	I	87	CYS
2	I	143	ALA
2	J	87	CYS

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Mol	Chain	Res	Type
2	K	87	CYS
2	L	87	CYS
2	L	143	ALA
2	G	12	GLN
2	G	55	THR
2	G	125	GLY
2	G	147	ASP
2	G	152	CYS
2	H	12	GLN
2	H	122	ASN
2	H	125	GLY
2	H	147	ASP
2	H	152	CYS
2	I	12	GLN
2	I	55	THR
2	I	125	GLY
2	I	147	ASP
2	I	152	CYS
2	J	12	GLN
2	J	55	THR
2	J	122	ASN
2	J	125	GLY
2	J	147	ASP
2	J	152	CYS
2	K	12	GLN
2	K	122	ASN
2	K	125	GLY
2	K	147	ASP
2	K	152	CYS
2	L	12	GLN
2	L	55	THR
2	L	125	GLY
2	L	147	ASP
2	L	152	CYS
2	G	17	PRO
2	G	122	ASN
2	G	176	SER
2	H	55	THR
2	H	130	SER
2	H	143	ALA
2	I	17	PRO
2	I	122	ASN

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Mol	Chain	Res	Type
2	I	176	SER
2	J	17	PRO
2	J	143	ALA
2	J	176	SER
2	K	55	THR
2	K	143	ALA
2	L	17	PRO
2	L	122	ASN
2	L	176	SER
2	G	188	ASN
2	H	17	PRO
2	I	188	ASN
2	K	17	PRO
2	K	176	SER
2	L	188	ASN
1	C	60	GLY
1	E	60	GLY
2	H	176	SER
2	K	130	SER
1	A	60	GLY
2	J	130	SER
1	D	60	GLY
2	L	50	PRO
2	G	50	PRO
1	B	60	GLY

### 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	234/234 (100%)	220 (94%)	14 (6%)	24	65
1	B	234/234 (100%)	220 (94%)	14 (6%)	24	65
1	C	234/234 (100%)	219 (94%)	15 (6%)	22	63
1	D	234/234 (100%)	220 (94%)	14 (6%)	24	65
1	E	234/234 (100%)	220 (94%)	14 (6%)	24	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	234/234 (100%)	220 (94%)	14 (6%)	24	65
2	G	189/192 (98%)	166 (88%)	23 (12%)	6	33
2	H	189/192 (98%)	165 (87%)	24 (13%)	5	31
2	I	189/192 (98%)	165 (87%)	24 (13%)	5	31
2	J	189/192 (98%)	166 (88%)	23 (12%)	6	33
2	K	189/192 (98%)	164 (87%)	25 (13%)	5	30
2	L	189/192 (98%)	164 (87%)	25 (13%)	5	30
All	All	2538/2556 (99%)	2309 (91%)	229 (9%)	12	49

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	10	ILE
1	A	11	LEU
1	A	19	MET
1	A	31	VAL
1	A	50	ASN
1	A	51	ILE
1	A	54	GLU
1	A	57	ASN
1	A	97	GLU
1	A	125	LYS
1	A	197	ASP
1	A	239	SER
1	A	276	LYS
1	B	7	ASN
1	B	10	ILE
1	B	11	LEU
1	B	19	MET
1	B	31	VAL
1	B	50	ASN
1	B	51	ILE
1	B	54	GLU
1	B	57	ASN
1	B	97	GLU
1	B	125	LYS
1	B	197	ASP
1	B	239	SER
1	B	276	LYS

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Mol	Chain	Res	Type
1	C	7	ASN
1	C	10	ILE
1	C	11	LEU
1	C	19	MET
1	C	31	VAL
1	C	50	ASN
1	C	51	ILE
1	C	54	GLU
1	C	57	ASN
1	C	97	GLU
1	C	125	LYS
1	C	197	ASP
1	C	239	SER
1	C	241	ILE
1	C	276	LYS
1	D	7	ASN
1	D	10	ILE
1	D	11	LEU
1	D	19	MET
1	D	31	VAL
1	D	50	ASN
1	D	51	ILE
1	D	54	GLU
1	D	57	ASN
1	D	97	GLU
1	D	125	LYS
1	D	197	ASP
1	D	239	SER
1	D	276	LYS
1	E	7	ASN
1	E	10	ILE
1	E	11	LEU
1	E	19	MET
1	E	31	VAL
1	E	50	ASN
1	E	51	ILE
1	E	54	GLU
1	E	57	ASN
1	E	97	GLU
1	E	125	LYS
1	E	197	ASP
1	E	239	SER

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Mol	Chain	Res	Type
1	E	276	LYS
1	F	7	ASN
1	F	10	ILE
1	F	11	LEU
1	F	19	MET
1	F	31	VAL
1	F	50	ASN
1	F	51	ILE
1	F	54	GLU
1	F	57	ASN
1	F	97	GLU
1	F	125	LYS
1	F	197	ASP
1	F	239	SER
1	F	276	LYS
2	G	11	LEU
2	G	15	PHE
2	G	21	HIS
2	G	53	GLU
2	G	54	SER
2	G	55	THR
2	G	99	ASN
2	G	102	LEU
2	G	103	TYR
2	G	105	ASN
2	G	109	LYS
2	G	110	PHE
2	G	119	ILE
2	G	120	CYS
2	G	121	ARG
2	G	128	ASN
2	G	130	SER
2	G	134	SER
2	G	135	LEU
2	G	136	ASN
2	G	146	LYS
2	G	154	ARG
2	G	176	SER
2	H	11	LEU
2	H	15	PHE
2	H	21	HIS
2	H	53	GLU

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Mol	Chain	Res	Type
2	H	54	SER
2	H	55	THR
2	H	99	ASN
2	H	102	LEU
2	H	103	TYR
2	H	105	ASN
2	H	109	LYS
2	H	119	ILE
2	H	120	CYS
2	H	121	ARG
2	H	128	ASN
2	H	129	ASP
2	H	130	SER
2	H	133	CYS
2	H	134	SER
2	H	135	LEU
2	H	136	ASN
2	H	146	LYS
2	H	154	ARG
2	H	176	SER
2	I	11	LEU
2	I	15	PHE
2	I	21	HIS
2	I	53	GLU
2	I	54	SER
2	I	55	THR
2	I	99	ASN
2	I	102	LEU
2	I	103	TYR
2	I	105	ASN
2	I	109	LYS
2	I	110	PHE
2	I	119	ILE
2	I	120	CYS
2	I	121	ARG
2	I	128	ASN
2	I	129	ASP
2	I	130	SER
2	I	134	SER
2	I	135	LEU
2	I	136	ASN
2	I	146	LYS

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Mol	Chain	Res	Type
2	I	154	ARG
2	I	176	SER
2	J	11	LEU
2	J	15	PHE
2	J	18	HIS
2	J	21	HIS
2	J	53	GLU
2	J	54	SER
2	J	55	THR
2	J	99	ASN
2	J	102	LEU
2	J	103	TYR
2	J	105	ASN
2	J	109	LYS
2	J	119	ILE
2	J	121	ARG
2	J	128	ASN
2	J	129	ASP
2	J	130	SER
2	J	134	SER
2	J	135	LEU
2	J	136	ASN
2	J	146	LYS
2	J	154	ARG
2	J	176	SER
2	K	11	LEU
2	K	12	GLN
2	K	15	PHE
2	K	18	HIS
2	K	21	HIS
2	K	53	GLU
2	K	54	SER
2	K	55	THR
2	K	99	ASN
2	K	102	LEU
2	K	103	TYR
2	K	105	ASN
2	K	109	LYS
2	K	119	ILE
2	K	120	CYS
2	K	121	ARG
2	K	128	ASN

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Mol	Chain	Res	Type
2	K	129	ASP
2	K	130	SER
2	K	134	SER
2	K	135	LEU
2	K	136	ASN
2	K	146	LYS
2	K	154	ARG
2	K	176	SER
2	L	11	LEU
2	L	15	PHE
2	L	18	HIS
2	L	21	HIS
2	L	53	GLU
2	L	54	SER
2	L	55	THR
2	L	99	ASN
2	L	102	LEU
2	L	103	TYR
2	L	105	ASN
2	L	109	LYS
2	L	110	PHE
2	L	119	ILE
2	L	120	CYS
2	L	121	ARG
2	L	128	ASN
2	L	129	ASP
2	L	130	SER
2	L	134	SER
2	L	135	LEU
2	L	136	ASN
2	L	146	LYS
2	L	154	ARG
2	L	176	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	14	HIS
1	A	50	ASN
1	A	269	ASN
1	A	281	ASN

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Mol	Chain	Res	Type
1	B	7	ASN
1	B	14	HIS
1	B	50	ASN
1	B	281	ASN
1	C	7	ASN
1	C	14	HIS
1	C	50	ASN
1	C	269	ASN
1	C	279	HIS
1	C	281	ASN
1	D	14	HIS
1	D	50	ASN
1	D	269	ASN
1	D	281	ASN
1	E	7	ASN
1	E	14	HIS
1	E	50	ASN
1	E	279	HIS
1	E	281	ASN
1	F	14	HIS
1	F	50	ASN
1	F	281	ASN
2	G	12	GLN
2	G	74	HIS
2	G	108	ASN
2	G	128	ASN
2	G	196	ASN
2	G	202	HIS
2	H	12	GLN
2	H	202	HIS
2	I	12	GLN
2	I	108	ASN
2	I	202	HIS
2	J	12	GLN
2	J	128	ASN
2	J	196	ASN
2	J	202	HIS
2	K	12	GLN
2	K	128	ASN
2	K	202	HIS
2	L	12	GLN
2	L	74	HIS

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Mol	Chain	Res	Type
2	L	108	ASN
2	L	128	ASN
2	L	202	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 ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PO4	A	301	-	4,4,4	0.74	0	6,6,6	0.27	0
3	PO4	A	302	-	4,4,4	0.44	0	6,6,6	0.28	0
3	PO4	B	301	-	4,4,4	0.74	0	6,6,6	0.27	0
3	PO4	B	302	-	4,4,4	0.51	0	6,6,6	0.29	0
3	PO4	C	301	-	4,4,4	0.92	0	6,6,6	0.27	0
3	PO4	C	302	-	4,4,4	0.49	0	6,6,6	0.29	0
3	PO4	D	301	-	4,4,4	0.66	0	6,6,6	0.27	0
3	PO4	D	302	-	4,4,4	0.85	0	6,6,6	0.30	0
3	PO4	E	301	-	4,4,4	0.81	0	6,6,6	0.27	0
3	PO4	E	302	-	4,4,4	0.70	0	6,6,6	0.29	0
3	PO4	F	301	-	4,4,4	0.70	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	F	302	-	4,4,4	0.75	0	6,6,6	0.28	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	A	301	-	-	0/0/0/0	0/0/0/0
3	PO4	A	302	-	-	0/0/0/0	0/0/0/0
3	PO4	B	301	-	-	0/0/0/0	0/0/0/0
3	PO4	B	302	-	-	0/0/0/0	0/0/0/0
3	PO4	C	301	-	-	0/0/0/0	0/0/0/0
3	PO4	C	302	-	-	0/0/0/0	0/0/0/0
3	PO4	D	301	-	-	0/0/0/0	0/0/0/0
3	PO4	D	302	-	-	0/0/0/0	0/0/0/0
3	PO4	E	301	-	-	0/0/0/0	0/0/0/0
3	PO4	E	302	-	-	0/0/0/0	0/0/0/0
3	PO4	F	301	-	-	0/0/0/0	0/0/0/0
3	PO4	F	302	-	-	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.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	282/282 (100%)	-0.16	7 (2%) 61 46	59, 81, 111, 129	0
1	B	282/282 (100%)	-0.21	7 (2%) 61 46	59, 81, 109, 127	0
1	C	282/282 (100%)	-0.21	5 (1%) 71 57	58, 78, 109, 128	0
1	D	282/282 (100%)	-0.19	5 (1%) 71 57	58, 80, 114, 135	0
1	E	282/282 (100%)	-0.14	3 (1%) 82 70	56, 77, 107, 126	0
1	F	282/282 (100%)	-0.17	6 (2%) 67 52	59, 80, 112, 128	0
2	G	217/217 (100%)	0.49	15 (6%) 20 13	87, 118, 167, 199	0
2	H	217/217 (100%)	0.33	14 (6%) 22 15	60, 98, 158, 188	0
2	I	217/217 (100%)	0.90	34 (15%) 3 3	83, 123, 187, 223	0
2	J	217/217 (100%)	0.16	3 (1%) 78 65	57, 88, 142, 195	0
2	K	217/217 (100%)	0.85	18 (8%) 14 10	76, 110, 165, 200	0
2	L	217/217 (100%)	1.39	50 (23%) 1 1	90, 109, 141, 161	217 (100%)
All	All	2994/2994 (100%)	0.20	167 (5%) 28 19	56, 91, 147, 223	217 (7%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	116	ASP	8.4
1	E	6	ASP	5.5
2	L	164	ASP	5.2
2	L	122	ASN	5.2
2	L	101	LYS	4.9
2	I	184	ALA	4.9
2	L	3	GLU	4.8
2	K	116	ASP	4.7
2	K	85	GLY	4.7
2	L	136	ASN	4.6
2	I	96	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	57	ASN	4.5
2	L	118	THR	4.5
1	B	53	SER	4.3
2	H	140	ASP	4.3
1	C	54	GLU	4.2
2	K	152	CYS	4.1
2	I	105	ASN	4.1
1	A	3	ASP	4.1
1	C	284	ALA	4.0
1	A	54	GLU	4.0
1	C	53	SER	4.0
2	I	147	ASP	3.9
2	L	108	ASN	3.9
2	L	152	CYS	3.8
2	K	182	ILE	3.7
2	I	186	GLU	3.7
2	L	147	ASP	3.7
2	I	107	GLY	3.7
2	H	202	HIS	3.7
2	L	109	LYS	3.6
2	I	60	CYS	3.6
1	D	6	ASP	3.6
2	L	120	CYS	3.6
2	L	210	TYR	3.6
2	L	121	ARG	3.6
1	A	53	SER	3.5
2	L	160	GLU	3.5
1	F	3	ASP	3.5
2	H	147	ASP	3.5
2	L	117	ILE	3.5
1	B	54	GLU	3.4
2	I	152	CYS	3.4
2	L	30	LEU	3.4
2	L	39	HIS	3.4
2	L	119	ILE	3.4
2	K	165	GLU	3.3
2	L	82	PRO	3.3
1	B	3	ASP	3.3
2	H	139	SER	3.3
1	F	55	LEU	3.3
1	D	3	ASP	3.3
1	B	57	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	79	LEU	3.2
2	L	162	LEU	3.2
1	F	57	ASN	3.2
2	H	175	GLU	3.1
2	I	190	CYS	3.1
2	I	183	ALA	3.1
2	L	45	ASP	3.1
2	J	152	CYS	3.0
2	H	148	LEU	3.0
2	G	206	GLN	3.0
2	G	147	ASP	3.0
2	L	142	SER	3.0
2	I	187	GLN	3.0
2	K	140	ASP	2.9
2	I	185	VAL	2.9
1	A	50	ASN	2.9
1	E	3	ASP	2.9
1	C	50	ASN	2.9
2	K	175	GLU	2.9
2	I	116	ASP	2.9
2	L	134	SER	2.9
2	L	158	ILE	2.9
2	I	94	SER	2.8
1	E	57	ASN	2.8
2	K	205	PHE	2.8
1	A	55	LEU	2.8
2	H	128	ASN	2.8
2	L	128	ASN	2.8
2	L	163	SER	2.8
2	H	149	THR	2.8
2	I	29	SER	2.7
2	H	134	SER	2.7
2	I	166	VAL	2.7
2	L	61	CYS	2.7
2	I	101	LYS	2.7
2	L	4	ILE	2.7
2	H	102	LEU	2.7
2	G	131	PHE	2.6
1	F	284	ALA	2.6
2	L	146	LYS	2.6
1	B	6	ASP	2.6
1	D	5	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	146	LYS	2.6
2	H	135	LEU	2.6
1	A	284	ALA	2.6
1	F	53	SER	2.6
2	L	216	TYR	2.6
2	G	128	ASN	2.6
2	I	163	SER	2.5
2	K	144	PHE	2.5
2	I	98	GLU	2.5
2	I	170	ALA	2.5
1	D	57	ASN	2.4
2	G	150	ALA	2.4
2	G	175	GLU	2.4
2	K	183	ALA	2.4
2	I	167	LYS	2.4
1	F	54	GLU	2.4
2	L	7	GLY	2.4
2	I	146	LYS	2.4
2	L	174	HIS	2.4
2	I	106	PHE	2.3
2	K	60	CYS	2.3
2	L	75	PHE	2.3
2	L	131	PHE	2.3
2	L	180	ASN	2.3
1	B	284	ALA	2.3
2	K	150	ALA	2.3
2	K	202	HIS	2.3
2	K	107	GLY	2.3
2	L	144	PHE	2.3
2	G	213	VAL	2.3
2	I	97	VAL	2.3
2	L	40	ASP	2.3
2	H	133	CYS	2.3
2	I	120	CYS	2.3
2	I	202	HIS	2.3
2	L	129	ASP	2.3
2	G	202	HIS	2.3
2	K	131	PHE	2.2
2	I	119	ILE	2.2
2	I	191	LEU	2.2
2	G	173	SER	2.2
2	I	140	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	40	ASP	2.2
2	I	164	ASP	2.2
2	L	102	LEU	2.2
2	I	150	ALA	2.2
2	L	52	GLY	2.2
2	K	190	CYS	2.2
2	G	183	ALA	2.2
2	J	64	GLU	2.2
2	G	4	ILE	2.1
2	I	162	LEU	2.1
1	D	7	ASN	2.1
2	G	184	ALA	2.1
1	B	55	LEU	2.1
2	I	195	PHE	2.1
2	K	146	LYS	2.1
2	G	30	LEU	2.1
2	L	133	CYS	2.1
2	L	189	ASN	2.1
2	L	25	LEU	2.1
2	H	25	LEU	2.1
2	I	128	ASN	2.1
2	G	152	CYS	2.1
2	J	147	ASP	2.0
2	L	66	ASP	2.0
2	L	137	ILE	2.0
2	L	161	ILE	2.0
2	L	78	VAL	2.0
1	C	6	ASP	2.0
2	L	140	ASP	2.0
2	H	122	ASN	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
3	PO4	D	302	5/5	0.93	0.29	1.00	73,74,78,79	0
3	PO4	F	302	5/5	0.94	0.20	-0.14	74,76,79,82	0
3	PO4	A	302	5/5	0.92	0.19	-0.80	78,80,83,86	0
3	PO4	E	302	5/5	0.95	0.18	-0.94	72,74,76,78	0
3	PO4	C	301	5/5	0.96	0.21	-1.12	78,80,82,83	0
3	PO4	B	302	5/5	0.93	0.17	-1.33	75,76,80,82	0
3	PO4	C	302	5/5	0.95	0.12	-1.47	74,75,79,80	0
3	PO4	B	301	5/5	0.96	0.17	-1.51	75,77,79,79	0
3	PO4	A	301	5/5	0.93	0.18	-1.71	74,76,79,79	0
3	PO4	E	301	5/5	0.93	0.17	-2.04	76,78,80,80	0
3	PO4	D	301	5/5	0.96	0.13	-2.38	79,81,83,83	0
3	PO4	F	301	5/5	0.94	0.18	-3.67	73,75,76,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.