



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:13 PM GMT

PDB ID : 3TAI  
Title : Crystal structure of NurA  
Authors : Chae, J.; Kim, Y.C.; Cho, Y.  
Deposited on : 2011-08-04  
Resolution : 2.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

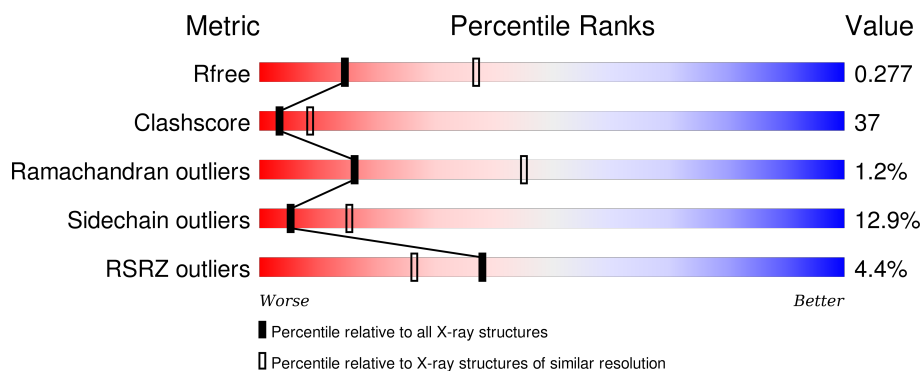
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	471	<div> <div>2%</div> <div>43%</div> <div>41%</div> <div>7%</div> <div>9%</div> </div>
1	B	471	<div> <div>6%</div> <div>38%</div> <div>46%</div> <div>8%</div> <div>9%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	452	-	-	-	X
2	GOL	A	454	-	-	-	X
2	GOL	A	455	-	-	X	-
2	GOL	A	456	-	-	-	X
2	GOL	A	457	-	-	-	X
2	GOL	B	452	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7002 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 DNA double-strand break repair protein nurA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	Se	0	0	0
			3471	2223	595	646	7			
1	B	430	Total	C	N	O	Se	0	0	0
			3470	2223	594	646	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
A	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
A	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
A	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
A	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
A	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
A	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
A	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
A	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-19	MSE	-	EXPRESSION TAG	UNP Q8U1N8
B	-18	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-17	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-16	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-15	HIS	-	EXPRESSION TAG	UNP Q8U1N8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-13	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-12	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-11	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-10	HIS	-	EXPRESSION TAG	UNP Q8U1N8
B	-9	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-8	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	-7	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-6	LEU	-	EXPRESSION TAG	UNP Q8U1N8
B	-5	VAL	-	EXPRESSION TAG	UNP Q8U1N8
B	-4	PRO	-	EXPRESSION TAG	UNP Q8U1N8
B	-3	ARG	-	EXPRESSION TAG	UNP Q8U1N8
B	-2	GLY	-	EXPRESSION TAG	UNP Q8U1N8
B	-1	SER	-	EXPRESSION TAG	UNP Q8U1N8
B	0	HIS	-	EXPRESSION TAG	UNP Q8U1N8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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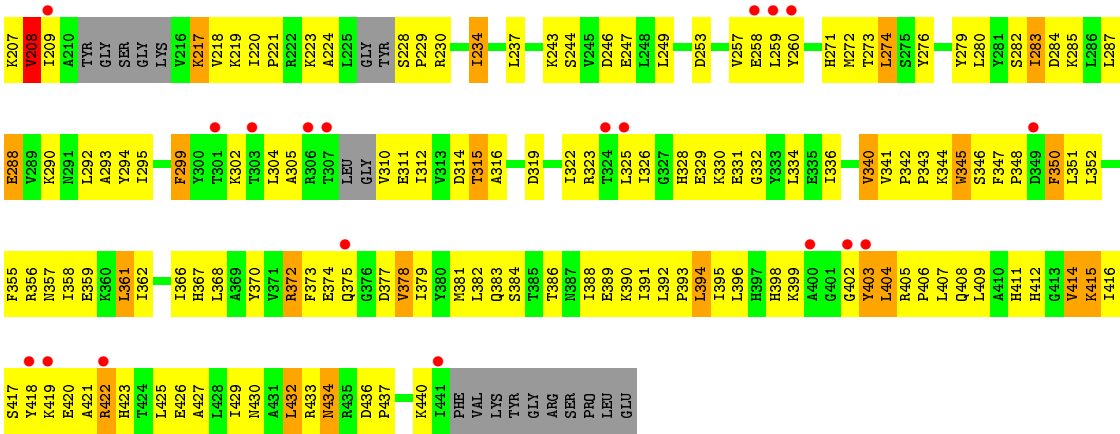
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	4	Total	O	0	0
			4	4		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.00Å 114.21Å 122.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.82 31.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.55-2.82) 89.0 (31.73-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.202 , 0.276 0.206 , 0.277	Depositor DCC
$R_{free}$ test set	1118 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 71.2	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 32315 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GOL

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	0/3523	0.72	1/4741 (0.0%)
1	B	0.46	0/3520	0.66	0/4738
All	All	0.49	0/7043	0.69	1/9479 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	62	THR	N-CA-C	5.19	125.02	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain

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

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3471	0	3587	271	0
1	B	3470	0	3586	295	0
2	A	36	0	48	9	0
2	B	6	0	8	2	0
3	A	15	0	0	3	0
3	B	4	0	0	0	0
All	All	7002	0	7229	522	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 37.

All (522) 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:A:54:ARG:HB3	1:A:101:MSE:HE3	1.26	1.11
1:A:138:VAL:HG13	1:A:142:ASP:OD1	1.54	1.07
1:B:347:PHE:HB3	1:B:352:LEU:HD11	1.37	1.05
1:A:135:ARG:NH2	1:B:90:TYR:HB2	1.73	1.04
1:B:67:LEU:HD22	1:B:101:MSE:HE2	1.39	1.03
1:A:54:ARG:HB3	1:A:101:MSE:CE	1.92	0.99
1:B:139:TYR:HB3	1:B:140:PRO:HD3	1.43	0.98
1:B:54:ARG:HB3	1:B:101:MSE:CE	1.94	0.97
1:A:67:LEU:HD22	1:A:101:MSE:HE2	1.43	0.97
1:B:50:VAL:HG13	1:B:125:MSE:HE1	1.48	0.96
1:B:345:TRP:HD1	1:B:346:SER:N	1.63	0.96
1:B:404:LEU:H	1:B:404:LEU:HD12	1.31	0.95
1:A:135:ARG:HH21	1:B:90:TYR:HB2	1.25	0.94
1:B:29:ILE:HG21	1:B:33:ILE:HG13	1.47	0.94
1:B:54:ARG:HB3	1:B:101:MSE:HE3	1.48	0.93
1:A:61:GLY:O	1:A:88:SER:HB2	1.68	0.93
1:A:425:LEU:HD11	1:B:12:ILE:HD13	1.52	0.90
1:A:440:LYS:NZ	1:B:378:VAL:HG22	1.87	0.88
1:A:67:LEU:HD22	1:A:101:MSE:CE	2.03	0.88
1:B:50:VAL:HG13	1:B:125:MSE:CE	2.03	0.88
1:B:50:VAL:CG1	1:B:125:MSE:HE1	2.05	0.87
1:A:139:TYR:OH	1:A:346:SER:HA	1.73	0.86
1:A:135:ARG:HH22	1:B:90:TYR:H	1.24	0.85
1:B:423:HIS:O	1:B:427:ALA:HB2	1.76	0.84
1:B:129:LEU:HG	1:B:294:TYR:CE2	2.12	0.84
1:B:29:ILE:HG13	1:B:33:ILE:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLY:O	1:A:88:SER:CB	2.26	0.83
1:B:54:ARG:CB	1:B:101:MSE:HE3	2.10	0.81
1:B:123:ILE:CG2	1:B:125:MSE:HE3	2.09	0.81
1:B:350:PHE:HD2	1:B:350:PHE:H	1.28	0.81
1:A:141:GLU:O	1:A:144:ARG:HG2	1.79	0.81
1:A:313:VAL:HG12	1:A:314:ASP:H	1.45	0.81
1:A:301:THR:HG22	1:A:303:THR:H	1.46	0.81
1:B:345:TRP:CD1	1:B:346:SER:N	2.48	0.80
1:A:301:THR:H	1:A:304:LEU:HG	1.44	0.80
1:B:422:ARG:HG3	1:B:423:HIS:N	1.96	0.80
1:A:162:LEU:HD21	1:A:354:LYS:HG3	1.62	0.80
1:B:201:LYS:HA	1:B:205:ASP:HB2	1.64	0.80
1:B:138:VAL:HG12	1:B:141:GLU:HB2	1.62	0.80
1:A:138:VAL:HA	1:A:142:ASP:OD2	1.82	0.80
1:A:223:LYS:H	1:A:223:LYS:HD2	1.46	0.80
1:A:136:PRO:HD2	1:A:139:TYR:CE2	2.18	0.79
1:A:436:ASP:HB2	1:A:437:PRO:HD3	1.64	0.78
1:A:386:THR:OG1	1:A:391:ILE:HD11	1.84	0.78
1:A:418:TYR:HD1	1:A:419:LYS:H	1.32	0.78
1:B:7:GLN:HG3	1:B:8:SER:H	1.47	0.77
1:B:422:ARG:HE	1:B:423:HIS:HD2	1.33	0.77
1:A:419:LYS:C	1:A:421:ALA:H	1.89	0.76
1:A:401:GLY:C	1:A:403:TYR:H	1.86	0.76
1:A:440:LYS:HZ1	1:B:378:VAL:HG22	1.46	0.76
1:B:422:ARG:HG3	1:B:423:HIS:H	1.49	0.75
1:A:11:ARG:NH1	1:B:82:TYR:OH	2.20	0.75
1:B:336:ILE:HD11	1:B:370:TYR:CE2	2.21	0.75
1:A:299:PHE:CZ	1:A:381:MSE:HE3	2.22	0.74
1:B:30:ARG:O	1:B:31:ASN:HB3	1.87	0.74
1:B:107:MSE:HE1	1:B:176:VAL:HG21	1.69	0.74
1:B:404:LEU:N	1:B:404:LEU:HD12	2.01	0.74
1:B:329:GLU:HG2	1:B:329:GLU:O	1.86	0.73
1:B:139:TYR:HB3	1:B:140:PRO:CD	2.18	0.73
1:B:326:ILE:HG22	1:B:328:HIS:NE2	2.03	0.73
1:A:347:PHE:HB3	1:A:352:LEU:HD11	1.70	0.73
1:A:49:ALA:HB1	1:A:407:LEU:HD13	1.70	0.73
1:A:172:HIS:O	1:A:176:VAL:HG23	1.90	0.72
1:A:316:ALA:HB2	1:B:440:LYS:HG3	1.71	0.72
1:B:92:THR:O	1:B:96:ILE:HG12	1.89	0.72
1:B:136:PRO:HG2	1:B:139:TYR:HD1	1.55	0.72
1:A:440:LYS:HE2	1:B:315:THR:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:C	1:A:138:VAL:H	1.93	0.72
1:B:220:ILE:HB	1:B:221:PRO:HD2	1.72	0.71
1:B:67:LEU:CD2	1:B:101:MSE:HE2	2.18	0.71
1:B:130:THR:H	1:B:383:GLN:HE22	1.39	0.70
1:B:419:LYS:NZ	1:B:421:ALA:HB3	2.06	0.70
1:A:222:ARG:HD2	1:A:255:GLU:HG3	1.73	0.70
1:A:299:PHE:H	1:A:299:PHE:HD1	1.41	0.69
1:A:301:THR:N	1:A:304:LEU:HG	2.05	0.69
1:B:422:ARG:O	1:B:426:GLU:HG3	1.90	0.69
1:B:193:ASP:OD1	1:B:271:HIS:HE1	1.74	0.69
1:B:95:GLN:HB3	1:B:138:VAL:HG22	1.74	0.69
1:A:11:ARG:NH2	3:A:469:HOH:O	2.25	0.69
1:B:423:HIS:O	1:B:427:ALA:CB	2.41	0.69
1:B:287:LEU:HD22	1:B:361:LEU:HD13	1.73	0.69
1:B:386:THR:OG1	1:B:391:ILE:HD11	1.92	0.69
1:A:135:ARG:HH12	1:A:301:THR:HG21	1.58	0.68
1:B:305:ALA:HA	1:B:310:VAL:O	1.92	0.68
1:B:123:ILE:HG22	1:B:125:MSE:HE3	1.74	0.68
1:B:146:LEU:CD1	1:B:273:THR:HG23	2.23	0.68
1:A:249:LEU:HD21	1:B:237:LEU:HB3	1.75	0.68
1:A:316:ALA:HA	1:B:440:LYS:HE3	1.74	0.68
1:B:19:GLU:O	1:B:23:VAL:HB	1.94	0.68
1:A:27:GLU:CG	1:A:28:GLN:H	2.07	0.68
1:B:319:ASP:OD2	1:B:372:ARG:NH1	2.26	0.68
1:A:135:ARG:NH1	1:A:301:THR:HG21	2.10	0.67
1:B:299:PHE:CE2	1:B:381:MSE:HG2	2.28	0.67
1:B:398:HIS:HB3	1:B:406:PRO:HD3	1.76	0.67
1:A:175:LYS:O	1:A:179:HIS:HD2	1.77	0.67
1:B:168:LYS:HD3	1:B:195:VAL:HG21	1.77	0.67
1:B:347:PHE:CB	1:B:352:LEU:HD11	2.22	0.66
1:B:336:ILE:HD11	1:B:370:TYR:HE2	1.61	0.66
1:A:419:LYS:O	1:A:421:ALA:N	2.29	0.66
1:A:132:SER:HB2	2:A:455:GOL:O2	1.96	0.66
1:A:374:GLU:HB2	1:A:402:GLY:HA2	1.78	0.66
1:A:136:PRO:HG2	1:A:138:VAL:HB	1.77	0.66
1:B:419:LYS:HB3	1:B:422:ARG:HB3	1.75	0.66
1:B:404:LEU:CD1	1:B:404:LEU:H	2.05	0.66
1:B:244:SER:OG	1:B:247:GLU:HG3	1.94	0.66
1:B:345:TRP:HD1	1:B:346:SER:H	1.41	0.66
1:A:298:SER:HB2	1:B:60:SER:HA	1.78	0.66
1:A:146:LEU:HD21	1:A:351:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:O	1:A:23:VAL:HG23	1.96	0.65
1:B:374:GLU:OE2	1:B:402:GLY:HA2	1.96	0.65
1:B:36:TRP:CZ2	1:B:332:GLY:HA3	2.31	0.65
1:A:138:VAL:CG2	1:A:276:TYR:HE1	2.09	0.65
1:A:420:GLU:O	1:A:424:THR:HG23	1.96	0.65
1:B:350:PHE:CD2	1:B:350:PHE:N	2.63	0.65
1:A:420:GLU:HG3	1:A:424:THR:CG2	2.27	0.65
1:A:102:GLU:OE1	2:A:455:GOL:H31	1.97	0.65
1:A:27:GLU:HG2	1:A:28:GLN:H	1.61	0.65
1:A:419:LYS:C	1:A:421:ALA:N	2.46	0.65
1:A:32:ILE:HG13	1:A:334:LEU:HD11	1.79	0.65
1:A:142:ASP:HB3	1:A:272:MSE:SE	2.48	0.65
1:A:314:ASP:OD1	1:B:60:SER:HB3	1.96	0.65
1:B:129:LEU:O	1:B:133:LEU:HG	1.97	0.64
1:B:395:ILE:HG23	1:B:404:LEU:HD21	1.80	0.64
1:B:54:ARG:CG	1:B:101:MSE:HE3	2.27	0.64
1:A:208:VAL:HG22	1:A:218:VAL:HG22	1.79	0.64
1:A:228:SER:N	1:A:229:PRO:HD3	2.12	0.64
1:A:116:LEU:HD23	1:A:121:ARG:HB3	1.79	0.64
1:B:395:ILE:CG2	1:B:404:LEU:HD21	2.27	0.64
1:A:149:MSE:HE1	1:A:204:ILE:HD11	1.81	0.63
1:A:139:TYR:OH	1:A:346:SER:CA	2.46	0.63
1:B:325:LEU:HD23	1:B:326:ILE:HD11	1.80	0.63
1:A:440:LYS:HE2	1:B:315:THR:HG23	1.80	0.63
1:A:223:LYS:NZ	1:A:230:ARG:HG2	2.13	0.63
1:A:195:VAL:CG1	1:A:199:LEU:HD22	2.28	0.63
1:A:316:ALA:CB	1:B:440:LYS:HG3	2.29	0.62
1:A:425:LEU:HD13	1:B:12:ILE:HG21	1.81	0.62
1:B:427:ALA:O	1:B:430:ASN:HB2	2.00	0.62
1:B:342:PRO:HD2	1:B:362:ILE:HA	1.80	0.62
1:B:416:ILE:HG13	1:B:417:SER:O	1.99	0.62
1:A:138:VAL:HG22	1:A:276:TYR:CE1	2.35	0.62
1:B:234:ILE:HD13	1:B:234:ILE:O	1.97	0.62
1:B:178:GLU:O	1:B:181:GLU:HG2	2.00	0.62
1:A:195:VAL:HG12	1:A:199:LEU:HD22	1.82	0.62
1:B:367:HIS:O	1:B:368:LEU:HD23	1.99	0.62
1:A:330:LYS:O	1:A:372:ARG:HD2	2.00	0.62
1:B:136:PRO:HD2	1:B:139:TYR:CD1	2.35	0.62
1:A:244:SER:OG	1:A:247:GLU:HG3	1.99	0.61
1:A:48:TYR:CD1	1:A:116:LEU:HD13	2.34	0.61
1:A:180:LEU:O	1:A:184:GLY:HA2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LEU:HD12	1:B:273:THR:HG23	1.82	0.61
1:A:88:SER:O	1:B:302:LYS:HE3	2.01	0.61
1:A:27:GLU:OE2	1:A:29:ILE:HG12	2.00	0.61
1:B:217:LYS:HZ2	1:B:260:TYR:HE2	1.47	0.61
1:A:138:VAL:CG2	1:A:276:TYR:CE1	2.84	0.60
1:A:99:MSE:HE2	1:A:137:PRO:HB2	1.82	0.60
1:B:419:LYS:HZ3	1:B:421:ALA:HB3	1.65	0.60
1:A:420:GLU:HG3	1:A:424:THR:HG23	1.83	0.60
1:A:144:ARG:HB2	1:B:230:ARG:HH21	1.67	0.60
1:A:440:LYS:HD3	1:B:316:ALA:HB2	1.84	0.60
1:A:299:PHE:N	1:A:299:PHE:CD1	2.69	0.60
1:B:129:LEU:HB3	1:B:366:ILE:HD13	1.84	0.60
1:B:33:ILE:HD13	1:B:326:ILE:HD11	1.83	0.59
1:B:7:GLN:HG3	1:B:8:SER:N	2.15	0.59
1:A:303:THR:O	1:A:307:THR:HG23	2.03	0.59
1:A:366:ILE:HG22	1:A:368:LEU:HD23	1.84	0.59
1:B:279:TYR:CZ	1:B:283:ILE:HD11	2.38	0.59
1:B:421:ALA:O	1:B:426:GLU:HG2	2.03	0.59
1:A:347:PHE:CB	1:A:352:LEU:HD11	2.33	0.59
1:A:301:THR:H	1:A:304:LEU:CG	2.15	0.59
1:A:354:LYS:O	2:A:452:GOL:H2	2.03	0.58
1:A:241:ARG:O	1:B:246:ASP:OD2	2.22	0.58
1:A:37:LYS:HB2	1:A:38:PRO:HD2	1.86	0.58
1:A:267:TYR:CD2	1:A:268:ASP:OD2	2.56	0.58
1:B:138:VAL:HG11	1:B:272:MSE:HE1	1.85	0.58
1:A:258:GLU:HG3	3:A:459:HOH:O	2.04	0.58
1:A:130:THR:O	1:A:134:VAL:HG12	2.03	0.58
1:B:54:ARG:HH22	1:B:98:ARG:NH2	2.01	0.58
1:A:48:TYR:CD1	1:A:112:ALA:HB1	2.39	0.58
1:B:434:ASN:HB3	1:B:437:PRO:HD2	1.87	0.57
1:B:425:LEU:O	1:B:429:ILE:HG13	2.03	0.57
1:B:18:ASP:O	1:B:22:ASN:HB2	2.03	0.57
1:B:29:ILE:O	1:B:30:ARG:HB2	2.03	0.57
1:B:219:LYS:HG3	1:B:258:GLU:HG2	1.84	0.57
1:A:60:SER:HB2	1:B:314:ASP:OD1	2.04	0.57
1:B:95:GLN:NE2	1:B:138:VAL:HA	2.19	0.57
1:A:240:SER:HB2	1:A:243:LYS:HD2	1.86	0.57
1:A:356:ARG:HD2	2:A:452:GOL:O3	2.05	0.57
1:B:299:PHE:CZ	1:B:381:MSE:HE3	2.39	0.57
1:B:183:ASN:HD22	1:B:183:ASN:N	2.02	0.57
1:B:146:LEU:HD21	1:B:351:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ILE:HG23	1:B:404:LEU:CD2	2.35	0.56
1:B:30:ARG:NH2	1:B:311:GLU:HB3	2.20	0.56
1:B:146:LEU:HD11	1:B:273:THR:HG23	1.88	0.56
1:B:323:ARG:CZ	1:B:329:GLU:HG3	2.36	0.56
1:B:392:LEU:HB3	1:B:393:PRO:HD3	1.88	0.56
1:A:54:ARG:HH22	1:A:98:ARG:NH2	2.03	0.56
1:A:313:VAL:HG12	1:A:314:ASP:N	2.19	0.56
1:A:61:GLY:O	1:A:88:SER:OG	2.24	0.56
1:A:425:LEU:O	1:A:429:ILE:HG23	2.06	0.56
1:A:208:VAL:HG13	1:A:216:VAL:HB	1.86	0.56
1:A:67:LEU:HA	1:A:101:MSE:HE1	1.88	0.56
1:A:130:THR:HG23	1:A:383:GLN:OE1	2.06	0.56
1:A:9:ILE:O	1:A:13:THR:HG23	2.06	0.56
1:A:43:GLU:O	1:A:397:HIS:HB2	2.06	0.55
1:B:65:TYR:OH	1:B:100:GLN:NE2	2.39	0.55
1:A:426:GLU:HG3	1:A:438:ALA:HB1	1.89	0.55
1:A:180:LEU:O	1:A:184:GLY:N	2.40	0.55
1:A:89:ASN:HB2	1:A:92:THR:HB	1.88	0.55
1:B:129:LEU:H	1:B:383:GLN:NE2	2.05	0.55
1:B:288:GLU:OE2	1:B:357:ASN:ND2	2.37	0.55
1:B:348:PRO:O	1:B:352:LEU:HD13	2.06	0.55
1:A:299:PHE:CG	1:A:300:TYR:N	2.74	0.55
1:A:299:PHE:N	1:A:299:PHE:HD1	2.03	0.55
1:A:340:VAL:HG23	1:A:366:ILE:HB	1.88	0.55
1:B:12:ILE:O	1:B:15:ILE:HG22	2.07	0.55
1:A:258:GLU:O	1:A:259:LEU:HD12	2.07	0.55
1:A:395:ILE:HG22	1:A:404:LEU:HD22	1.89	0.55
1:B:36:TRP:HZ2	1:B:331:GLU:O	1.89	0.55
1:A:307:THR:O	1:A:308:LEU:HB2	2.07	0.54
1:B:54:ARG:HG2	1:B:101:MSE:HE3	1.90	0.54
1:B:139:TYR:O	1:B:142:ASP:OD2	2.25	0.54
1:A:425:LEU:O	1:A:429:ILE:N	2.35	0.54
1:B:326:ILE:CG2	1:B:328:HIS:CE1	2.91	0.54
1:A:138:VAL:HG12	1:A:139:TYR:N	2.22	0.54
1:A:302:LYS:HD3	1:B:87:LYS:HE3	1.88	0.54
1:A:178:GLU:O	1:A:182:LYS:HG3	2.07	0.54
1:B:133:LEU:HD22	1:B:347:PHE:HZ	1.71	0.54
1:A:378:VAL:HG13	1:A:379:ILE:N	2.23	0.54
1:A:133:LEU:CD2	1:A:347:PHE:HZ	2.20	0.54
1:B:326:ILE:HG22	1:B:328:HIS:CE1	2.42	0.53
1:B:138:VAL:HG11	1:B:272:MSE:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TYR:CD1	1:B:116:LEU:HD13	2.44	0.53
1:A:81:SER:O	1:A:189:PRO:HD3	2.08	0.53
1:B:367:HIS:C	1:B:368:LEU:HD23	2.29	0.53
1:A:418:TYR:CD1	1:A:419:LYS:N	2.75	0.53
1:B:45:SER:HB3	1:B:394:LEU:HB3	1.90	0.53
1:A:357:ASN:HA	1:A:360:LYS:HD2	1.90	0.53
1:A:328:HIS:CD2	1:A:330:LYS:HE2	2.43	0.53
1:B:416:ILE:HD11	1:B:420:GLU:OE1	2.08	0.53
1:A:300:TYR:HA	1:A:304:LEU:HD12	1.91	0.53
1:B:136:PRO:CG	1:B:139:TYR:HD1	2.19	0.53
1:A:102:GLU:HG2	2:A:455:GOL:O3	2.08	0.53
1:B:217:LYS:HA	1:B:259:LEU:O	2.07	0.53
1:B:229:PRO:O	1:B:230:ARG:HB2	2.08	0.53
1:B:95:GLN:CB	1:B:138:VAL:HG22	2.37	0.53
1:A:11:ARG:NH1	1:B:82:TYR:CZ	2.76	0.53
1:A:267:TYR:CD2	1:A:268:ASP:N	2.77	0.53
1:A:27:GLU:CG	1:A:28:GLN:N	2.72	0.52
1:A:422:ARG:O	1:A:426:GLU:HB3	2.09	0.52
1:A:307:THR:O	1:A:308:LEU:CD1	2.58	0.52
1:A:148:VAL:HG21	1:B:230:ARG:NH1	2.24	0.52
1:A:436:ASP:N	1:A:436:ASP:OD1	2.42	0.52
1:A:440:LYS:CE	1:B:378:VAL:HG22	2.39	0.52
1:B:96:ILE:HD11	1:B:272:MSE:HE1	1.92	0.52
1:A:27:GLU:HG2	1:A:28:GLN:N	2.24	0.52
1:A:183:ASN:H	1:A:183:ASN:HD22	1.56	0.52
1:B:433:ARG:C	1:B:433:ARG:HH11	2.13	0.52
1:A:433:ARG:NH1	1:B:17:LEU:HD13	2.24	0.52
1:B:294:TYR:O	1:B:295:ILE:HD13	2.10	0.52
1:A:180:LEU:O	1:A:184:GLY:CA	2.58	0.52
1:B:129:LEU:HG	1:B:294:TYR:CZ	2.45	0.52
1:A:299:PHE:CD2	1:A:304:LEU:CD1	2.93	0.52
1:A:284:ASP:OD2	1:A:355:PHE:HB3	2.10	0.52
1:B:37:LYS:HB3	1:B:38:PRO:HD2	1.92	0.52
1:B:220:ILE:HD12	1:B:224:ALA:HB3	1.91	0.51
1:A:136:PRO:C	1:A:138:VAL:N	2.63	0.51
1:B:217:LYS:HE3	1:B:260:TYR:OH	2.11	0.51
1:A:139:TYR:CZ	1:A:345:TRP:CD1	2.98	0.51
1:B:422:ARG:HE	1:B:423:HIS:CD2	2.19	0.51
1:A:267:TYR:HD2	1:A:268:ASP:OD2	1.92	0.51
1:B:219:LYS:HA	1:B:257:VAL:O	2.11	0.51
1:A:135:ARG:HG2	1:A:135:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:OG	1:A:61:GLY:N	2.44	0.51
1:A:144:ARG:CB	1:B:230:ARG:HH21	2.22	0.51
1:A:378:VAL:CG1	1:A:379:ILE:N	2.73	0.51
1:A:217:LYS:HE3	1:A:258:GLU:OE2	2.11	0.51
1:A:138:VAL:HG21	1:A:276:TYR:HE1	1.73	0.51
1:A:223:LYS:HZ1	1:A:230:ARG:HG2	1.74	0.51
1:B:125:MSE:HE2	1:B:125:MSE:HA	1.92	0.51
1:B:326:ILE:HG22	1:B:328:HIS:CD2	2.45	0.51
1:B:176:VAL:HG22	1:B:186:TYR:CE2	2.46	0.51
1:A:302:LYS:HB2	1:B:87:LYS:HD3	1.93	0.51
1:B:32:ILE:HG22	1:B:334:LEU:HD11	1.92	0.51
1:B:30:ARG:O	1:B:31:ASN:CB	2.59	0.51
1:B:285:LYS:O	1:B:288:GLU:HB2	2.10	0.51
1:B:342:PRO:HB2	1:B:362:ILE:HD13	1.93	0.51
1:A:240:SER:CB	1:A:243:LYS:HD2	2.40	0.51
1:B:29:ILE:O	1:B:30:ARG:CB	2.58	0.51
1:A:54:ARG:CB	1:A:101:MSE:HE3	2.19	0.50
1:A:135:ARG:NH1	1:A:135:ARG:HG2	2.25	0.50
1:A:284:ASP:CG	1:A:355:PHE:HB3	2.31	0.50
1:B:55:SER:OG	1:B:419:LYS:HE2	2.10	0.50
1:A:40:PRO:HD2	1:A:396:LEU:HD11	1.93	0.50
1:B:207:LYS:C	1:B:208:VAL:HG12	2.32	0.50
1:A:222:ARG:HD2	1:A:255:GLU:CG	2.41	0.50
1:A:127:GLY:O	1:A:296:ALA:HB2	2.12	0.50
1:B:326:ILE:HG22	1:B:326:ILE:O	2.11	0.50
1:B:137:PRO:C	1:B:138:VAL:HG23	2.32	0.50
1:B:419:LYS:HG2	1:B:421:ALA:H	1.76	0.50
1:A:182:LYS:HB2	1:A:183:ASN:ND2	2.27	0.50
1:B:368:LEU:HD22	1:B:383:GLN:HG2	1.93	0.50
1:B:374:GLU:HG2	1:B:375:GLN:H	1.77	0.50
1:A:319:ASP:OD1	1:A:372:ARG:NH1	2.45	0.50
1:A:136:PRO:HB2	1:A:138:VAL:HG23	1.92	0.50
1:B:336:ILE:HB	1:B:368:LEU:O	2.12	0.49
1:B:139:TYR:CB	1:B:140:PRO:HD3	2.29	0.49
1:B:326:ILE:CG2	1:B:328:HIS:NE2	2.75	0.49
1:A:369:ALA:HB2	1:A:388:ILE:HG13	1.93	0.49
1:A:146:LEU:CD2	1:A:351:LEU:HD11	2.40	0.49
1:A:139:TYR:CE2	1:A:345:TRP:NE1	2.78	0.49
1:A:267:TYR:C	1:A:267:TYR:CD2	2.85	0.49
1:A:23:VAL:HG21	1:A:317:LEU:HD13	1.94	0.49
1:B:228:SER:N	1:B:229:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:HG23	1:A:96:ILE:HD11	1.94	0.49
1:B:9:ILE:H	1:B:9:ILE:HD12	1.76	0.49
1:A:347:PHE:HB3	1:A:352:LEU:CD1	2.40	0.49
1:B:183:ASN:N	1:B:183:ASN:ND2	2.60	0.49
1:A:433:ARG:HH11	1:B:17:LEU:HD13	1.78	0.49
1:B:25:GLU:C	1:B:27:GLU:H	2.16	0.49
1:A:142:ASP:O	1:A:146:LEU:HD13	2.13	0.49
1:B:284:ASP:HB2	1:B:355:PHE:HB3	1.95	0.49
1:B:419:LYS:HZ2	1:B:421:ALA:HB3	1.78	0.49
1:A:342:PRO:HG2	1:A:362:ILE:CD1	2.42	0.49
1:A:368:LEU:HD22	1:A:383:GLN:HG2	1.95	0.49
1:B:280:LEU:HA	1:B:283:ILE:HG13	1.95	0.49
1:B:39:LEU:HD11	1:B:331:GLU:OE2	2.12	0.49
1:B:319:ASP:OD2	1:B:379:ILE:HG13	2.13	0.48
1:B:125:MSE:O	1:B:294:TYR:HA	2.13	0.48
1:B:398:HIS:HB3	1:B:406:PRO:CD	2.44	0.48
1:A:144:ARG:HB2	1:B:230:ARG:NH2	2.29	0.48
1:A:436:ASP:HB2	1:A:437:PRO:CD	2.40	0.48
1:B:414:VAL:O	1:B:414:VAL:HG13	2.13	0.48
1:A:139:TYR:CZ	1:A:346:SER:HA	2.47	0.48
1:B:421:ALA:HB1	1:B:425:LEU:HB3	1.96	0.48
1:B:132:SER:OG	2:B:452:GOL:H2	2.14	0.48
1:A:160:ASN:ND2	2:A:453:GOL:O3	2.38	0.48
1:B:54:ARG:NH2	1:B:98:ARG:NH2	2.62	0.48
1:B:392:LEU:O	1:B:396:LEU:HG	2.14	0.48
1:A:29:ILE:O	1:A:29:ILE:HG22	2.13	0.48
1:A:223:LYS:HZ2	1:A:230:ARG:HD3	1.79	0.48
1:B:374:GLU:HB3	1:B:377:ASP:HB2	1.95	0.48
1:B:390:LYS:O	1:B:393:PRO:HD2	2.14	0.48
1:B:24:ARG:O	1:B:25:GLU:HB2	2.13	0.48
1:B:143:ILE:O	1:B:147:ASN:ND2	2.46	0.48
1:B:67:LEU:HD21	1:B:97:VAL:HG13	1.96	0.48
1:B:196:VAL:HG12	1:B:274:LEU:HD23	1.95	0.48
1:B:70:LEU:HG	1:B:414:VAL:HB	1.96	0.47
1:A:183:ASN:ND2	1:A:183:ASN:N	2.61	0.47
1:B:53:SER:OG	1:B:414:VAL:HG22	2.14	0.47
1:B:41:SER:HA	1:B:42:PRO:HD3	1.63	0.47
1:B:110:TYR:CD2	1:B:111:LEU:HD23	2.48	0.47
1:A:92:THR:HG23	1:A:96:ILE:CD1	2.44	0.47
1:A:70:LEU:HD22	1:A:71:ALA:N	2.29	0.47
1:A:313:VAL:HG12	1:A:317:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ILE:HD12	1:B:388:ILE:H	1.80	0.47
1:A:245:VAL:HG23	1:B:243:LYS:O	2.15	0.47
1:B:358:ILE:O	1:B:362:ILE:HG12	2.15	0.47
1:B:204:ILE:O	1:B:208:VAL:HG12	2.15	0.47
1:B:72:VAL:HG11	1:B:409:LEU:HB3	1.96	0.47
1:A:428:LEU:O	1:A:431:ALA:HB3	2.14	0.47
1:A:130:THR:HG23	1:A:383:GLN:CD	2.35	0.47
1:B:373:PHE:CE1	1:B:404:LEU:HD11	2.49	0.47
1:A:366:ILE:HG22	1:A:368:LEU:CD2	2.44	0.46
1:B:391:ILE:HA	1:B:394:LEU:HD11	1.97	0.46
1:B:420:GLU:H	1:B:420:GLU:CD	2.17	0.46
1:A:183:ASN:ND2	1:A:183:ASN:H	2.13	0.46
1:B:102:GLU:OE1	2:B:452:GOL:O3	2.33	0.46
1:B:274:LEU:HA	1:B:274:LEU:HD12	1.79	0.46
1:B:115:LYS:HA	1:B:115:LYS:HD3	1.61	0.46
1:A:62:THR:HG21	1:B:16:LEU:HD21	1.96	0.46
1:A:102:GLU:HG2	2:A:455:GOL:C3	2.45	0.46
1:B:218:VAL:O	1:B:258:GLU:HA	2.16	0.46
1:A:134:VAL:C	1:A:135:ARG:HG3	2.35	0.46
1:A:92:THR:O	1:A:96:ILE:HD12	2.16	0.46
1:B:293:ALA:HB2	1:B:395:ILE:HD11	1.98	0.46
1:A:237:LEU:HB3	1:B:249:LEU:HD21	1.97	0.46
2:A:455:GOL:H2	2:A:456:GOL:O1	2.16	0.46
1:B:192:THR:HG23	1:B:196:VAL:HG13	1.97	0.46
1:A:323:ARG:HA	1:A:327:GLY:HA2	1.96	0.46
1:A:88:SER:O	1:B:302:LYS:CE	2.64	0.46
1:A:425:LEU:CD1	1:B:12:ILE:HG21	2.44	0.46
1:A:401:GLY:C	1:A:403:TYR:N	2.56	0.46
1:B:176:VAL:HG22	1:B:186:TYR:CD2	2.51	0.46
1:B:295:ILE:HD11	1:B:382:LEU:HD13	1.97	0.45
1:B:89:ASN:O	1:B:90:TYR:C	2.54	0.45
1:B:405:ARG:N	1:B:406:PRO:HD2	2.31	0.45
1:B:106:ASN:HB2	1:B:282:SER:HB2	1.96	0.45
1:B:356:ARG:HD3	1:B:359:GLU:OE2	2.15	0.45
1:A:134:VAL:HG22	1:A:135:ARG:HG3	1.98	0.45
1:A:81:SER:O	1:A:189:PRO:CD	2.65	0.45
1:A:113:TYR:CG	1:A:289:VAL:HG22	2.50	0.45
1:A:260:TYR:CD2	1:A:260:TYR:N	2.83	0.45
1:A:27:GLU:H	1:A:27:GLU:CD	2.18	0.45
1:A:312:ILE:HD13	1:A:312:ILE:O	2.16	0.45
1:B:340:VAL:HG11	1:B:368:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:CG2	1:B:16:LEU:N	2.80	0.45
1:A:144:ARG:CG	1:B:230:ARG:HH21	2.30	0.45
1:B:201:LYS:HA	1:B:205:ASP:CB	2.41	0.45
1:A:133:LEU:CD2	1:A:347:PHE:CZ	2.99	0.45
1:A:281:TYR:CZ	1:A:285:LYS:CE	3.00	0.45
1:A:29:ILE:HA	1:A:32:ILE:HG22	1.98	0.45
1:B:341:VAL:HA	1:B:342:PRO:HD3	1.76	0.45
1:A:152:LEU:HD21	1:A:261:LEU:HD12	1.99	0.45
1:A:144:ARG:HG3	1:B:230:ARG:HH21	1.81	0.45
1:A:220:ILE:HA	1:A:221:PRO:HD3	1.85	0.45
1:B:202:LYS:HD3	1:B:203:TYR:CE1	2.52	0.44
1:A:405:ARG:O	1:A:408:GLN:HB3	2.17	0.44
1:A:159:GLU:HG3	1:A:163:ASN:ND2	2.32	0.44
1:A:27:GLU:CD	1:A:28:GLN:H	2.20	0.44
1:B:83:ALA:O	1:B:84:ASN:HB2	2.17	0.44
1:B:418:TYR:O	1:B:419:LYS:C	2.56	0.44
1:A:418:TYR:HD1	1:A:419:LYS:N	2.07	0.44
1:A:329:GLU:O	1:A:375:GLN:O	2.35	0.44
1:A:85:ALA:HB3	1:B:15:ILE:HG21	1.99	0.44
1:B:287:LEU:HB3	1:B:357:ASN:HB3	1.99	0.44
1:B:330:LYS:O	1:B:372:ARG:HD2	2.18	0.44
1:A:220:ILE:HD11	1:A:259:LEU:HD22	1.98	0.44
1:B:285:LYS:HA	1:B:285:LYS:HD2	1.85	0.44
1:A:267:TYR:CE2	1:A:268:ASP:OD2	2.71	0.44
1:B:110:TYR:HD2	1:B:111:LEU:HD23	1.83	0.44
1:B:399:LYS:HA	1:B:404:LEU:HA	1.99	0.44
1:B:393:PRO:O	1:B:396:LEU:HB2	2.17	0.44
1:A:295:ILE:HA	1:A:295:ILE:HD13	1.85	0.44
1:A:423:HIS:O	1:A:427:ALA:HB3	2.18	0.44
1:B:129:LEU:HB2	1:B:383:GLN:HE21	1.82	0.44
1:B:433:ARG:O	1:B:433:ARG:NH1	2.47	0.44
1:B:421:ALA:CB	1:B:425:LEU:HB3	2.48	0.44
1:A:44:LYS:HA	1:A:397:HIS:CD2	2.53	0.43
1:B:21:GLU:O	1:B:24:ARG:NE	2.50	0.43
1:B:403:TYR:HD1	1:B:407:LEU:HD23	1.83	0.43
1:B:315:THR:HG22	1:B:316:ALA:N	2.34	0.43
1:A:321:VAL:O	1:A:324:THR:HB	2.18	0.43
1:A:146:LEU:HD11	1:A:273:THR:HG23	2.00	0.43
1:A:386:THR:HG1	1:A:391:ILE:HD11	1.83	0.43
1:B:299:PHE:HZ	1:B:381:MSE:HE3	1.83	0.43
1:B:39:LEU:HD12	1:B:39:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:N	1:A:34:ASN:OD1	2.50	0.43
1:A:8:SER:OG	3:A:469:HOH:O	2.21	0.43
1:B:104:LEU:HD22	1:B:189:PRO:HB2	2.00	0.43
1:A:64:ILE:HG21	1:A:425:LEU:HD12	2.00	0.43
1:B:284:ASP:O	1:B:287:LEU:HB2	2.18	0.43
1:A:281:TYR:CZ	1:A:285:LYS:HE3	2.53	0.43
1:B:299:PHE:N	1:B:299:PHE:CD1	2.85	0.43
1:B:70:LEU:HB3	1:B:79:ARG:HG2	2.01	0.43
1:B:403:TYR:CD1	1:B:407:LEU:HD23	2.54	0.43
1:B:14:LYS:HB3	1:B:14:LYS:HE3	1.79	0.43
1:B:80:LEU:HG	1:B:108:LEU:HD13	2.01	0.43
1:B:60:SER:HB3	1:B:61:GLY:H	1.66	0.43
1:A:60:SER:CB	1:B:314:ASP:OD1	2.66	0.43
1:A:347:PHE:HA	1:A:348:PRO:HD3	1.84	0.43
1:A:320:ALA:HB2	1:B:436:ASP:HB2	2.01	0.43
1:A:307:THR:O	1:A:308:LEU:CB	2.67	0.42
1:B:136:PRO:HD2	1:B:139:TYR:CE1	2.54	0.42
1:B:325:LEU:HB3	1:B:326:ILE:HD12	2.01	0.42
1:B:326:ILE:HG21	1:B:328:HIS:CE1	2.54	0.42
1:B:329:GLU:O	1:B:375:GLN:O	2.36	0.42
1:B:221:PRO:HB2	1:B:223:LYS:HE2	2.01	0.42
1:A:195:VAL:O	1:A:195:VAL:CG1	2.67	0.42
1:A:300:TYR:HD2	1:B:61:GLY:HA3	1.84	0.42
1:B:15:ILE:HG22	1:B:16:LEU:N	2.34	0.42
1:A:223:LYS:CD	1:A:223:LYS:H	2.15	0.42
1:B:244:SER:OG	1:B:247:GLU:CG	2.64	0.42
1:B:208:VAL:O	1:B:209:ILE:HG12	2.20	0.42
1:A:49:ALA:HA	1:A:124:LEU:O	2.20	0.42
1:A:104:LEU:HD21	1:A:189:PRO:HG2	2.01	0.42
1:B:208:VAL:CG2	1:B:209:ILE:N	2.81	0.42
1:A:135:ARG:NH2	1:B:90:TYR:H	2.04	0.42
1:A:420:GLU:C	1:A:424:THR:HG23	2.39	0.42
1:A:340:VAL:CG2	1:A:366:ILE:HB	2.50	0.42
1:A:65:TYR:OH	1:A:100:GLN:NE2	2.51	0.42
1:A:54:ARG:HB3	1:A:101:MSE:HE1	1.92	0.42
1:B:50:VAL:HG11	1:B:125:MSE:HE1	1.96	0.42
1:A:306:ARG:HG3	1:A:307:THR:N	2.33	0.42
1:B:182:LYS:CB	1:B:183:ASN:HD22	2.33	0.42
1:B:143:ILE:HG23	1:B:147:ASN:HD21	1.85	0.42
1:A:108:LEU:HA	1:A:108:LEU:HD12	1.82	0.42
1:A:392:LEU:N	1:A:393:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLN:O	1:B:29:ILE:HB	2.18	0.42
1:A:45:SER:H	1:A:397:HIS:CD2	2.38	0.42
1:A:372:ARG:HB2	1:A:379:ILE:HG12	2.01	0.41
1:A:4:LEU:N	1:A:4:LEU:HD12	2.35	0.41
1:A:249:LEU:HD22	1:B:234:ILE:HD11	2.02	0.41
1:A:307:THR:O	1:A:308:LEU:HD13	2.21	0.41
1:A:416:ILE:O	1:A:416:ILE:CG2	2.67	0.41
1:A:153:ILE:HD13	1:A:153:ILE:HG21	1.81	0.41
1:B:395:ILE:HG22	1:B:404:LEU:HD21	2.00	0.41
1:A:202:LYS:HD2	1:A:203:TYR:CE1	2.56	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.86	0.41
1:A:130:THR:HG23	1:A:383:GLN:NE2	2.36	0.41
1:B:325:LEU:HD23	1:B:326:ILE:CD1	2.46	0.41
1:A:138:VAL:HG21	1:A:276:TYR:CE1	2.52	0.41
1:B:283:ILE:HG22	1:B:287:LEU:HD11	2.02	0.41
1:A:102:GLU:HG2	2:A:455:GOL:H31	2.01	0.41
1:A:79:ARG:O	1:A:185:ASN:HA	2.21	0.41
1:B:319:ASP:O	1:B:322:ILE:HB	2.21	0.41
1:B:153:ILE:O	1:B:157:ASP:HB2	2.20	0.41
1:B:292:LEU:HD12	1:B:293:ALA:H	1.85	0.41
1:A:162:LEU:HD23	1:A:354:LYS:HE2	2.02	0.41
1:B:47:ILE:HG22	1:B:398:HIS:CE1	2.55	0.41
1:B:134:VAL:HA	1:B:343:PRO:HG2	2.02	0.41
1:B:414:VAL:O	1:B:415:LYS:C	2.59	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.89	0.41
1:A:281:TYR:O	1:A:285:LYS:HG2	2.21	0.41
1:A:138:VAL:HG12	1:A:139:TYR:CD1	2.56	0.41
1:B:310:VAL:HG22	1:B:311:GLU:N	2.36	0.41
1:B:419:LYS:HD3	1:B:422:ARG:N	2.35	0.41
1:B:323:ARG:NH1	1:B:329:GLU:HG3	2.36	0.41
1:B:276:TYR:CE2	1:B:280:LEU:HD11	2.56	0.41
1:B:164:GLU:O	1:B:167:GLU:HB2	2.20	0.41
1:B:106:ASN:CB	1:B:282:SER:HB2	2.51	0.41
1:A:192:THR:HG23	1:A:274:LEU:HB2	2.03	0.41
1:B:130:THR:HG22	1:B:366:ILE:HD12	2.03	0.40
1:B:394:LEU:H	1:B:394:LEU:HG	1.55	0.40
1:B:342:PRO:HA	1:B:343:PRO:HD3	1.83	0.40
1:A:232:ILE:HD13	1:A:232:ILE:HG21	1.83	0.40
1:A:11:ARG:NH1	1:B:82:TYR:CE1	2.81	0.40
1:A:379:ILE:H	1:B:440:LYS:NZ	2.19	0.40
1:A:241:ARG:HD3	1:A:241:ARG:HH11	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:O	1:A:362:ILE:HG12	2.21	0.40
1:A:125:MSE:HB3	1:A:125:MSE:HE3	2.02	0.40
1:B:292:LEU:HD12	1:B:293:ALA:N	2.36	0.40
1:A:96:ILE:O	1:A:100:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/471 (90%)	390 (92%)	31 (7%)	3 (1%)	26	60
1	B	422/471 (90%)	382 (90%)	33 (8%)	7 (2%)	11	34
All	All	846/942 (90%)	772 (91%)	64 (8%)	10 (1%)	16	45

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	B	43	GLU
1	B	139	TYR
1	A	420	GLU
1	B	42	PRO
1	B	208	VAL
1	A	300	TYR
1	A	424	THR
1	B	432	LEU
1	B	138	VAL



### 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	385/410 (94%)	337 (88%)	48 (12%)	6	17
1	B	385/410 (94%)	334 (87%)	51 (13%)	5	14
All	All	770/820 (94%)	671 (87%)	99 (13%)	5	15

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	21	GLU
1	A	27	GLU
1	A	34	ASN
1	A	35	SER
1	A	50	VAL
1	A	55	SER
1	A	56	VAL
1	A	66	PHE
1	A	70	LEU
1	A	79	ARG
1	A	90	TYR
1	A	102	GLU
1	A	129	LEU
1	A	135	ARG
1	A	141	GLU
1	A	144	ARG
1	A	156	SER
1	A	167	GLU
1	A	174	ARG
1	A	183	ASN
1	A	185	ASN
1	A	188	SER
1	A	199	LEU
1	A	222	ARG
1	A	223	LYS
1	A	230	ARG

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Mol	Chain	Res	Type
1	A	231	VAL
1	A	267	TYR
1	A	288	GLU
1	A	299	PHE
1	A	302	LYS
1	A	308	LEU
1	A	312	ILE
1	A	328	HIS
1	A	341	VAL
1	A	345	TRP
1	A	352	LEU
1	A	353	SER
1	A	374	GLU
1	A	386	THR
1	A	387	ASN
1	A	404	LEU
1	A	405	ARG
1	A	414	VAL
1	A	428	LEU
1	A	432	LEU
1	A	436	ASP
1	B	7	GLN
1	B	19	GLU
1	B	26	ASN
1	B	39	LEU
1	B	41	SER
1	B	50	VAL
1	B	60	SER
1	B	62	THR
1	B	68	SER
1	B	90	TYR
1	B	104	LEU
1	B	129	LEU
1	B	135	ARG
1	B	138	VAL
1	B	142	ASP
1	B	183	ASN
1	B	195	VAL
1	B	199	LEU
1	B	200	ARG
1	B	208	VAL
1	B	217	LYS

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Mol	Chain	Res	Type
1	B	234	ILE
1	B	253	ASP
1	B	274	LEU
1	B	283	ILE
1	B	288	GLU
1	B	290	LYS
1	B	299	PHE
1	B	304	LEU
1	B	312	ILE
1	B	315	THR
1	B	340	VAL
1	B	344	LYS
1	B	345	TRP
1	B	350	PHE
1	B	361	LEU
1	B	372	ARG
1	B	378	VAL
1	B	384	SER
1	B	389	GLU
1	B	394	LEU
1	B	403	TYR
1	B	404	LEU
1	B	408	GLN
1	B	411	HIS
1	B	412	HIS
1	B	414	VAL
1	B	415	LYS
1	B	422	ARG
1	B	432	LEU
1	B	434	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	106	ASN
1	A	179	HIS
1	A	183	ASN
1	A	271	HIS
1	A	328	HIS
1	A	397	HIS
1	B	95	GLN

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Mol	Chain	Res	Type
1	B	100	GLN
1	B	106	ASN
1	B	147	ASN
1	B	163	ASN
1	B	183	ASN
1	B	185	ASN
1	B	271	HIS
1	B	291	ASN
1	B	383	GLN
1	B	408	GLN
1	B	412	HIS
1	B	423	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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	452	-	5,5,5	0.34	0	5,5,5	0.23	0
2	GOL	A	453	-	5,5,5	0.36	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	454	-	5,5,5	0.43	0	5,5,5	0.39	0
2	GOL	A	455	-	5,5,5	0.25	0	5,5,5	0.80	0
2	GOL	A	456	-	5,5,5	0.38	0	5,5,5	0.33	0
2	GOL	A	457	-	5,5,5	0.35	0	5,5,5	0.24	0
2	GOL	B	452	-	5,5,5	0.38	0	5,5,5	0.38	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
2	GOL	A	452	-	-	0/4/4/4	0/0/0/0
2	GOL	A	453	-	-	0/4/4/4	0/0/0/0
2	GOL	A	454	-	-	0/4/4/4	0/0/0/0
2	GOL	A	455	-	-	0/4/4/4	0/0/0/0
2	GOL	A	456	-	-	0/4/4/4	0/0/0/0
2	GOL	A	457	-	-	0/4/4/4	0/0/0/0
2	GOL	B	452	-	-	0/4/4/4	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.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	452	GOL	2	0
2	A	453	GOL	1	0
2	A	455	GOL	6	0
2	A	456	GOL	1	0
2	B	452	GOL	2	0

## 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	423/471 (89%)	-0.30	11 (2%) 59 47	41, 79, 150, 209	0
1	B	423/471 (89%)	0.03	26 (6%) 25 15	51, 104, 174, 265	0
All	All	846/942 (89%)	-0.13	37 (4%) 38 26	41, 91, 162, 265	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	LEU	7.0
1	B	403	TYR	7.0
1	A	139	TYR	4.1
1	B	31	ASN	3.9
1	B	258	GLU	3.7
1	B	26	ASN	3.6
1	B	441	ILE	3.6
1	B	324	THR	3.6
1	A	418	TYR	3.5
1	B	260	TYR	3.4
1	B	306	ARG	3.4
1	A	306	ARG	3.3
1	A	429	ILE	3.2
1	A	90	TYR	3.2
1	B	303	THR	2.9
1	B	402	GLY	2.9
1	B	400	ALA	2.8
1	B	301	THR	2.7
1	B	119	GLU	2.7
1	A	426	GLU	2.7
1	B	418	TYR	2.7
1	B	181	GLU	2.6
1	B	27	GLU	2.6
1	A	26	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	375	GLN	2.4
1	B	32	ILE	2.4
1	A	416	ILE	2.3
1	A	91	GLY	2.3
1	B	419	LYS	2.3
1	B	209	ILE	2.3
1	B	259	LEU	2.3
1	B	307	THR	2.2
1	B	139	TYR	2.2
1	B	349	ASP	2.2
1	B	422	ARG	2.1
1	A	4	LEU	2.0
1	A	345	TRP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	B	452	6/6	0.92	0.69	13.73	110,131,142,147	0
2	GOL	A	456	6/6	0.88	0.46	12.12	83,96,100,103	0
2	GOL	A	454	6/6	0.86	0.27	8.21	77,104,111,117	0
2	GOL	A	452	6/6	0.60	0.31	2.38	83,118,124,130	0
2	GOL	A	457	6/6	0.84	0.26	2.25	93,115,118,121	0
2	GOL	A	455	6/6	0.87	0.29	1.64	68,78,79,91	0
2	GOL	A	453	6/6	0.85	0.13	-	96,115,118,118	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.