



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:25 AM UTC

PDB ID : 1M5Q / pdb_00001m5q
Title : Crystal structure of a novel Sm-like archaeal protein from *Pyrobaculum aerophilum*
Authors : Mura, C.; Phillips, M.; Kozhukhovskiy, A.; Eisenberg, D.
Deposited on : 2002-07-09
Resolution : 2.00 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

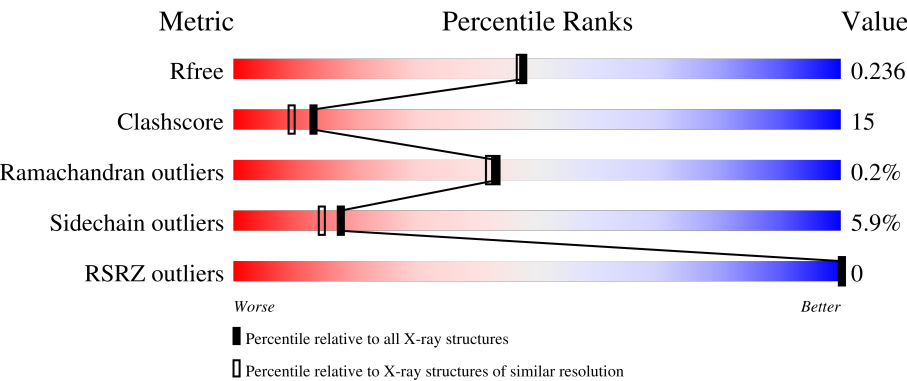
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	130	65%26%6% .
1	2	130	68%25%5% .
1	A	130	75%18% . . .
1	B	130	69%26% . .
1	C	130	72%22% . . .

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Mol	Chain	Length	Quality of chain
1	D	130	
1	E	130	
1	F	130	
1	G	130	
1	H	130	
1	I	130	
1	J	130	
1	K	130	
1	L	130	
1	M	130	
1	N	130	
1	O	130	
1	P	130	
1	Q	130	
1	R	130	
1	S	130	
1	T	130	
1	U	130	
1	V	130	
1	W	130	
1	X	130	
1	Y	130	
1	Z	130	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	1	4010	-	X	-	-
4	GOL	2	4009	-	X	-	-
4	GOL	A	4012	-	X	-	-
4	GOL	G	4001	-	X	-	-
4	GOL	H	4002	-	X	X	-
4	GOL	H	4011	-	X	-	-
4	GOL	J	4005	-	X	-	-
4	GOL	M	4003	-	X	-	-
4	GOL	R	4007	-	X	-	-
4	GOL	V	4008	-	X	-	-
4	GOL	W	4006	-	X	-	-
4	GOL	X	4004	-	X	-	-
5	ACY	K	5013	-	-	X	-
5	ACY	W	5011	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30641 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 small nuclear ribonucleoprotein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	Se	0	0	0
			1008	644	177	184	3			
1	B	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	C	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	D	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	E	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	F	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	G	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	H	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	I	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	J	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	K	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	L	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	M	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	N	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	O	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	P	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	R	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	S	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	T	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	U	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	V	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	W	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	X	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	Y	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	Z	128	Total	C	N	O	Se	0	0	0
			1028	656	183	186	3			
1	1	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			
1	2	127	Total	C	N	O	Se	0	0	0
			1017	650	179	185	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	MSE	MET	cloning artifact	UNP Q8ZVU2
A	82	MSE	MET	cloning artifact	UNP Q8ZVU2
A	96	MSE	MET	cloning artifact	UNP Q8ZVU2
B	66	MSE	MET	cloning artifact	UNP Q8ZVU2
B	82	MSE	MET	cloning artifact	UNP Q8ZVU2
B	96	MSE	MET	cloning artifact	UNP Q8ZVU2
C	66	MSE	MET	cloning artifact	UNP Q8ZVU2
C	82	MSE	MET	cloning artifact	UNP Q8ZVU2
C	96	MSE	MET	cloning artifact	UNP Q8ZVU2
D	66	MSE	MET	cloning artifact	UNP Q8ZVU2
D	82	MSE	MET	cloning artifact	UNP Q8ZVU2
D	96	MSE	MET	cloning artifact	UNP Q8ZVU2
E	66	MSE	MET	cloning artifact	UNP Q8ZVU2
E	82	MSE	MET	cloning artifact	UNP Q8ZVU2
E	96	MSE	MET	cloning artifact	UNP Q8ZVU2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	66	MSE	MET	cloning artifact	UNP Q8ZVU2
F	82	MSE	MET	cloning artifact	UNP Q8ZVU2
F	96	MSE	MET	cloning artifact	UNP Q8ZVU2
G	66	MSE	MET	cloning artifact	UNP Q8ZVU2
G	82	MSE	MET	cloning artifact	UNP Q8ZVU2

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cd 2 2	0	0
2	B	1	Total Cd 1 1	0	0
2	D	2	Total Cd 2 2	0	0
2	E	1	Total Cd 1 1	0	0
2	F	1	Total Cd 1 1	0	0
2	H	2	Total Cd 2 2	0	0
2	I	1	Total Cd 1 1	0	0
2	J	1	Total Cd 1 1	0	0
2	K	1	Total Cd 1 1	0	0
2	L	1	Total Cd 1 1	0	0
2	M	1	Total Cd 1 1	0	0
2	O	1	Total Cd 1 1	0	0
2	P	2	Total Cd 2 2	0	0
2	Q	1	Total Cd 1 1	0	0
2	R	1	Total Cd 1 1	0	0
2	S	1	Total Cd 1 1	0	0
2	U	1	Total Cd 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	V	1	Total 1	Cd 1	0	0
2	W	1	Total 1	Cd 1	0	0
2	X	1	Total 1	Cd 1	0	0
2	Y	1	Total 1	Cd 1	0	0
2	Z	1	Total 1	Cd 1	0	0
2	1	1	Total 1	Cd 1	0	0
2	2	1	Total 1	Cd 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

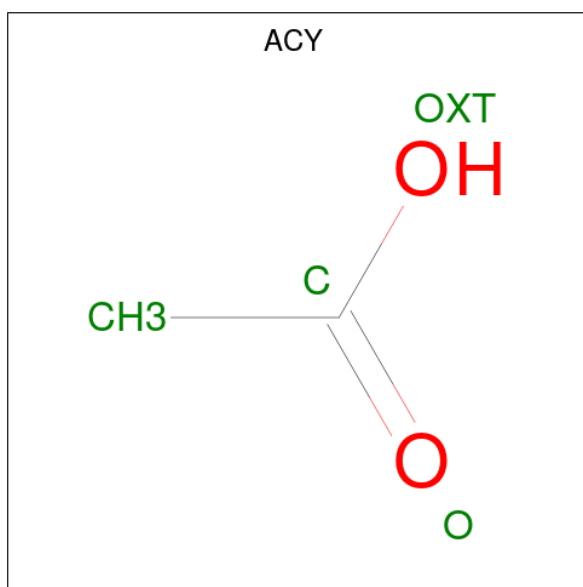
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	R	1	Total 1	Na 1	0	0
3	S	1	Total 1	Na 1	0	0
3	V	1	Total 1	Na 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		
4	M	1	Total	C	O	0	0
			6	3	3		
4	R	1	Total	C	O	0	0
			6	3	3		
4	V	1	Total	C	O	0	0
			6	3	3		
4	W	1	Total	C	O	0	0
			6	3	3		
4	X	1	Total	C	O	0	0
			6	3	3		
4	1	1	Total	C	O	0	0
			6	3	3		
4	2	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		
5	V	1	Total	C	O	0	0
			4	2	2		
5	W	1	Total	C	O	0	0
			4	2	2		
5	W	1	Total	C	O	0	0
			4	2	2		
5	X	1	Total	C	O	0	0
			4	2	2		
5	Y	1	Total	C	O	0	0
			4	2	2		
5	Z	1	Total	C	O	0	0
			4	2	2		
5	1	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	2	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		
6	B	64	Total	O	0	0
			64	64		
6	C	64	Total	O	0	0
			64	64		
6	D	46	Total	O	0	0
			46	46		
6	E	48	Total	O	0	0
			48	48		
6	F	69	Total	O	0	0
			69	69		
6	G	74	Total	O	0	0
			74	74		
6	H	67	Total	O	0	0
			67	67		
6	I	58	Total	O	0	0
			58	58		
6	J	47	Total	O	0	0
			47	47		
6	K	42	Total	O	0	0
			42	42		
6	L	59	Total	O	0	0
			59	59		
6	M	98	Total	O	0	0
			98	98		
6	N	89	Total	O	0	0
			89	89		
6	O	72	Total	O	0	0
			72	72		
6	P	63	Total	O	0	0
			63	63		
6	Q	63	Total	O	0	0
			63	63		
6	R	52	Total	O	0	0
			52	52		

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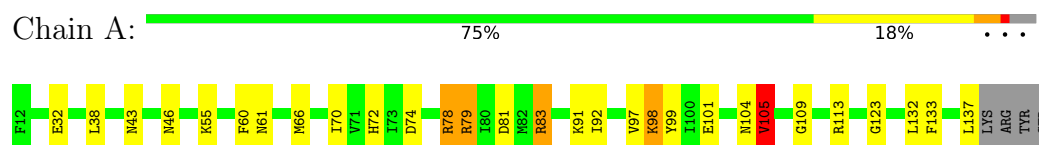
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	52	Total 52	O 52	0	0
6	T	63	Total 63	O 63	0	0
6	U	69	Total 69	O 69	0	0
6	V	115	Total 115	O 115	0	0
6	W	86	Total 86	O 86	0	0
6	X	93	Total 93	O 93	0	0
6	Y	77	Total 77	O 77	0	0
6	Z	64	Total 64	O 64	0	0
6	1	52	Total 52	O 52	0	0
6	2	75	Total 75	O 75	0	0

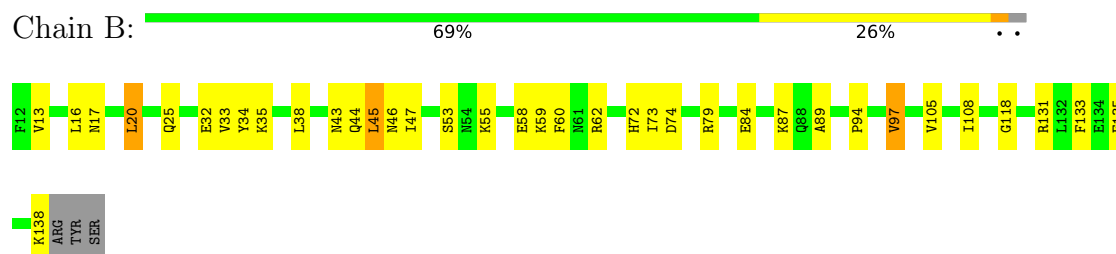
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

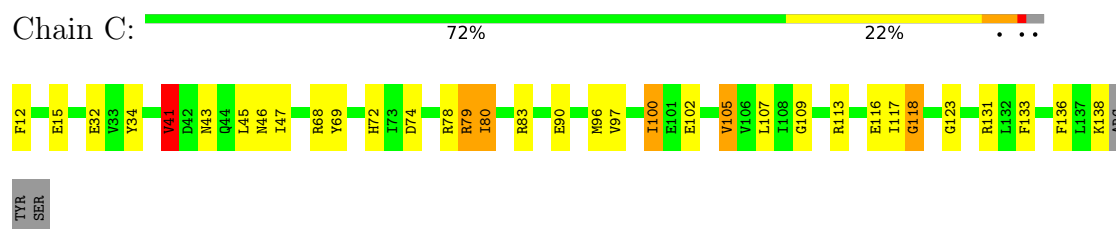
- Molecule 1: small nuclear ribonucleoprotein homolog



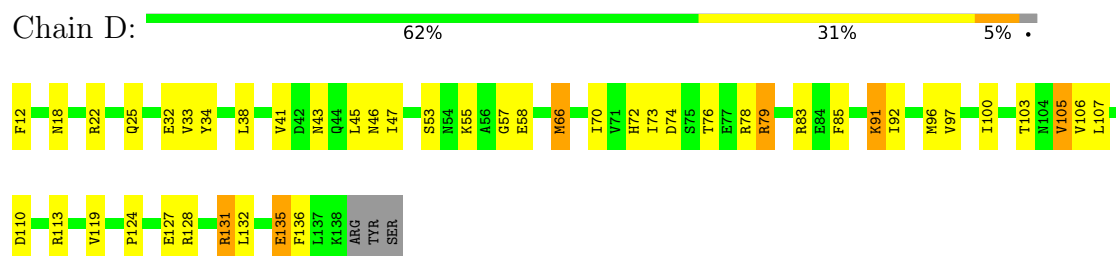
- Molecule 1: small nuclear ribonucleoprotein homolog



- Molecule 1: small nuclear ribonucleoprotein homolog

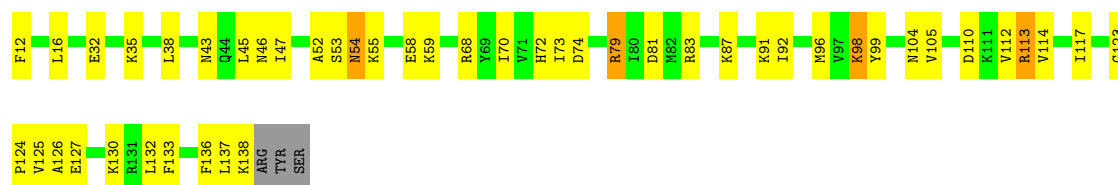


- Molecule 1: small nuclear ribonucleoprotein homolog



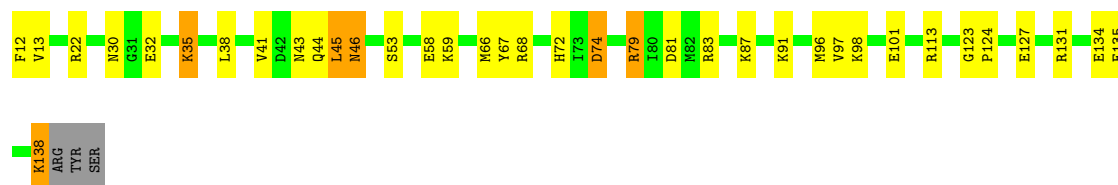
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain E:  62% 33% . .



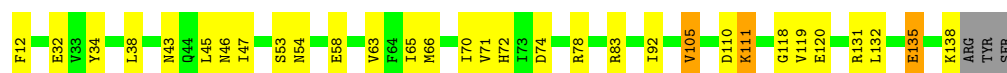
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain F:  69% 24% 5% .



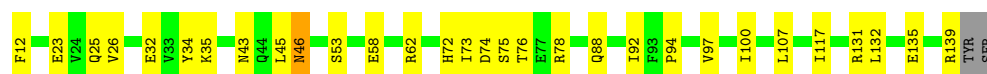
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain G:  74% 22% . .



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain H:  75% 22% . .



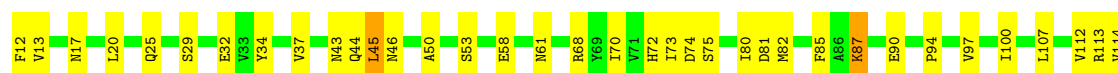
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain I:  63% 32% . .



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain J:  62% 32% . .

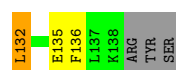
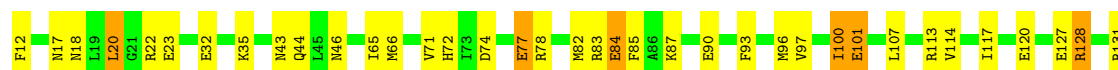




- Molecule 1: small nuclear ribonucleoprotein homolog



- Molecule 1: small nuclear ribonucleoprotein homolog



- Molecule 1: small nuclear ribonucleoprotein homolog



- Molecule 1: small nuclear ribonucleoprotein homolog

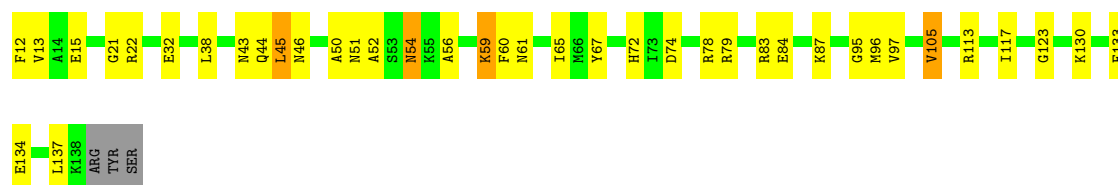


- Molecule 1: small nuclear ribonucleoprotein homolog



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain P:  68% 27% ..



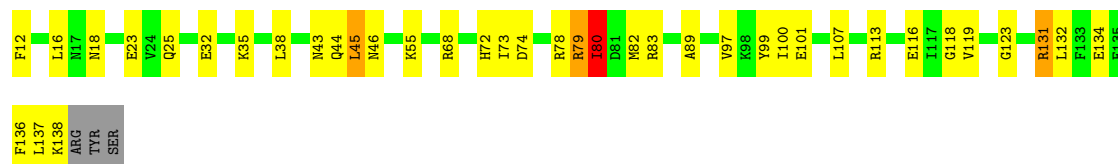
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain Q:  65% 31% ..



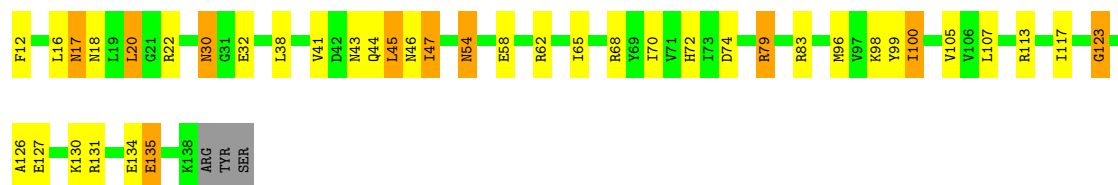
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain R:  68% 27% ...



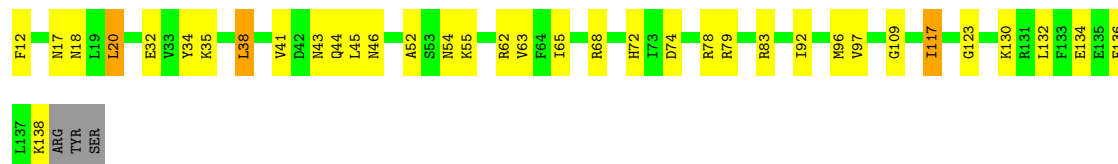
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain S:  67% 23% 8% .



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain T:  70% 25% ..



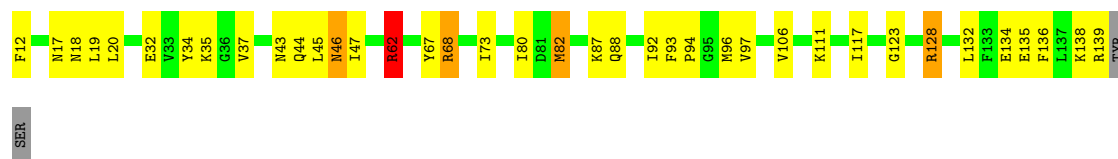
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain U:  69% 25%



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain V:  69% 25%



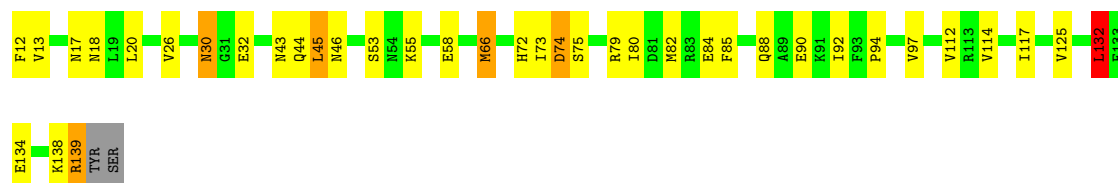
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain W:  80% 18%



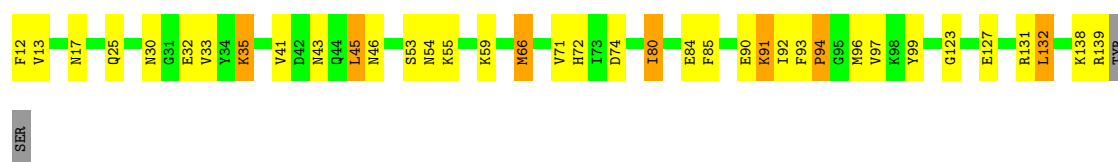
- Molecule 1: small nuclear ribonucleoprotein homolog

Chain X:  69% 25%



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain Y:  70% 23% 5%



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain Z:  64% 28% 7%





- Molecule 1: small nuclear ribonucleoprotein homolog

Chain 1: 65% 26% 6% .



- Molecule 1: small nuclear ribonucleoprotein homolog

Chain 2: 68% 25% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.32Å 172.43Å 148.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.00 19.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (19.97-2.00) 93.6 (19.97-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.236 0.191 , 0.236	Depositor DCC
R_{free} test set	13431 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30641	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CD, NA, ACY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.95	0/1028	1.16	8/1377 (0.6%)
1	2	1.00	0/1028	1.21	9/1377 (0.7%)
1	A	0.97	0/1019	1.16	9/1366 (0.7%)
1	B	1.04	0/1028	1.14	2/1377 (0.1%)
1	C	0.95	0/1028	1.10	6/1377 (0.4%)
1	D	0.90	0/1028	1.16	8/1377 (0.6%)
1	E	0.88	0/1028	1.12	2/1377 (0.1%)
1	F	0.91	0/1028	1.16	6/1377 (0.4%)
1	G	1.02	0/1028	1.17	10/1377 (0.7%)
1	H	0.98	0/1039	1.13	3/1391 (0.2%)
1	I	1.01	1/1039 (0.1%)	1.15	7/1391 (0.5%)
1	J	0.86	0/1039	1.14	6/1391 (0.4%)
1	K	0.82	0/1039	1.12	4/1391 (0.3%)
1	L	0.88	1/1028 (0.1%)	1.10	2/1377 (0.1%)
1	M	0.98	0/1039	1.18	3/1391 (0.2%)
1	N	0.99	1/1039 (0.1%)	1.18	3/1391 (0.2%)
1	O	0.94	1/1028 (0.1%)	1.13	5/1377 (0.4%)
1	P	1.00	0/1028	1.15	6/1377 (0.4%)
1	Q	0.93	0/1028	1.10	5/1377 (0.4%)
1	R	0.90	0/1028	1.15	7/1377 (0.5%)
1	S	0.92	1/1028 (0.1%)	1.15	7/1377 (0.5%)
1	T	0.94	0/1028	1.10	5/1377 (0.4%)
1	U	0.96	0/1028	1.13	3/1377 (0.2%)
1	V	1.30	3/1039 (0.3%)	1.21	5/1391 (0.4%)
1	W	1.02	1/1039 (0.1%)	1.19	6/1391 (0.4%)
1	X	1.02	1/1039 (0.1%)	1.18	3/1391 (0.2%)
1	Y	1.03	0/1039	1.19	7/1391 (0.5%)
1	Z	0.94	0/1039	1.15	7/1391 (0.5%)
All	All	0.97	10/28896 (0.0%)	1.15	154/38699 (0.4%)

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	2	0	1
1	B	0	1
1	C	0	2
1	H	0	1
1	I	0	1
1	V	0	1
1	W	0	1
All	All	0	8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	82	MSE	SE-CE	-23.01	1.26	1.95
1	W	66	MSE	SE-CE	-7.29	1.73	1.95
1	V	37	VAL	CA-C	5.95	1.59	1.52
1	O	96	MSE	SE-CE	-5.94	1.77	1.95
1	L	71	VAL	CA-CB	5.51	1.61	1.54
1	I	73	ILE	C-O	5.42	1.29	1.24
1	V	106	VAL	CA-CB	5.41	1.61	1.54
1	N	119	VAL	CA-CB	5.24	1.60	1.54
1	S	100	ILE	CA-CB	5.23	1.60	1.53
1	X	80	ILE	CA-CB	5.17	1.59	1.54

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASN	N-CA-C	-9.44	96.50	110.48
1	C	46	ASN	N-CA-C	-9.43	97.20	110.50
1	Q	46	ASN	N-CA-C	-9.37	96.62	110.48
1	R	46	ASN	N-CA-C	-9.32	96.69	110.48
1	X	46	ASN	N-CA-C	-9.22	97.50	110.50
1	O	46	ASN	N-CA-C	-9.09	97.69	110.50
1	K	46	ASN	N-CA-C	-8.93	97.91	110.50
1	B	46	ASN	N-CA-C	-8.93	97.91	110.50
1	Y	46	ASN	N-CA-C	-8.90	97.95	110.50
1	T	46	ASN	N-CA-C	-8.89	97.97	110.50
1	N	46	ASN	N-CA-C	-8.80	97.45	110.48
1	H	46	ASN	N-CA-C	-8.61	98.36	110.50
1	V	46	ASN	N-CA-C	-8.57	98.42	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	46	ASN	N-CA-C	-8.51	98.50	110.50
1	F	41	VAL	CB-CA-C	-8.39	97.02	110.28
1	W	46	ASN	N-CA-C	-8.38	98.68	110.50
1	J	46	ASN	N-CA-C	-8.37	98.70	110.50
1	E	46	ASN	N-CA-C	-8.27	98.84	110.50
1	S	123	GLY	CA-C-N	8.13	128.08	119.05
1	S	123	GLY	C-N-CA	8.13	128.08	119.05
1	S	46	ASN	N-CA-C	-7.98	99.99	110.53
1	2	46	ASN	N-CA-C	-7.79	99.51	110.50
1	I	97	VAL	N-CA-C	7.78	119.48	108.36
1	Z	46	ASN	N-CA-C	-7.77	98.78	110.28
1	L	46	ASN	N-CA-C	-7.63	99.74	110.50
1	M	46	ASN	N-CA-C	-7.62	99.76	110.50
1	J	97	VAL	N-CA-C	7.59	119.21	108.36
1	G	118	GLY	N-CA-C	7.58	121.45	111.52
1	2	22	ARG	NE-CZ-NH2	-7.52	112.43	119.20
1	Y	97	VAL	N-CA-C	7.51	118.69	108.17
1	R	123	GLY	CA-C-N	7.45	127.82	119.32
1	R	123	GLY	C-N-CA	7.45	127.82	119.32
1	F	123	GLY	CA-C-N	7.45	127.32	119.05
1	F	123	GLY	C-N-CA	7.45	127.32	119.05
1	2	97	VAL	N-CA-C	7.36	118.89	108.36
1	M	97	VAL	N-CA-C	7.24	118.71	108.36
1	D	97	VAL	N-CA-C	7.05	118.05	108.17
1	U	46	ASN	N-CA-C	-6.99	100.64	110.50
1	F	46	ASN	N-CA-C	-6.96	100.69	110.50
1	G	46	ASN	N-CA-C	-6.95	100.71	110.50
1	P	46	ASN	N-CA-C	-6.94	100.01	110.28
1	R	118	GLY	N-CA-C	6.88	120.54	111.52
1	D	76	THR	N-CA-C	-6.85	104.91	112.72
1	1	41	VAL	CB-CA-C	-6.78	99.58	110.28
1	V	97	VAL	N-CA-C	6.71	118.71	108.71
1	Q	123	GLY	CA-C-N	6.67	126.45	119.05
1	Q	123	GLY	C-N-CA	6.67	126.45	119.05
1	1	46	ASN	N-CA-C	-6.65	101.13	110.50
1	F	30	ASN	N-CA-C	-6.50	105.22	113.02
1	S	41	VAL	CB-CA-C	-6.44	100.10	110.28
1	I	132	LEU	N-CA-C	-6.40	104.38	111.36
1	A	83	ARG	N-CA-C	-6.40	104.39	111.82
1	C	123	GLY	CA-C-N	6.38	126.59	119.32
1	C	123	GLY	C-N-CA	6.38	126.59	119.32
1	Z	75	SER	N-CA-C	-6.34	99.68	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	VAL	N-CA-C	6.31	117.00	108.17
1	G	119	VAL	N-CA-C	6.24	117.57	108.58
1	O	105	VAL	N-CA-CB	-6.23	103.79	112.52
1	T	65	ILE	N-CA-C	6.22	116.77	107.51
1	D	46	ASN	N-CA-C	-6.21	101.75	110.50
1	U	65	ILE	N-CA-C	6.20	117.04	107.99
1	N	41	VAL	CB-CA-C	-6.20	100.49	110.28
1	P	123	GLY	CA-C-N	6.18	126.36	119.32
1	P	123	GLY	C-N-CA	6.18	126.36	119.32
1	J	123	GLY	CA-C-N	6.15	125.64	119.24
1	J	123	GLY	C-N-CA	6.15	125.64	119.24
1	Q	97	VAL	N-CA-C	6.12	116.73	108.17
1	D	41	VAL	CB-CA-C	-6.11	101.09	110.50
1	C	118	GLY	N-CA-C	6.07	119.58	110.97
1	A	123	GLY	CA-C-N	6.06	125.54	119.24
1	A	123	GLY	C-N-CA	6.06	125.54	119.24
1	X	97	VAL	N-CA-C	5.96	116.89	108.36
1	R	119	VAL	N-CA-C	5.94	117.28	109.21
1	V	123	GLY	CA-C-N	5.93	125.64	119.05
1	V	123	GLY	C-N-CA	5.93	125.64	119.05
1	O	123	GLY	CA-C-N	5.92	125.40	119.24
1	O	123	GLY	C-N-CA	5.92	125.40	119.24
1	Z	123	GLY	CA-C-N	5.92	125.62	119.05
1	Z	123	GLY	C-N-CA	5.92	125.62	119.05
1	Y	30	ASN	N-CA-C	-5.90	105.94	113.02
1	H	97	VAL	N-CA-C	5.89	116.78	108.36
1	M	41	VAL	CB-CA-C	-5.89	100.53	110.71
1	2	123	GLY	CA-C-N	5.88	126.02	119.32
1	2	123	GLY	C-N-CA	5.88	126.02	119.32
1	R	97	VAL	N-CA-C	5.87	116.93	108.48
1	N	67	TYR	N-CA-C	5.86	118.41	111.33
1	A	105	VAL	N-CA-CB	-5.85	102.61	112.44
1	D	135	GLU	N-CA-C	-5.84	104.60	110.97
1	T	123	GLY	CA-C-N	5.84	125.32	119.24
1	T	123	GLY	C-N-CA	5.84	125.32	119.24
1	H	75	SER	N-CA-C	-5.83	102.28	110.50
1	Q	117	ILE	CB-CA-C	-5.82	102.67	112.16
1	1	65	ILE	N-CA-C	5.81	116.47	107.99
1	2	119	VAL	N-CA-C	5.81	116.30	108.17
1	F	97	VAL	N-CA-C	5.78	116.92	108.53
1	K	123	GLY	CA-C-N	5.78	125.91	119.32
1	K	123	GLY	C-N-CA	5.78	125.91	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	82	MSE	N-CA-C	5.75	118.32	111.71
1	E	117	ILE	CB-CA-C	-5.75	104.54	112.24
1	Y	123	GLY	CA-C-N	5.72	125.84	119.32
1	Y	123	GLY	C-N-CA	5.72	125.84	119.32
1	W	93	PHE	CA-C-N	5.69	126.02	119.93
1	W	93	PHE	C-N-CA	5.69	126.02	119.93
1	D	105	VAL	CB-CA-C	-5.62	102.80	110.90
1	2	67	TYR	N-CA-C	5.59	118.09	111.33
1	V	62	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	C	41	VAL	CB-CA-C	-5.57	101.49	110.28
1	Z	65	ILE	N-CA-C	5.55	116.09	107.99
1	2	114	VAL	N-CA-C	5.54	115.97	107.77
1	Y	71	VAL	N-CA-C	-5.50	106.33	111.45
1	G	65	ILE	N-CA-C	5.47	115.66	107.51
1	1	123	GLY	CA-C-N	5.46	125.11	119.05
1	1	123	GLY	C-N-CA	5.46	125.11	119.05
1	2	22	ARG	CG-CD-NE	-5.46	99.99	112.00
1	I	123	GLY	CA-C-N	5.41	124.92	119.19
1	I	123	GLY	C-N-CA	5.41	124.92	119.19
1	B	97	VAL	N-CA-C	5.38	116.33	108.53
1	1	67	TYR	N-CA-C	5.33	117.84	111.71
1	I	75	SER	N-CA-C	-5.33	102.98	110.50
1	A	109	GLY	CA-C-N	-5.31	114.22	122.67
1	A	109	GLY	C-N-CA	-5.31	114.22	122.67
1	P	97	VAL	N-CA-C	5.31	115.60	108.17
1	K	41	VAL	CB-CA-C	-5.30	101.54	110.71
1	A	97	VAL	N-CA-C	5.30	116.11	108.48
1	D	119	VAL	N-CA-C	5.29	115.88	108.89
1	W	71	VAL	N-CA-C	-5.28	106.54	111.45
1	S	99	TYR	N-CA-C	-5.25	101.14	109.96
1	P	65	ILE	N-CA-C	5.22	115.61	107.99
1	L	65	ILE	N-CA-C	5.19	115.57	107.99
1	Z	132	LEU	N-CA-C	-5.19	105.51	111.07
1	G	71	VAL	N-CA-C	-5.19	106.63	111.45
1	G	78	ARG	N-CA-C	-5.18	98.82	107.99
1	W	65	ILE	N-CA-C	5.17	115.54	107.99
1	G	135	GLU	CB-CA-C	-5.17	102.74	110.90
1	J	130	LYS	N-CA-C	-5.17	105.73	111.36
1	P	21	GLY	N-CA-C	-5.16	108.51	115.21
1	S	47	ILE	N-CA-C	5.15	116.08	108.45
1	Z	83	ARG	N-CA-C	-5.15	105.57	111.14
1	J	75	SER	N-CA-C	-5.15	102.65	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	132	LEU	N-CA-C	-5.15	105.75	111.36
1	G	111	LYS	CA-C-N	-5.15	115.95	123.06
1	G	111	LYS	C-N-CA	-5.15	115.95	123.06
1	R	80	ILE	N-CA-C	5.14	116.69	108.87
1	G	105	VAL	N-CA-CB	-5.12	103.83	112.44
1	T	97	VAL	N-CA-C	5.12	115.96	108.53
1	A	61	ASN	N-CA-C	-5.09	105.73	111.28
1	O	99	TYR	N-CA-C	-5.09	101.41	109.96
1	Y	99	TYR	N-CA-C	-5.09	100.87	108.96
1	I	30	ASN	N-CA-C	-5.08	106.93	113.02
1	W	56	ALA	N-CA-C	-5.07	106.88	113.16
1	S	65	ILE	N-CA-C	5.06	115.38	107.99
1	D	79	ARG	N-CA-C	-5.05	102.09	109.81
1	U	97	VAL	N-CA-C	5.02	115.20	108.17
1	1	79	ARG	N-CA-C	-5.01	103.06	110.48

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	34	TYR	Sidechain
1	B	34	TYR	Sidechain
1	C	34	TYR	Sidechain
1	C	69	TYR	Sidechain
1	H	34	TYR	Sidechain
1	I	34	TYR	Sidechain
1	V	34	TYR	Sidechain
1	W	34	TYR	Sidechain

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	1	1017	0	1042	38	0
1	2	1017	0	1042	30	0
1	A	1008	0	1029	21	0
1	B	1017	0	1042	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1017	0	1042	30	0
1	D	1017	0	1042	55	0
1	E	1017	0	1042	44	0
1	F	1017	0	1042	33	0
1	G	1017	0	1042	19	0
1	H	1028	0	1055	26	0
1	I	1028	0	1055	55	0
1	J	1028	0	1055	37	0
1	K	1028	0	1055	50	0
1	L	1017	0	1042	41	0
1	M	1028	0	1055	29	0
1	N	1028	0	1055	39	0
1	O	1017	0	1042	27	0
1	P	1017	0	1042	31	0
1	Q	1017	0	1042	32	0
1	R	1017	0	1042	41	0
1	S	1017	0	1042	41	0
1	T	1017	0	1042	36	0
1	U	1017	0	1042	42	0
1	V	1028	0	1055	29	0
1	W	1028	0	1055	23	0
1	X	1028	0	1055	43	0
1	Y	1028	0	1055	38	0
1	Z	1028	0	1055	43	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	O	1	0	0	0	0
2	P	2	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	V	1	0	0	0	0
4	1	6	0	5	0	0
4	2	6	0	4	0	0
4	A	6	0	4	1	0
4	G	6	0	4	0	0
4	H	12	0	9	5	0
4	J	6	0	4	0	0
4	M	6	0	4	0	0
4	R	6	0	4	0	0
4	V	6	0	4	0	0
4	W	6	0	5	2	0
4	X	6	0	4	2	0
5	1	4	0	3	0	0
5	2	4	0	3	1	0
5	F	4	0	3	0	0
5	H	4	0	3	0	0
5	I	8	0	6	0	0
5	K	4	0	3	4	0
5	M	4	0	3	0	0
5	N	4	0	4	0	0
5	V	4	0	3	0	0
5	W	8	0	6	7	0
5	X	4	0	3	0	0
5	Y	4	0	3	0	0
5	Z	4	0	3	0	0
6	1	52	0	0	5	0
6	2	75	0	0	2	0
6	A	67	0	0	3	0
6	B	64	0	0	4	0
6	C	64	0	0	5	0
6	D	46	0	0	3	0
6	E	48	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	69	0	0	4	0
6	G	74	0	0	3	0
6	H	67	0	0	1	0
6	I	58	0	0	6	1
6	J	47	0	0	2	0
6	K	42	0	0	2	0
6	L	59	0	0	5	0
6	M	98	0	0	2	0
6	N	89	0	0	2	0
6	O	72	0	0	1	0
6	P	63	0	0	1	0
6	Q	63	0	0	5	0
6	R	52	0	0	5	0
6	S	52	0	0	3	0
6	T	63	0	0	5	0
6	U	69	0	0	5	0
6	V	115	0	0	5	1
6	W	86	0	0	3	0
6	X	93	0	0	5	0
6	Y	77	0	0	4	0
6	Z	64	0	0	2	0
All	All	30641	0	29403	868	1

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 15.

All (868) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:4006:GOL:O1	4:W:4006:GOL:C1	1.63	1.47
1:V:82:MSE:SE	1:V:82:MSE:CE	1.26	1.45
1:R:80:ILE:HD11	1:R:116:GLU:HG2	1.25	1.14
1:V:82:MSE:SE	1:V:82:MSE:HE3	1.83	1.14
1:E:79:ARG:HH11	1:E:79:ARG:HB2	1.11	1.10
1:V:82:MSE:SE	1:V:82:MSE:HE2	1.83	1.10
1:S:107:LEU:HD13	1:Z:138:LYS:HZ3	1.16	1.10
1:V:82:MSE:SE	1:V:82:MSE:HE1	1.83	1.09
1:X:66:MSE:HE2	6:X:5006:HOH:O	1.51	1.07
1:Y:66:MSE:HE2	6:Y:5030:HOH:O	1.53	1.06
1:R:100:ILE:HD11	1:R:107:LEU:HD11	1.39	1.05
1:B:87:LYS:HG2	6:M:5096:HOH:O	1.56	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:127:GLU:HG3	1:L:131:ARG:NH1	1.77	1.00
1:I:20:LEU:HD23	1:I:38:LEU:HD22	1.41	0.99
1:E:79:ARG:HB2	1:E:79:ARG:NH1	1.77	0.99
1:B:62:ARG:HH22	1:C:138:LYS:HE3	1.28	0.98
1:H:88:GLN:HE22	1:H:139:ARG:HH12	1.10	0.98
1:S:113:ARG:NH1	1:Z:131:ARG:HG3	1.79	0.97
1:F:79:ARG:HG2	1:F:79:ARG:HH11	1.28	0.97
1:V:82:MSE:CE	1:V:82:MSE:CG	2.41	0.96
1:J:112:VAL:HG21	1:J:125:VAL:HG12	1.49	0.95
1:D:92:ILE:HD12	1:D:132:LEU:HD22	1.48	0.94
1:D:66:MSE:HE2	6:D:2012:HOH:O	1.68	0.94
1:Y:80:ILE:HG22	6:Y:5015:HOH:O	1.65	0.93
1:R:100:ILE:HD11	1:R:107:LEU:CD1	1.99	0.93
1:S:107:LEU:HD13	1:Z:138:LYS:NZ	1.85	0.91
1:S:72:HIS:HD2	1:S:74:ASP:OD2	1.52	0.90
1:R:79:ARG:HB3	1:R:79:ARG:NH1	1.87	0.89
1:D:66:MSE:CE	1:D:66:MSE:HA	2.03	0.89
1:Z:82:MSE:HE1	1:Z:114:VAL:HG12	1.55	0.89
1:P:83:ARG:HD2	1:V:17:ASN:ND2	1.88	0.88
1:B:25:GLN:HE21	1:B:35:LYS:HZ2	1.20	0.88
1:R:68:ARG:HG2	6:R:4014:HOH:O	1.73	0.87
6:T:175:HOH:O	1:Y:138:LYS:HE3	1.74	0.87
1:I:72:HIS:HD2	1:I:74:ASP:OD1	1.58	0.86
1:T:62:ARG:HH22	1:U:138:LYS:HE2	1.40	0.86
1:B:25:GLN:HE21	1:B:35:LYS:NZ	1.72	0.86
4:H:4002:GOL:H12	1:I:79:ARG:HH21	1.40	0.85
1:G:72:HIS:HD2	1:G:74:ASP:OD1	1.60	0.84
1:2:72:HIS:HD2	1:2:74:ASP:OD1	1.61	0.83
1:P:51:ASN:HA	1:P:59:LYS:HE2	1.61	0.83
1:I:20:LEU:HD23	1:I:38:LEU:CD2	2.08	0.83
1:C:80:ILE:HD12	1:C:116:GLU:HB2	1.60	0.83
1:E:72:HIS:HD2	1:E:74:ASP:OD1	1.61	0.83
1:P:83:ARG:HD2	1:V:17:ASN:HD21	1.42	0.82
1:X:72:HIS:HD2	1:X:74:ASP:OD2	1.62	0.82
1:B:62:ARG:NH2	1:C:138:LYS:HE3	1.93	0.82
1:Y:72:HIS:HD2	1:Y:74:ASP:OD1	1.63	0.82
1:L:72:HIS:HD2	1:L:74:ASP:OD1	1.64	0.81
1:Z:72:HIS:HD2	1:Z:74:ASP:OD1	1.62	0.81
1:O:119:VAL:HG21	1:O:130:LYS:HG3	1.61	0.81
1:C:68:ARG:NH2	6:C:189:HOH:O	2.13	0.81
1:D:66:MSE:HE2	1:D:66:MSE:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:HIS:HD2	1:F:74:ASP:OD1	1.63	0.81
1:W:72:HIS:HD2	1:W:74:ASP:OD1	1.65	0.80
1:T:72:HIS:HD2	1:T:74:ASP:OD1	1.64	0.80
1:2:23:GLU:HG2	1:2:35:LYS:NZ	1.95	0.80
1:E:137:LEU:O	1:E:138:LYS:HG3	1.82	0.80
1:D:100:ILE:HD11	1:D:107:LEU:HG	1.64	0.80
1:M:72:HIS:HD2	1:M:74:ASP:OD1	1.64	0.80
1:R:80:ILE:CD1	1:R:116:GLU:HG2	2.09	0.80
1:N:95:GLY:O	1:N:96:MSE:HE2	1.82	0.79
1:Z:88:GLN:HA	1:Z:91:LYS:HE3	1.64	0.79
1:F:79:ARG:HG2	1:F:79:ARG:NH1	1.93	0.79
1:K:35:LYS:HE3	1:K:76:THR:HG21	1.65	0.78
1:X:66:MSE:HA	1:X:66:MSE:CE	2.14	0.78
1:R:79:ARG:HB3	1:R:79:ARG:HH11	1.47	0.78
1:N:72:HIS:HD2	1:N:74:ASP:OD1	1.66	0.78
1:N:26:VAL:HG13	1:N:73:ILE:CD1	2.14	0.77
1:C:80:ILE:HD11	1:C:116:GLU:OE2	1.84	0.77
1:1:72:HIS:HD2	1:1:74:ASP:OD1	1.67	0.77
1:C:102:GLU:OE1	1:L:22:ARG:NH2	2.17	0.77
1:N:22:ARG:HB3	1:N:22:ARG:HH11	1.50	0.77
1:K:72:HIS:HD2	1:K:74:ASP:OD1	1.67	0.76
1:H:23:GLU:OE2	1:H:35:LYS:HE2	1.85	0.76
1:2:93:PHE:HB3	1:2:96:MSE:HE3	1.67	0.76
1:D:105:VAL:HG11	1:D:113:ARG:HG3	1.67	0.76
1:U:131:ARG:HD2	6:U:2069:HOH:O	1.86	0.76
1:Z:32:GLU:OE2	1:1:72:HIS:HE1	1.68	0.76
1:I:139:ARG:HB3	1:I:139:ARG:NH1	2.00	0.76
1:A:72:HIS:HD2	1:A:74:ASP:OD1	1.69	0.75
1:Y:66:MSE:HE3	1:Z:12:PHE:CZ	2.22	0.75
1:D:18:ASN:HD22	1:D:83:ARG:HH12	1.34	0.75
1:J:72:HIS:HD2	1:J:74:ASP:OD1	1.68	0.75
1:E:54:ASN:C	1:E:54:ASN:HD22	1.94	0.75
1:R:32:GLU:OE2	1:S:72:HIS:HE1	1.70	0.75
1:H:72:HIS:HD2	1:H:74:ASP:OD1	1.68	0.75
1:W:61:ASN:HB3	6:W:5022:HOH:O	1.87	0.75
1:E:55:LYS:O	1:V:111:LYS:HD3	1.87	0.74
1:B:72:HIS:HD2	1:B:74:ASP:OD1	1.71	0.74
1:L:32:GLU:OE2	1:M:72:HIS:HE1	1.69	0.74
1:L:127:GLU:HG3	1:L:131:ARG:HH12	1.51	0.74
1:Q:102:GLU:OE2	1:2:22:ARG:NH2	2.20	0.74
1:D:100:ILE:CD1	1:D:107:LEU:HG	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:77:GLU:HB2	5:W:5011:ACY:H3	1.69	0.73
1:B:59:LYS:HD2	1:B:60:PHE:N	2.03	0.73
1:Z:135:GLU:O	1:Z:139:ARG:HG3	1.88	0.73
1:1:61:ASN:OD1	6:1:5019:HOH:O	2.04	0.73
1:A:32:GLU:OE2	1:B:72:HIS:HE1	1.71	0.73
1:R:80:ILE:HD11	1:R:116:GLU:CG	2.14	0.73
1:S:113:ARG:HH11	1:Z:131:ARG:HG3	1.50	0.73
1:X:66:MSE:HE3	1:Y:12:PHE:CZ	2.24	0.73
1:P:72:HIS:HD2	1:P:74:ASP:OD1	1.71	0.73
1:D:47:ILE:HD12	1:D:70:ILE:HD13	1.70	0.73
1:K:91:LYS:NZ	1:K:91:LYS:HB3	2.03	0.73
1:O:119:VAL:HG21	1:O:130:LYS:CG	2.18	0.73
1:M:131:ARG:HG2	6:M:5044:HOH:O	1.89	0.73
1:1:127:GLU:O	1:1:131:ARG:HD3	1.89	0.72
1:Q:80:ILE:HD12	1:Q:116:GLU:OE1	1.90	0.72
1:2:72:HIS:CD2	1:2:74:ASP:OD1	2.42	0.72
1:E:123:GLY:O	1:E:127:GLU:HG2	1.90	0.72
1:Q:32:GLU:OE2	1:R:72:HIS:HE1	1.71	0.72
1:D:103:THR:OG1	1:D:105:VAL:HG23	1.89	0.72
1:A:72:HIS:HE1	1:G:32:GLU:OE2	1.72	0.72
1:B:32:GLU:OE2	1:C:72:HIS:HE1	1.73	0.72
1:J:82:MSE:HE1	1:J:114:VAL:HG12	1.70	0.72
1:K:132:LEU:HD22	1:K:136:PHE:CE1	2.24	0.72
1:W:66:MSE:HE1	1:X:45:LEU:HG	1.72	0.72
1:O:72:HIS:HD2	1:O:74:ASP:OD1	1.72	0.71
1:I:38:LEU:C	1:I:38:LEU:HD23	2.14	0.71
1:M:15:GLU:CD	1:M:15:GLU:H	1.96	0.71
1:E:47:ILE:HD12	1:E:70:ILE:HD13	1.70	0.71
1:H:88:GLN:NE2	1:H:139:ARG:HH12	1.86	0.71
1:O:72:HIS:HE1	1:U:32:GLU:OE2	1.73	0.70
1:U:72:HIS:HD2	1:U:74:ASP:OD1	1.73	0.70
1:D:66:MSE:HE3	1:E:12:PHE:CZ	2.27	0.70
1:Q:131:ARG:HD2	6:Q:2071:HOH:O	1.91	0.70
1:F:135:GLU:O	1:F:138:LYS:HB3	1.91	0.70
1:L:23:GLU:OE1	1:L:35:LYS:HD2	1.92	0.69
1:V:32:GLU:OE2	1:W:72:HIS:HE1	1.75	0.69
1:G:131:ARG:HD2	6:G:4068:HOH:O	1.92	0.69
1:I:110:ASP:C	1:I:111:LYS:HD2	2.17	0.69
1:S:105:VAL:HG11	1:S:113:ARG:HH21	1.58	0.69
1:J:100:ILE:HD11	1:J:107:LEU:CD1	2.23	0.68
1:O:92:ILE:HD12	1:O:92:ILE:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:72:HIS:CD2	1:S:74:ASP:OD2	2.43	0.68
1:G:72:HIS:CD2	1:G:74:ASP:OD1	2.46	0.68
1:R:100:ILE:CD1	1:R:107:LEU:HD11	2.19	0.68
1:T:136:PHE:C	1:T:138:LYS:H	2.00	0.68
1:L:72:HIS:CD2	1:L:74:ASP:OD1	2.46	0.68
1:S:43:ASN:HD21	1:Z:12:PHE:N	1.90	0.68
1:X:66:MSE:CE	6:X:5006:HOH:O	2.25	0.68
1:Z:68:ARG:NH2	6:Z:5048:HOH:O	2.27	0.68
1:W:45:LEU:N	1:W:45:LEU:HD22	2.09	0.68
1:P:52:ALA:O	1:P:59:LYS:HD3	1.94	0.68
1:R:83:ARG:HD3	1:I:18:ASN:OD1	1.92	0.67
1:F:113:ARG:NH1	1:I:134:GLU:OE2	2.27	0.67
1:F:113:ARG:NH1	1:I:134:GLU:OE1	2.28	0.67
1:C:32:GLU:OE2	1:D:72:HIS:HE1	1.78	0.66
1:F:81:ASP:OD1	1:F:83:ARG:HD2	1.96	0.66
1:K:35:LYS:CE	1:K:76:THR:HG21	2.26	0.66
1:R:79:ARG:HH11	1:R:79:ARG:CB	2.08	0.66
1:T:12:PHE:N	1:Y:43:ASN:HD21	1.94	0.66
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.61	0.66
1:P:32:GLU:OE1	1:Q:72:HIS:HE1	1.79	0.66
1:D:47:ILE:CD1	1:D:73:ILE:HD11	2.25	0.66
1:U:138:LYS:NZ	6:U:2079:HOH:O	2.29	0.66
1:Y:66:MSE:HE1	1:Z:45:LEU:HD23	1.78	0.66
1:R:72:HIS:HD2	1:R:74:ASP:OD1	1.79	0.66
1:J:37:VAL:HG23	1:J:50:ALA:HB3	1.78	0.65
1:2:23:GLU:HG2	1:2:35:LYS:HZ2	1.57	0.65
1:F:113:ARG:NH1	1:I:134:GLU:CD	2.55	0.65
1:E:70:ILE:HG21	1:E:73:ILE:HD11	1.79	0.65
1:F:131:ARG:NH1	6:F:5074:HOH:O	2.28	0.65
1:K:132:LEU:HD22	1:K:136:PHE:HE1	1.61	0.65
1:L:85:PHE:CE1	1:L:132:LEU:HD13	2.32	0.65
1:D:124:PRO:HG2	1:L:100:ILE:HD13	1.79	0.65
1:S:113:ARG:HH11	1:Z:131:ARG:CG	2.10	0.65
1:S:131:ARG:HA	1:S:134:GLU:CD	2.22	0.65
1:C:72:HIS:HD2	1:C:74:ASP:OD1	1.79	0.65
1:L:113:ARG:NH1	6:L:2026:HOH:O	2.30	0.65
1:W:82:MSE:HE1	1:W:114:VAL:HG12	1.78	0.65
1:X:26:VAL:HG13	1:X:73:ILE:CD1	2.26	0.64
1:D:66:MSE:HA	1:D:66:MSE:HE3	1.79	0.64
1:T:72:HIS:CD2	1:T:74:ASP:OD1	2.50	0.64
1:X:66:MSE:HA	1:X:66:MSE:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:ILE:HD12	1:I:70:ILE:HD13	1.80	0.64
1:I:134:GLU:O	1:I:138:LYS:HG3	1.97	0.64
1:I:72:HIS:CD2	1:I:74:ASP:OD1	2.48	0.64
1:R:136:PHE:C	1:R:138:LYS:H	2.05	0.64
1:M:26:VAL:HG13	1:M:73:ILE:CD1	2.28	0.64
1:C:96:MSE:HE3	1:C:109:GLY:HA2	1.78	0.64
1:I:139:ARG:HB3	1:I:139:ARG:CZ	2.28	0.63
1:K:100:ILE:HD11	1:K:107:LEU:CD1	2.27	0.63
1:N:17:ASN:O	1:N:20:LEU:HD22	1.99	0.63
1:L:84:GLU:OE2	1:L:87:LYS:HD2	1.99	0.63
1:W:32:GLU:OE1	1:X:72:HIS:HE1	1.80	0.63
1:W:75:SER:HB2	5:W:5011:ACY:CH3	2.28	0.63
1:Y:91:LYS:HB3	1:Y:91:LYS:NZ	2.13	0.63
1:D:32:GLU:OE2	1:E:72:HIS:HE1	1.82	0.63
1:F:91:LYS:O	1:J:117:ILE:HD11	1.99	0.63
1:Y:80:ILE:HD11	1:Y:85:PHE:HB2	1.80	0.63
1:J:37:VAL:CG2	1:J:50:ALA:HB3	2.29	0.63
1:Y:72:HIS:CD2	1:Y:74:ASP:OD1	2.50	0.63
1:D:47:ILE:HD11	1:D:73:ILE:HD11	1.80	0.63
1:U:13:VAL:HG22	1:U:45:LEU:HD13	1.80	0.62
1:P:51:ASN:CA	1:P:59:LYS:HE2	2.28	0.62
1:I:111:LYS:HD2	1:I:111:LYS:N	2.13	0.62
1:U:79:ARG:HD3	6:U:2067:HOH:O	1.98	0.62
1:S:22:ARG:HG3	1:S:79:ARG:HD2	1.81	0.62
1:D:100:ILE:N	1:D:100:ILE:HD12	2.14	0.62
1:I:56:ALA:HA	6:I:5051:HOH:O	1.98	0.62
1:Y:35:LYS:NZ	6:Y:5031:HOH:O	2.32	0.62
1:2:79:ARG:NH2	1:2:117:ILE:HD11	2.14	0.62
1:P:83:ARG:HD3	1:V:18:ASN:OD1	1.98	0.62
1:D:91:LYS:HE3	1:D:91:LYS:HA	1.81	0.62
1:F:124:PRO:HD2	6:J:4025:HOH:O	2.00	0.62
1:Y:32:GLU:OE2	1:Z:72:HIS:HE1	1.83	0.62
4:A:4012:GOL:O2	1:B:33:VAL:HG21	2.00	0.61
1:M:88:GLN:HE22	1:M:139:ARG:HH12	1.47	0.61
1:I:32:GLU:OE2	1:J:72:HIS:HE1	1.83	0.61
1:J:32:GLU:OE2	1:K:72:HIS:HE1	1.83	0.61
1:I:13:VAL:HG22	1:I:45:LEU:HD13	1.82	0.61
1:J:70:ILE:HG21	1:J:73:ILE:HD11	1.82	0.61
1:M:110:ASP:OD2	1:M:111:LYS:HG3	2.01	0.61
1:W:77:GLU:H	5:W:5011:ACY:H1	1.65	0.61
1:B:25:GLN:NE2	1:B:35:LYS:NZ	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LYS:O	1:L:117:ILE:HD11	2.00	0.61
1:E:112:VAL:HG21	1:E:125:VAL:HG12	1.81	0.61
1:Z:72:HIS:CD2	1:Z:74:ASP:OD1	2.51	0.61
1:K:127:GLU:OE1	1:K:131:ARG:NH1	2.34	0.60
1:A:105:VAL:HG21	1:A:113:ARG:CZ	2.31	0.60
1:2:23:GLU:HG2	1:2:35:LYS:HZ1	1.66	0.60
1:2:77:GLU:OE2	6:2:5034:HOH:O	2.16	0.60
1:C:116:GLU:HG2	6:C:195:HOH:O	2.00	0.60
1:E:43:ASN:HD21	1:J:12:PHE:N	1.99	0.60
1:X:82:MSE:HE1	1:X:114:VAL:HG12	1.83	0.60
1:F:43:ASN:HD21	1:I:12:PHE:N	1.99	0.60
1:D:124:PRO:HD2	6:L:2024:HOH:O	2.02	0.60
1:I:35:LYS:HE2	1:I:76:THR:HG21	1.84	0.60
1:C:80:ILE:CD1	1:C:116:GLU:HB2	2.31	0.60
1:T:17:ASN:HA	1:T:20:LEU:CD2	2.31	0.60
1:U:136:PHE:C	1:U:138:LYS:H	2.10	0.60
1:B:131:ARG:O	1:B:135:GLU:HG3	2.03	0.59
1:N:57:GLY:O	1:N:59:LYS:HD2	2.02	0.59
1:I:93:PHE:HB3	1:I:96:MSE:SE	2.51	0.59
1:B:62:ARG:HH22	1:C:138:LYS:CE	2.08	0.59
1:R:43:ASN:HD21	1:I:12:PHE:N	2.00	0.59
1:U:105:VAL:HG12	1:U:106:VAL:N	2.16	0.59
1:I:127:GLU:OE1	1:I:131:ARG:NH1	2.33	0.59
1:I:80:ILE:HD13	1:I:136:PHE:CB	2.32	0.59
1:L:127:GLU:CG	1:L:131:ARG:HH12	2.15	0.59
1:P:22:ARG:HG3	1:P:79:ARG:HD2	1.83	0.59
1:C:43:ASN:HD21	1:L:12:PHE:N	2.01	0.59
1:M:15:GLU:CD	1:M:15:GLU:N	2.61	0.59
1:A:66:MSE:HE1	1:B:45:LEU:HB3	1.85	0.59
1:B:97:VAL:HG22	1:B:108:ILE:HD13	1.84	0.59
1:D:92:ILE:HD11	1:D:132:LEU:HD13	1.84	0.59
1:S:62:ARG:HH12	1:T:138:LYS:HZ1	1.50	0.59
1:Q:12:PHE:N	1:2:43:ASN:HD21	2.01	0.59
1:A:79:ARG:HD3	6:A:4047:HOH:O	2.03	0.59
1:Z:116:GLU:HG3	1:Z:117:ILE:HD13	1.85	0.59
1:F:59:LYS:HB3	6:F:5062:HOH:O	2.03	0.58
1:P:59:LYS:HD3	1:P:60:PHE:H	1.68	0.58
1:T:20:LEU:HD13	1:T:38:LEU:HD13	1.84	0.58
1:S:113:ARG:HH12	1:Z:131:ARG:HG3	1.65	0.58
1:I:102:GLU:OE1	6:I:5047:HOH:O	2.17	0.58
1:P:54:ASN:C	1:P:54:ASN:HD22	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:83:ARG:HD3	1:2:18:ASN:OD1	2.03	0.58
1:U:22:ARG:HD3	1:U:79:ARG:HH11	1.67	0.58
1:X:66:MSE:HE2	1:X:66:MSE:HA	1.85	0.58
1:H:26:VAL:HG13	1:H:73:ILE:HD13	1.85	0.58
1:S:30:ASN:N	1:S:30:ASN:HD22	2.02	0.58
1:K:131:ARG:O	1:K:135:GLU:HG2	2.04	0.58
1:V:93:PHE:HZ	1:V:128:ARG:HB3	1.68	0.57
1:X:26:VAL:HG13	1:X:73:ILE:HD13	1.85	0.57
1:X:72:HIS:CD2	1:X:74:ASP:OD2	2.52	0.57
1:L:93:PHE:HB3	1:L:96:MSE:HG3	1.86	0.57
1:K:93:PHE:CA	1:K:96:MSE:HE3	2.34	0.57
1:D:92:ILE:CD1	1:D:132:LEU:HD13	2.33	0.57
1:I:80:ILE:CD1	1:I:136:PHE:HB3	2.34	0.57
1:S:83:ARG:NE	6:S:3052:HOH:O	2.37	0.57
1:G:43:ASN:HD21	1:H:12:PHE:N	2.01	0.57
1:J:37:VAL:HG22	1:J:50:ALA:O	2.05	0.57
1:Q:102:GLU:CD	1:2:22:ARG:HH22	2.12	0.57
1:W:45:LEU:HD23	6:W:5043:HOH:O	2.04	0.57
1:I:15:GLU:OE2	6:I:5054:HOH:O	2.18	0.57
1:F:83:ARG:HG3	1:F:83:ARG:HH11	1.69	0.57
1:K:32:GLU:OE2	1:L:72:HIS:HE1	1.87	0.56
1:O:119:VAL:HG22	6:O:2058:HOH:O	2.05	0.56
1:Y:66:MSE:HA	1:Y:66:MSE:CE	2.35	0.56
1:I:97:VAL:HG22	1:I:108:ILE:HG12	1.85	0.56
1:E:126:ALA:HB1	1:E:130:LYS:NZ	2.20	0.56
1:G:120:GLU:CD	1:H:131:ARG:HH21	2.13	0.56
1:H:88:GLN:HE22	1:H:139:ARG:NH1	1.91	0.56
1:H:100:ILE:HD11	1:H:107:LEU:HD12	1.87	0.56
1:Q:120:GLU:OE1	1:2:131:ARG:NH2	2.37	0.56
1:U:136:PHE:C	1:U:138:LYS:N	2.63	0.56
1:Z:17:ASN:ND2	1:Z:41:VAL:CG1	2.68	0.56
1:I:55:LYS:C	6:I:5051:HOH:O	2.47	0.56
1:J:85:PHE:CE1	1:J:132:LEU:HD13	2.40	0.56
1:Z:55:LYS:HD2	6:Z:5020:HOH:O	2.05	0.56
1:J:128:ARG:O	1:J:128:ARG:HD3	2.06	0.56
1:R:136:PHE:C	1:R:138:LYS:N	2.62	0.56
1:S:30:ASN:HD22	1:S:30:ASN:H	1.53	0.56
1:G:83:ARG:HD3	6:G:4055:HOH:O	2.06	0.56
1:D:12:PHE:N	1:K:43:ASN:HD21	2.04	0.56
1:O:110:ASP:OD1	1:O:111:LYS:HE3	2.06	0.56
1:T:32:GLU:OE2	1:U:72:HIS:HE1	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:96:MSE:HE3	1:U:109:GLY:HA2	1.88	0.56
1:M:12:PHE:HB2	1:M:15:GLU:HG2	1.87	0.56
1:Q:23:GLU:OE1	1:Q:35:LYS:HE3	2.06	0.56
1:F:113:ARG:HH12	1:I:134:GLU:CD	2.14	0.55
1:A:43:ASN:HD21	1:N:12:PHE:N	2.04	0.55
1:E:113:ARG:NH2	6:E:2037:HOH:O	2.39	0.55
1:K:91:LYS:HB3	1:K:91:LYS:HZ2	1.70	0.55
1:S:12:PHE:N	1:Z:43:ASN:HD21	2.04	0.55
1:S:18:ASN:HD22	1:S:83:ARG:HH21	1.53	0.55
1:D:105:VAL:HG12	1:D:106:VAL:N	2.21	0.55
1:Q:98:LYS:HE3	6:Q:2043:HOH:O	2.06	0.55
1:U:80:ILE:HD12	1:U:116:GLU:HG2	1.87	0.55
4:W:4006:GOL:C1	4:W:4006:GOL:HO1	2.07	0.55
1:X:32:GLU:OE2	1:Y:72:HIS:HE1	1.89	0.55
1:J:44:GLN:O	1:J:45:LEU:HB2	2.06	0.55
1:M:32:GLU:OE2	1:N:72:HIS:HE1	1.89	0.55
1:Y:85:PHE:CE1	1:Y:132:LEU:HD13	2.42	0.55
1:A:133:PHE:CE2	1:A:137:LEU:HD11	2.41	0.55
1:E:79:ARG:NH1	1:E:79:ARG:CB	2.63	0.55
1:E:98:LYS:HB2	1:E:98:LYS:NZ	2.21	0.55
1:R:80:ILE:CD1	1:R:82:MSE:HE3	2.37	0.55
1:W:66:MSE:CE	1:X:12:PHE:HE2	2.20	0.55
1:I:93:PHE:CE2	1:I:125:VAL:HG13	2.42	0.55
1:E:53:SER:HA	1:E:58:GLU:O	2.07	0.55
1:F:12:PHE:N	1:I:43:ASN:HD21	2.05	0.55
1:P:87:LYS:HD3	6:V:5080:HOH:O	2.07	0.55
1:S:123:GLY:O	1:S:127:GLU:HG3	2.06	0.55
1:U:22:ARG:HD3	1:U:79:ARG:NH1	2.21	0.55
1:M:26:VAL:HG22	1:M:73:ILE:HD12	1.89	0.55
1:T:92:ILE:HG13	1:T:132:LEU:HD13	1.89	0.54
1:X:84:GLU:OE1	1:X:88:GLN:NE2	2.39	0.54
1:2:100:ILE:HD11	1:2:107:LEU:CD1	2.37	0.54
1:C:90:GLU:OE2	6:C:163:HOH:O	2.19	0.54
1:H:32:GLU:OE2	1:I:72:HIS:HE1	1.91	0.54
1:S:79:ARG:HD3	6:S:3024:HOH:O	2.07	0.54
1:U:72:HIS:CD2	1:U:74:ASP:OD1	2.57	0.54
1:H:100:ILE:HD11	1:H:107:LEU:CD1	2.37	0.54
1:T:136:PHE:C	1:T:138:LYS:N	2.66	0.54
1:U:105:VAL:CG1	1:U:106:VAL:N	2.70	0.54
1:W:75:SER:HB2	5:W:5011:ACY:H1	1.89	0.54
1:D:66:MSE:CE	6:D:2012:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:72:HIS:CD2	1:O:74:ASP:OD1	2.58	0.53
1:X:55:LYS:NZ	6:X:5049:HOH:O	2.40	0.53
1:Z:111:LYS:HD2	1:Z:111:LYS:N	2.23	0.53
1:O:32:GLU:OE2	1:P:72:HIS:HE1	1.91	0.53
1:P:61:ASN:ND2	1:Q:78:ARG:HD3	2.23	0.53
1:2:55:LYS:NZ	6:2:5070:HOH:O	2.28	0.53
1:2:93:PHE:CB	1:2:96:MSE:HE3	2.37	0.53
1:E:12:PHE:N	1:J:43:ASN:HD21	2.06	0.53
1:S:107:LEU:CD1	1:Z:138:LYS:HZ3	2.06	0.53
1:Z:136:PHE:HA	1:Z:139:ARG:HD2	1.91	0.53
1:E:81:ASP:OD1	1:E:83:ARG:HB2	2.08	0.53
1:N:22:ARG:HH11	1:N:22:ARG:CB	2.20	0.53
1:U:43:ASN:HD21	1:X:12:PHE:N	2.06	0.53
1:C:100:ILE:HD13	1:C:107:LEU:HG	1.91	0.53
1:X:66:MSE:HE1	1:Y:45:LEU:HD23	1.89	0.53
1:X:79:ARG:HH21	4:X:4004:GOL:H11	1.74	0.53
1:X:139:ARG:HD2	1:X:139:ARG:N	2.23	0.53
1:S:54:ASN:HD22	1:S:54:ASN:C	2.17	0.53
1:S:113:ARG:NH1	1:Z:131:ARG:CZ	2.71	0.53
1:H:78:ARG:HG2	6:H:5067:HOH:O	2.09	0.53
1:T:62:ARG:HH22	1:U:138:LYS:CE	2.16	0.53
1:Z:13:VAL:HG22	1:Z:45:LEU:HD13	1.91	0.53
1:C:83:ARG:NE	1:L:18:ASN:OD1	2.41	0.53
1:E:99:TYR:OH	1:E:104:ASN:ND2	2.41	0.53
1:L:17:ASN:O	1:L:20:LEU:HD13	2.09	0.53
1:N:26:VAL:HG22	1:N:73:ILE:HD12	1.90	0.53
1:D:72:HIS:HD2	1:D:74:ASP:OD1	1.93	0.52
1:D:131:ARG:O	1:D:135:GLU:HG2	2.08	0.52
1:K:83:ARG:NH1	1:K:101:GLU:OE2	2.42	0.52
1:L:83:ARG:HH22	1:L:101:GLU:HG3	1.74	0.52
1:M:12:PHE:CB	1:M:15:GLU:HG2	2.39	0.52
1:X:13:VAL:HG22	1:X:45:LEU:HD13	1.91	0.52
1:D:18:ASN:ND2	1:D:83:ARG:HH12	2.04	0.52
1:O:70:ILE:HG21	1:O:73:ILE:HD11	1.91	0.52
1:F:32:GLU:OE2	1:G:72:HIS:HE1	1.91	0.52
1:I:89:ALA:O	1:I:93:PHE:HD1	1.92	0.52
1:F:79:ARG:HH11	1:F:79:ARG:CG	2.11	0.52
1:K:47:ILE:HD12	1:K:70:ILE:HD13	1.92	0.52
1:M:113:ARG:HD3	1:M:120:GLU:OE2	2.08	0.52
1:N:95:GLY:C	1:N:96:MSE:HE2	2.34	0.52
1:N:131:ARG:O	1:N:135:GLU:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:17:ASN:HA	1:T:20:LEU:HD22	1.92	0.52
1:F:66:MSE:SE	1:G:45:LEU:HD13	2.60	0.52
1:H:72:HIS:HE1	1:N:32:GLU:OE2	1.93	0.52
1:O:12:PHE:N	1:W:43:ASN:HD21	2.05	0.52
1:T:17:ASN:O	1:T:20:LEU:CD2	2.57	0.52
1:W:72:HIS:CD2	1:W:74:ASP:OD1	2.55	0.52
1:I:38:LEU:CD2	1:I:38:LEU:C	2.81	0.52
1:O:43:ASN:HD21	1:W:12:PHE:N	2.08	0.52
1:2:93:PHE:HB3	1:2:96:MSE:CE	2.39	0.52
1:R:131:ARG:NE	6:R:4020:HOH:O	2.21	0.52
1:G:12:PHE:N	1:H:43:ASN:HD21	2.08	0.52
1:I:98:LYS:HE3	6:I:5050:HOH:O	2.10	0.52
1:K:80:ILE:HD12	1:K:133:PHE:CE2	2.44	0.52
1:L:22:ARG:NH1	1:L:77:GLU:OE2	2.43	0.52
1:O:18:ASN:HD22	1:O:83:ARG:HH21	1.57	0.52
1:O:88:GLN:O	1:O:92:ILE:HD13	2.09	0.52
1:P:130:LYS:O	1:P:134:GLU:HG2	2.09	0.52
1:U:41:VAL:HG12	1:U:47:ILE:HD12	1.91	0.52
1:U:78:ARG:O	1:U:79:ARG:HB2	2.10	0.52
1:P:44:GLN:O	1:P:45:LEU:HB2	2.08	0.52
1:U:41:VAL:HG12	1:U:47:ILE:CD1	2.40	0.52
1:D:47:ILE:HD12	1:D:70:ILE:CD1	2.39	0.51
1:M:67:TYR:OH	1:M:68:ARG:NH1	2.43	0.51
1:S:113:ARG:NH1	1:Z:131:ARG:CG	2.61	0.51
1:N:26:VAL:HG13	1:N:73:ILE:HD11	1.92	0.51
1:F:53:SER:HA	1:F:58:GLU:O	2.10	0.51
1:K:16:LEU:HD21	1:K:73:ILE:HD13	1.91	0.51
1:N:72:HIS:C	1:N:73:ILE:HD13	2.35	0.51
1:P:54:ASN:ND2	1:P:56:ALA:H	2.07	0.51
1:E:133:PHE:O	1:E:136:PHE:HB3	2.10	0.51
1:K:76:THR:HG22	1:K:76:THR:O	2.09	0.51
1:T:96:MSE:HE3	1:T:109:GLY:HA2	1.92	0.51
1:C:12:PHE:N	1:L:43:ASN:HD21	2.09	0.51
1:E:32:GLU:OE2	1:F:72:HIS:HE1	1.94	0.51
1:G:47:ILE:HD12	1:G:70:ILE:HD13	1.93	0.51
1:S:135:GLU:HA	1:S:135:GLU:OE1	2.11	0.51
1:E:124:PRO:HB2	5:K:5013:ACY:H1	1.92	0.51
1:K:82:MSE:HE1	1:K:114:VAL:HG12	1.91	0.51
1:2:82:MSE:HE1	1:2:114:VAL:HG12	1.93	0.51
1:A:55:LYS:HE2	6:A:4063:HOH:O	2.11	0.51
1:W:66:MSE:HE2	1:X:12:PHE:HE2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:89:ALA:O	1:Z:93:PHE:HD1	1.94	0.51
1:J:72:HIS:CD2	1:J:74:ASP:OD1	2.58	0.51
1:K:15:GLU:O	1:K:19:LEU:HD22	2.11	0.51
1:N:15:GLU:H	1:N:15:GLU:CD	2.18	0.51
1:W:135:GLU:O	1:W:139:ARG:HG3	2.11	0.51
1:E:92:ILE:HD13	1:E:132:LEU:HD13	1.91	0.50
1:G:92:ILE:HG13	1:G:132:LEU:HD13	1.93	0.50
1:K:100:ILE:HD11	1:K:107:LEU:HG	1.92	0.50
1:R:12:PHE:N	1:I:43:ASN:HD21	2.08	0.50
1:B:118:GLY:HA2	1:B:133:PHE:CE2	2.47	0.50
1:R:25:GLN:NE2	6:R:4049:HOH:O	2.39	0.50
1:B:17:ASN:HA	1:B:20:LEU:HD22	1.94	0.50
1:C:118:GLY:HA2	1:C:133:PHE:CE2	2.46	0.50
1:D:110:ASP:HB2	1:K:138:LYS:HE3	1.92	0.50
1:F:68:ARG:HB2	6:F:5018:HOH:O	2.11	0.50
1:S:62:ARG:HH22	1:T:138:LYS:NZ	2.09	0.50
1:F:44:GLN:O	1:F:45:LEU:HB2	2.12	0.50
1:H:72:HIS:CD2	1:H:74:ASP:OD1	2.57	0.50
1:N:22:ARG:NH1	1:N:77:GLU:OE1	2.44	0.50
1:P:87:LYS:NZ	6:P:2042:HOH:O	2.41	0.50
1:D:85:PHE:HB2	1:D:136:PHE:CE2	2.47	0.50
1:I:139:ARG:NH1	1:I:139:ARG:CB	2.72	0.50
1:O:91:LYS:O	1:X:117:ILE:HD11	2.12	0.50
1:W:45:LEU:N	1:W:45:LEU:CD2	2.74	0.50
1:X:66:MSE:HE3	1:Y:12:PHE:HZ	1.71	0.50
1:B:13:VAL:HG22	1:B:45:LEU:HD13	1.93	0.50
1:I:80:ILE:CD1	1:I:136:PHE:CB	2.89	0.50
1:N:72:HIS:CD2	1:N:74:ASP:OD1	2.56	0.50
1:Q:13:VAL:HG22	1:Q:45:LEU:HD13	1.94	0.50
1:Q:72:HIS:HD2	1:Q:74:ASP:OD1	1.95	0.50
1:R:80:ILE:HD12	1:R:82:MSE:HE3	1.94	0.50
1:Y:92:ILE:C	1:Y:94:PRO:HD3	2.37	0.50
1:E:112:VAL:HG21	1:E:125:VAL:CG1	2.42	0.50
1:F:83:ARG:HG3	1:F:83:ARG:NH1	2.27	0.50
1:E:72:HIS:CD2	1:E:74:ASP:OD1	2.52	0.50
1:B:44:GLN:O	1:B:45:LEU:HB2	2.12	0.49
1:F:22:ARG:CZ	1:F:79:ARG:HH22	2.25	0.49
1:K:72:HIS:CD2	1:K:74:ASP:OD1	2.57	0.49
1:O:92:ILE:N	1:O:92:ILE:CD1	2.75	0.49
1:N:25:GLN:NE2	6:N:5062:HOH:O	2.45	0.49
1:V:68:ARG:HB2	6:V:5010:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:87:LYS:NZ	6:V:5108:HOH:O	2.45	0.49
1:W:66:MSE:HE2	1:X:12:PHE:CE2	2.47	0.49
1:A:91:LYS:O	1:H:117:ILE:HD11	2.13	0.49
1:D:47:ILE:HD11	1:D:73:ILE:CD1	2.43	0.49
1:K:16:LEU:HA	1:K:19:LEU:HD23	1.94	0.49
1:U:22:ARG:HG3	1:U:79:ARG:HD2	1.94	0.49
1:D:43:ASN:HD21	1:K:12:PHE:N	2.09	0.49
1:L:82:MSE:HE1	1:L:114:VAL:HG12	1.93	0.49
1:L:100:ILE:HD11	1:L:107:LEU:HD11	1.94	0.49
1:T:34:TYR:CE1	1:T:54:ASN:HB3	2.47	0.49
1:I:80:ILE:HD13	1:I:136:PHE:HB3	1.94	0.49
1:J:100:ILE:HD11	1:J:107:LEU:HD11	1.94	0.49
1:K:92:ILE:HD13	1:K:128:ARG:NH2	2.27	0.49
1:K:93:PHE:HA	1:K:96:MSE:HE3	1.94	0.49
1:B:94:PRO:HG3	1:N:117:ILE:HB	1.94	0.49
1:M:46:ASN:HD22	1:M:67:TYR:H	1.59	0.49
1:N:57:GLY:O	1:N:59:LYS:CD	2.61	0.49
1:C:113:ARG:NH2	6:L:2062:HOH:O	2.42	0.49
1:C:131:ARG:HD2	6:C:193:HOH:O	2.11	0.49
4:H:4002:GOL:H12	1:I:79:ARG:NH2	2.20	0.49
1:J:80:ILE:HG12	1:J:136:PHE:HB3	1.94	0.48
1:U:12:PHE:N	1:X:43:ASN:HD21	2.11	0.48
1:U:96:MSE:CE	1:U:109:GLY:HA2	2.43	0.48
1:U:118:GLY:HA2	1:U:133:PHE:CE2	2.48	0.48
1:Y:127:GLU:HB3	1:Y:131:ARG:NH2	2.28	0.48
1:N:53:SER:HA	1:N:58:GLU:O	2.13	0.48
1:Q:53:SER:HA	1:Q:58:GLU:O	2.13	0.48
1:2:100:ILE:HD12	5:2:5005:ACY:H3	1.94	0.48
1:L:127:GLU:CD	1:L:131:ARG:HH12	2.20	0.48
1:T:43:ASN:HD21	1:Y:12:PHE:N	2.11	0.48
1:M:46:ASN:ND2	1:M:67:TYR:H	2.10	0.48
1:O:61:ASN:ND2	1:P:78:ARG:HE	2.11	0.48
1:Z:139:ARG:HH11	1:Z:139:ARG:HB3	1.78	0.48
1:O:119:VAL:O	1:O:119:VAL:HG23	2.13	0.48
1:M:13:VAL:HG22	1:M:45:LEU:HD13	1.95	0.48
1:R:18:ASN:HD22	1:R:83:ARG:HH21	1.61	0.48
1:V:88:GLN:HG3	1:V:136:PHE:HZ	1.78	0.48
1:Y:93:PHE:HB3	1:Y:96:MSE:SE	2.62	0.48
5:W:5011:ACY:H2	6:W:5031:HOH:O	2.14	0.48
1:V:93:PHE:HA	1:V:96:MSE:HE3	1.96	0.48
1:V:134:GLU:O	1:V:138:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:138:LYS:O	1:Y:139:ARG:HB2	2.13	0.48
1:1:131:ARG:O	1:1:135:GLU:HG2	2.13	0.48
1:E:54:ASN:HD21	1:E:58:GLU:H	1.62	0.48
1:2:127:GLU:OE2	1:2:131:ARG:NH1	2.43	0.48
1:G:135:GLU:HA	1:G:138:LYS:HE2	1.95	0.48
1:J:122:VAL:HG12	1:J:123:GLY:N	2.29	0.48
1:K:35:LYS:HE3	1:K:76:THR:CG2	2.40	0.48
1:L:127:GLU:CG	1:L:131:ARG:NH1	2.62	0.48
1:N:116:GLU:HG3	1:N:117:ILE:HD13	1.96	0.48
1:T:63:VAL:HG13	1:U:74:ASP:OD1	2.14	0.48
1:2:79:ARG:CZ	1:2:117:ILE:HD11	2.44	0.47
1:B:43:ASN:HD21	1:M:12:PHE:N	2.12	0.47
1:H:92:ILE:C	1:H:94:PRO:HD3	2.39	0.47
1:M:72:HIS:CD2	1:M:74:ASP:OD1	2.54	0.47
1:S:100:ILE:HD13	1:S:107:LEU:HG	1.96	0.47
1:V:46:ASN:ND2	1:V:67:TYR:H	2.12	0.47
1:Z:113:ARG:HD3	1:Z:120:GLU:OE1	2.14	0.47
1:F:13:VAL:HG22	1:F:45:LEU:HD13	1.95	0.47
1:1:92:ILE:C	1:1:94:PRO:HD3	2.39	0.47
1:V:62:ARG:HD3	6:V:5095:HOH:O	2.13	0.47
1:Z:79:ARG:CZ	1:Z:117:ILE:HD11	2.44	0.47
1:1:128:ARG:HD2	1:1:128:ARG:HA	1.65	0.47
1:A:72:HIS:CD2	1:A:74:ASP:OD1	2.59	0.47
1:L:85:PHE:HA	1:L:136:PHE:CZ	2.50	0.47
1:1:85:PHE:CE1	1:1:132:LEU:HD13	2.49	0.47
1:2:93:PHE:CA	1:2:96:MSE:HE3	2.45	0.47
1:L:90:GLU:HG2	1:L:97:VAL:HB	1.96	0.47
1:P:54:ASN:HD22	1:P:56:ALA:H	1.63	0.47
1:I:67:TYR:CD1	1:I:67:TYR:C	2.93	0.47
1:N:34:TYR:CE1	1:N:54:ASN:HB3	2.50	0.47
1:P:59:LYS:CD	1:P:60:PHE:N	2.78	0.47
1:S:126:ALA:O	1:S:130:LYS:HG3	2.15	0.47
1:T:41:VAL:O	1:T:41:VAL:HG13	2.13	0.47
1:V:44:GLN:O	1:V:45:LEU:HB2	2.14	0.47
1:W:77:GLU:H	5:W:5011:ACY:CH3	2.26	0.47
1:1:124:PRO:HG3	6:1:5056:HOH:O	2.15	0.47
1:B:131:ARG:NE	6:B:3030:HOH:O	2.44	0.47
4:H:4002:GOL:C1	1:I:79:ARG:HH21	2.21	0.47
1:I:80:ILE:HD13	1:I:136:PHE:HB2	1.96	0.47
1:P:43:ASN:HD21	1:V:12:PHE:N	2.13	0.47
1:X:66:MSE:CE	1:Y:12:PHE:CZ	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:HD3	1:D:79:ARG:HH11	1.79	0.47
1:D:66:MSE:CE	1:D:66:MSE:CA	2.85	0.47
1:J:81:ASP:OD2	1:J:81:ASP:C	2.58	0.47
1:J:113:ARG:HD3	1:J:120:GLU:OE2	2.14	0.47
1:O:130:LYS:O	1:O:134:GLU:HG3	2.14	0.47
1:Q:16:LEU:HD11	1:Q:73:ILE:HD12	1.97	0.47
1:K:93:PHE:HZ	1:K:128:ARG:HB3	1.80	0.46
1:M:135:GLU:O	1:M:139:ARG:HG3	2.15	0.46
1:R:136:PHE:O	1:R:138:LYS:N	2.48	0.46
1:T:130:LYS:O	1:T:134:GLU:HG3	2.14	0.46
1:K:100:ILE:HD11	1:K:107:LEU:CG	2.46	0.46
1:X:26:VAL:HG22	1:X:73:ILE:HD12	1.96	0.46
1:D:124:PRO:HG2	1:L:100:ILE:CD1	2.45	0.46
1:F:72:HIS:CD2	1:F:74:ASP:OD1	2.55	0.46
1:J:90:GLU:OE2	1:J:94:PRO:HA	2.15	0.46
1:L:113:ARG:HB3	1:L:120:GLU:HB2	1.97	0.46
1:X:55:LYS:HB2	6:X:5016:HOH:O	2.14	0.46
1:Y:53:SER:HB2	1:Y:59:LYS:CE	2.45	0.46
1:D:66:MSE:HE3	1:E:12:PHE:HZ	1.76	0.46
1:H:35:LYS:HE3	1:H:76:THR:HG21	1.97	0.46
1:N:79:ARG:CZ	1:N:117:ILE:HD11	2.46	0.46
1:Q:118:GLY:HA2	1:Q:133:PHE:CE2	2.50	0.46
1:T:35:LYS:O	1:T:52:ALA:HA	2.16	0.46
1:A:74:ASP:OD1	1:G:63:VAL:HG13	2.16	0.46
1:I:92:ILE:HG22	1:I:93:PHE:CD1	2.50	0.46
1:P:59:LYS:HD3	1:P:60:PHE:N	2.30	0.46
1:R:82:MSE:HE1	1:R:136:PHE:CE2	2.50	0.46
1:Y:66:MSE:HE1	1:Z:45:LEU:CD2	2.44	0.46
1:I:44:GLN:O	1:I:45:LEU:HB2	2.15	0.46
1:I:93:PHE:HB3	1:I:96:MSE:CG	2.46	0.46
1:C:136:PHE:C	1:C:138:LYS:H	2.22	0.46
1:E:92:ILE:CD1	1:E:132:LEU:HD13	2.45	0.46
1:T:17:ASN:O	1:T:20:LEU:HD23	2.15	0.46
1:D:66:MSE:CE	1:E:12:PHE:CZ	2.98	0.46
1:C:41:VAL:HG13	1:C:47:ILE:CD1	2.46	0.46
1:D:53:SER:HA	1:D:58:GLU:O	2.16	0.46
1:E:35:LYS:O	1:E:52:ALA:HA	2.16	0.46
1:K:89:ALA:C	1:K:97:VAL:HG21	2.41	0.46
1:N:70:ILE:HG21	1:N:73:ILE:HD11	1.97	0.46
1:I:61:ASN:HB3	6:I:5019:HOH:O	2.16	0.46
1:A:99:TYR:OH	1:A:104:ASN:ND2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:75:SER:HB2	5:W:5011:ACY:H2	1.98	0.46
1:E:52:ALA:O	1:E:59:LYS:HA	2.16	0.46
1:R:113:ARG:NH1	1:1:134:GLU:OE1	2.48	0.46
1:2:122:VAL:HG12	1:2:123:GLY:H	1.81	0.46
1:I:85:PHE:HA	1:I:136:PHE:CZ	2.52	0.45
1:I:139:ARG:CB	1:I:139:ARG:HH11	2.30	0.45
1:M:82:MSE:HE1	1:M:114:VAL:HG12	1.98	0.45
1:V:93:PHE:CA	1:V:96:MSE:HE3	2.46	0.45
1:Z:83:ARG:NH1	1:Z:99:TYR:CE2	2.84	0.45
1:D:55:LYS:C	1:D:57:GLY:H	2.24	0.45
1:K:67:TYR:CD1	1:K:67:TYR:C	2.94	0.45
6:T:175:HOH:O	1:Y:138:LYS:CE	2.48	0.45
1:E:68:ARG:HG3	6:E:2007:HOH:O	2.15	0.45
1:I:56:ALA:N	6:I:5051:HOH:O	2.49	0.45
1:N:116:GLU:HG3	1:N:117:ILE:CD1	2.46	0.45
1:R:18:ASN:HD22	1:R:83:ARG:NH2	2.14	0.45
1:R:44:GLN:O	1:R:45:LEU:HB2	2.16	0.45
1:S:32:GLU:OE2	1:T:72:HIS:HE1	1.98	0.45
1:C:100:ILE:CD1	1:C:107:LEU:HG	2.46	0.45
1:I:113:ARG:HD3	1:I:120:GLU:OE2	2.16	0.45
1:N:72:HIS:O	1:N:73:ILE:HD13	2.17	0.45
1:Q:55:LYS:HB2	6:Q:2045:HOH:O	2.16	0.45
1:R:79:ARG:HH11	1:R:79:ARG:CA	2.29	0.45
1:1:78:ARG:NH1	1:1:81:ASP:HB2	2.31	0.45
1:D:22:ARG:HD3	1:D:79:ARG:NH1	2.32	0.45
1:M:44:GLN:O	1:M:45:LEU:HB2	2.16	0.45
1:T:45:LEU:N	1:T:45:LEU:HD22	2.32	0.45
1:1:132:LEU:HD22	1:1:136:PHE:CE1	2.52	0.45
1:A:60:PHE:CD2	1:B:74:ASP:HB3	2.52	0.45
1:D:92:ILE:HD12	1:D:132:LEU:CD2	2.32	0.45
1:T:18:ASN:O	1:T:79:ARG:HD3	2.17	0.45
1:U:17:ASN:ND2	6:U:2088:HOH:O	2.40	0.45
1:V:93:PHE:CZ	1:V:128:ARG:HB3	2.50	0.45
1:A:81:ASP:OD1	1:A:83:ARG:NH1	2.49	0.45
1:E:87:LYS:O	1:E:91:LYS:HD3	2.17	0.45
1:H:26:VAL:HG13	1:H:73:ILE:CD1	2.47	0.45
1:N:15:GLU:CD	1:N:15:GLU:N	2.74	0.45
1:1:17:ASN:O	1:1:20:LEU:HG	2.17	0.45
1:B:79:ARG:HD3	6:B:3057:HOH:O	2.16	0.45
1:I:66:MSE:HE1	1:J:45:LEU:HB3	1.99	0.45
1:K:28:LEU:HD21	1:K:65:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:LYS:HB3	1:K:91:LYS:HZ3	1.78	0.45
1:N:135:GLU:O	1:N:139:ARG:HG3	2.17	0.45
1:O:119:VAL:CG2	1:O:130:LYS:HG2	2.47	0.45
1:K:23:GLU:OE2	1:K:35:LYS:HE2	2.17	0.45
1:L:83:ARG:HH22	1:L:101:GLU:CG	2.29	0.45
1:T:44:GLN:O	1:T:45:LEU:HB2	2.17	0.45
1:U:113:ARG:HD2	1:X:134:GLU:OE1	2.17	0.45
1:O:89:ALA:HA	1:O:132:LEU:HD21	1.98	0.45
1:C:96:MSE:CE	1:C:109:GLY:HA2	2.44	0.44
1:S:98:LYS:HE3	1:S:98:LYS:HB2	1.71	0.44
1:Z:16:LEU:HD12	1:Z:16:LEU:HA	1.71	0.44
1:D:22:ARG:HG3	1:D:79:ARG:HD2	1.99	0.44
1:O:44:GLN:O	1:O:45:LEU:HB2	2.16	0.44
1:S:44:GLN:O	1:S:45:LEU:HB2	2.17	0.44
1:S:54:ASN:HD21	1:S:58:GLU:H	1.64	0.44
1:I:72:HIS:CD2	1:I:74:ASP:OD1	2.57	0.44
1:D:47:ILE:CD1	1:D:73:ILE:CD1	2.94	0.44
1:F:101:GLU:OE2	1:I:18:ASN:HB3	2.18	0.44
1:G:34:TYR:CE1	1:G:54:ASN:HB3	2.52	0.44
1:H:135:GLU:O	1:H:139:ARG:HG3	2.17	0.44
1:L:44:GLN:NE2	6:L:2017:HOH:O	2.49	0.44
1:X:53:SER:HA	1:X:58:GLU:O	2.17	0.44
1:2:53:SER:HA	1:2:58:GLU:O	2.17	0.44
1:U:105:VAL:HG21	1:U:113:ARG:NH1	2.32	0.44
1:X:30:ASN:ND2	1:X:32:GLU:H	2.16	0.44
1:2:93:PHE:CE2	1:2:125:VAL:HG13	2.53	0.44
1:V:47:ILE:HD11	1:V:73:ILE:CD1	2.48	0.44
1:Z:91:LYS:NZ	1:Z:91:LYS:HB2	2.33	0.44
1:I:117:ILE:O	1:I:117:ILE:HG23	2.17	0.44
1:2:100:ILE:HD11	1:2:107:LEU:HD11	2.00	0.44
1:E:73:ILE:HD12	1:E:73:ILE:N	2.32	0.44
1:S:30:ASN:H	1:S:30:ASN:ND2	2.16	0.44
1:T:68:ARG:HB2	6:T:147:HOH:O	2.16	0.44
1:I:132:LEU:HD22	1:I:136:PHE:HE1	1.82	0.44
1:C:113:ARG:NH1	1:L:131:ARG:HD2	2.33	0.44
1:E:91:LYS:HD2	1:E:91:LYS:N	2.33	0.44
1:F:87:LYS:HZ1	1:I:20:LEU:HD11	1.82	0.44
1:G:110:ASP:C	1:G:111:LYS:HD2	2.43	0.44
1:Q:134:GLU:OE1	1:Q:134:GLU:HA	2.18	0.44
1:T:55:LYS:HB2	6:T:178:HOH:O	2.17	0.44
1:B:47:ILE:HD12	1:B:73:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LYS:C	1:D:57:GLY:N	2.76	0.44
1:E:16:LEU:HD23	1:E:16:LEU:HA	1.80	0.44
1:E:125:VAL:CG2	5:K:5013:ACY:H3	2.48	0.44
1:Q:43:ASN:HD21	1:2:12:PHE:N	2.16	0.44
1:Q:96:MSE:HE3	1:Q:109:GLY:HA2	1.99	0.44
1:U:131:ARG:HG3	6:U:2065:HOH:O	2.17	0.44
1:Y:13:VAL:HG22	1:Y:45:LEU:HD13	1.99	0.44
1:Z:17:ASN:ND2	1:Z:41:VAL:HG13	2.33	0.44
1:1:46:ASN:HD22	1:1:67:TYR:H	1.66	0.44
1:1:115:SER:C	1:1:117:ILE:H	2.26	0.44
1:A:101:GLU:OE2	1:N:18:ASN:HB3	2.18	0.44
1:J:13:VAL:HG22	1:J:45:LEU:HD13	2.00	0.44
1:O:119:VAL:HG21	1:O:130:LYS:HG2	1.98	0.44
1:T:79:ARG:HB2	6:T:173:HOH:O	2.17	0.44
1:Y:55:LYS:HD3	6:Y:5027:HOH:O	2.18	0.44
1:1:78:ARG:HH12	1:1:81:ASP:HB2	1.82	0.44
1:B:53:SER:HA	1:B:58:GLU:O	2.18	0.43
1:J:87:LYS:HE3	1:J:87:LYS:HB2	1.77	0.43
1:P:12:PHE:N	1:V:43:ASN:HD21	2.16	0.43
1:U:83:ARG:HD2	1:X:18:ASN:OD1	2.17	0.43
1:Y:53:SER:HB2	1:Y:59:LYS:HE2	2.00	0.43
1:1:88:GLN:O	1:1:92:ILE:HD13	2.18	0.43
1:G:53:SER:HA	1:G:58:GLU:O	2.18	0.43
1:J:139:ARG:NH1	1:J:139:ARG:HG2	2.33	0.43
1:K:46:ASN:HB3	1:L:12:PHE:CE1	2.53	0.43
1:O:119:VAL:CG2	1:O:130:LYS:CG	2.94	0.43
1:R:99:TYR:CE2	1:R:101:GLU:HA	2.53	0.43
1:S:47:ILE:HD12	1:S:70:ILE:HD13	2.01	0.43
1:W:53:SER:HA	1:W:58:GLU:O	2.18	0.43
1:B:17:ASN:O	1:B:20:LEU:HD22	2.19	0.43
1:Q:98:LYS:CE	6:Q:2043:HOH:O	2.63	0.43
1:U:67:TYR:CD1	1:U:67:TYR:C	2.96	0.43
1:V:92:ILE:C	1:V:94:PRO:HD3	2.43	0.43
1:Z:80:ILE:HD12	1:Z:133:PHE:CZ	2.53	0.43
1:B:131:ARG:HD2	6:B:3030:HOH:O	2.17	0.43
1:1:12:PHE:HB3	1:1:15:GLU:OE1	2.18	0.43
1:P:105:VAL:HG21	1:P:113:ARG:NH2	2.34	0.43
1:X:92:ILE:C	1:X:94:PRO:HD3	2.43	0.43
1:Z:53:SER:HA	1:Z:58:GLU:O	2.19	0.43
1:K:100:ILE:HD11	1:K:107:LEU:HD11	1.99	0.43
1:L:100:ILE:HD11	1:L:107:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:O	1:G:66:MSE:HG3	2.19	0.43
1:E:126:ALA:O	1:E:130:LYS:HG3	2.19	0.43
1:H:62:ARG:HD3	4:H:4002:GOL:H11	2.00	0.43
1:R:16:LEU:HD11	1:R:73:ILE:HD12	2.00	0.43
1:1:79:ARG:NH2	1:1:117:ILE:HD11	2.33	0.43
1:A:98:LYS:CB	1:A:98:LYS:NZ	2.81	0.43
1:I:68:ARG:HB2	6:I:5013:HOH:O	2.18	0.43
1:M:93:PHE:HB3	1:M:96:MSE:SE	2.69	0.43
1:Q:50:ALA:O	1:Q:51:ASN:C	2.62	0.43
1:X:112:VAL:HG21	1:X:125:VAL:HG12	2.01	0.43
1:D:110:ASP:HB2	1:K:138:LYS:CE	2.48	0.43
1:F:46:ASN:OD1	1:F:67:TYR:HD2	2.02	0.43
1:H:62:ARG:CD	4:H:4002:GOL:H11	2.48	0.43
1:H:100:ILE:CD1	1:H:107:LEU:CD1	2.97	0.43
1:V:62:ARG:CD	6:V:5095:HOH:O	2.66	0.43
1:Y:33:VAL:O	1:Y:54:ASN:HA	2.18	0.43
1:H:26:VAL:HG22	1:H:73:ILE:CD1	2.49	0.43
1:L:93:PHE:HZ	1:L:128:ARG:HB3	1.84	0.43
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.83	0.43
1:R:83:ARG:NE	6:R:4044:HOH:O	2.52	0.43
1:Y:91:LYS:HB3	1:Y:91:LYS:HZ2	1.83	0.43
1:B:47:ILE:CD1	1:B:73:ILE:CD1	2.97	0.42
1:C:96:MSE:HE2	1:M:102:GLU:O	2.18	0.42
1:O:108:ILE:HB	1:O:112:VAL:HG22	2.00	0.42
1:S:17:ASN:HA	1:S:20:LEU:HD22	2.01	0.42
1:U:83:ARG:NH1	1:X:17:ASN:HD22	2.17	0.42
1:A:83:ARG:HD2	6:A:4070:HOH:O	2.18	0.42
1:F:98:LYS:HE3	1:F:98:LYS:HB2	1.58	0.42
1:J:139:ARG:HG2	1:J:139:ARG:HH11	1.84	0.42
1:K:47:ILE:HD11	1:K:73:ILE:CD1	2.49	0.42
1:N:26:VAL:HG13	1:N:73:ILE:HD12	1.95	0.42
1:Z:93:PHE:HB3	1:Z:96:MSE:CG	2.49	0.42
1:I:35:LYS:O	1:I:52:ALA:HA	2.20	0.42
1:2:90:GLU:OE2	1:2:95:GLY:N	2.47	0.42
1:B:89:ALA:HB1	1:B:108:ILE:HD11	2.00	0.42
1:I:20:LEU:HA	1:I:38:LEU:HD22	2.01	0.42
1:I:55:LYS:HA	1:I:55:LYS:HD3	1.73	0.42
1:K:47:ILE:HD11	1:K:73:ILE:HD11	2.00	0.42
1:M:20:LEU:HA	1:M:20:LEU:HD23	1.82	0.42
1:N:58:GLU:C	1:N:59:LYS:HD2	2.44	0.42
1:P:50:ALA:O	1:P:51:ASN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:22:ARG:HD3	1:Q:79:ARG:NH1	2.34	0.42
1:R:79:ARG:HB3	1:R:79:ARG:CZ	2.48	0.42
1:Y:91:LYS:HB3	1:Y:91:LYS:HZ3	1.82	0.42
1:I:66:MSE:HG3	1:J:70:ILE:O	2.20	0.42
1:P:13:VAL:HG22	1:P:45:LEU:HD13	2.01	0.42
1:T:83:ARG:HD3	1:Y:17:ASN:HD22	1.84	0.42
1:N:100:ILE:HD11	1:N:107:LEU:CD1	2.49	0.42
1:U:96:MSE:HE3	1:U:96:MSE:HB3	1.91	0.42
1:Z:79:ARG:NH2	1:Z:117:ILE:HD11	2.34	0.42
1:I:93:PHE:HB3	1:I:96:MSE:HG3	2.01	0.42
1:L:93:PHE:HB3	1:L:96:MSE:CG	2.48	0.42
1:P:133:PHE:CE2	1:P:137:LEU:HD11	2.55	0.42
1:Q:96:MSE:CE	1:Q:109:GLY:HA2	2.50	0.42
1:2:51:ASN:O	1:2:59:LYS:HE3	2.20	0.42
1:M:69:TYR:CE2	1:N:29:SER:HB3	2.54	0.42
1:Y:93:PHE:N	1:Y:94:PRO:HD3	2.35	0.42
1:E:72:HIS:C	1:E:73:ILE:HD12	2.45	0.42
1:I:69:TYR:CE2	1:J:29:SER:HB3	2.55	0.42
1:K:100:ILE:HD12	5:K:5013:ACY:H2	2.01	0.42
1:R:23:GLU:OE1	1:R:35:LYS:HD3	2.20	0.42
1:R:89:ALA:HA	1:R:132:LEU:HD21	2.02	0.42
1:X:79:ARG:NH2	4:X:4004:GOL:H11	2.34	0.42
1:H:53:SER:HA	1:H:58:GLU:O	2.19	0.42
1:J:17:ASN:O	1:J:20:LEU:HG	2.20	0.42
1:K:100:ILE:CD1	5:K:5013:ACY:H2	2.50	0.42
1:O:61:ASN:ND2	1:P:78:ARG:HG2	2.35	0.42
1:S:68:ARG:NH2	6:S:3045:HOH:O	2.52	0.42
1:X:44:GLN:O	1:X:45:LEU:HB2	2.20	0.42
1:D:66:MSE:HG3	1:E:70:ILE:O	2.20	0.41
1:J:61:ASN:HB3	6:J:4023:HOH:O	2.20	0.41
1:R:113:ARG:NH1	1:I:134:GLU:OE2	2.53	0.41
1:S:62:ARG:HH22	1:T:138:LYS:HZ2	1.67	0.41
1:I:79:ARG:CZ	1:I:117:ILE:HD11	2.50	0.41
1:C:133:PHE:O	1:C:136:PHE:HB3	2.20	0.41
1:Q:34:TYR:CE1	1:Q:54:ASN:HB3	2.55	0.41
1:Q:98:LYS:HG2	1:Q:100:ILE:HD13	2.02	0.41
1:U:91:LYS:HE3	6:X:5070:HOH:O	2.19	0.41
1:V:19:LEU:HD23	1:V:19:LEU:HA	1.90	0.41
1:Y:66:MSE:HE2	1:Y:66:MSE:HA	2.02	0.41
1:D:128:ARG:HG2	1:L:113:ARG:NH1	2.36	0.41
1:F:35:LYS:HG3	6:F:5035:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ARG:O	1:F:134:GLU:HG2	2.21	0.41
1:I:138:LYS:O	1:I:139:ARG:C	2.63	0.41
1:J:53:SER:HA	1:J:58:GLU:O	2.20	0.41
1:K:15:GLU:HG2	6:K:5019:HOH:O	2.20	0.41
1:N:53:SER:HB3	1:N:59:LYS:HG3	2.03	0.41
1:R:72:HIS:CD2	1:R:74:ASP:OD1	2.66	0.41
1:B:55:LYS:HB2	6:B:3021:HOH:O	2.20	0.41
1:C:105:VAL:HG11	1:C:113:ARG:HG3	2.01	0.41
1:D:105:VAL:HG11	1:D:113:ARG:CG	2.42	0.41
1:K:90:GLU:N	1:K:97:VAL:HG21	2.35	0.41
1:L:83:ARG:NH2	1:L:101:GLU:HG3	2.34	0.41
1:Q:137:LEU:HD23	1:Q:137:LEU:HA	1.81	0.41
1:K:100:ILE:CD1	1:K:107:LEU:HG	2.50	0.41
1:P:67:TYR:CD1	1:P:67:TYR:C	2.98	0.41
1:Q:98:LYS:NZ	6:Q:2043:HOH:O	2.49	0.41
1:R:16:LEU:HD23	1:R:16:LEU:HA	1.87	0.41
1:U:113:ARG:NH1	1:X:134:GLU:OE2	2.53	0.41
1:U:126:ALA:O	1:U:130:LYS:HG3	2.21	0.41
1:D:131:ARG:NH1	6:D:2042:HOH:O	2.37	0.41
1:N:81:ASP:C	1:N:81:ASP:OD1	2.64	0.41
1:Q:34:TYR:CZ	1:Q:54:ASN:HB3	2.56	0.41
1:R:82:MSE:HE1	1:R:136:PHE:HE2	1.84	0.41
1:T:17:ASN:O	1:T:20:LEU:HD22	2.19	0.41
1:I:81:ASP:OD1	1:I:81:ASP:C	2.63	0.41
1:B:16:LEU:HD23	1:B:16:LEU:HA	1.85	0.41
1:N:75:SER:HB2	6:N:5039:HOH:O	2.20	0.41
1:P:95:GLY:O	1:P:96:MSE:HE2	2.20	0.41
1:Y:41:VAL:O	1:Y:41:VAL:HG13	2.19	0.41
1:D:25:GLN:HG3	1:D:33:VAL:CG1	2.50	0.41
1:L:93:PHE:CB	1:L:96:MSE:HG3	2.49	0.41
1:Q:37:VAL:HB	1:Q:50:ALA:HB3	2.03	0.41
1:U:107:LEU:HD13	1:X:138:LYS:HD3	2.03	0.41
1:D:105:VAL:HG12	1:D:106:VAL:H	1.83	0.41
1:J:132:LEU:O	1:J:132:LEU:HD22	2.21	0.41
1:K:77:GLU:CB	6:K:5047:HOH:O	2.69	0.41
1:R:55:LYS:HD3	1:R:55:LYS:HA	1.89	0.41
1:S:16:LEU:HD23	1:S:16:LEU:HA	1.85	0.41
1:S:130:LYS:O	1:S:134:GLU:HG3	2.21	0.41
1:T:138:LYS:HB3	1:T:138:LYS:HE2	1.92	0.41
1:U:16:LEU:HD23	1:U:16:LEU:HA	1.80	0.41
1:U:38:LEU:HD23	1:U:38:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:135:GLU:O	1:V:139:ARG:HG3	2.21	0.41
1:I:56:ALA:CA	6:I:5051:HOH:O	2.61	0.41
1:J:85:PHE:HA	1:J:136:PHE:CZ	2.56	0.41
1:J:112:VAL:HG21	1:J:125:VAL:CG1	2.35	0.41
1:S:117:ILE:O	1:S:117:ILE:CG2	2.68	0.41
1:T:96:MSE:CE	1:T:109:GLY:HA2	2.51	0.41
1:U:20:LEU:HD23	1:U:20:LEU:HA	1.95	0.41
1:Z:41:VAL:HG13	1:Z:41:VAL:O	2.21	0.41
1:Z:117:ILE:HA	1:Z:117:ILE:HD12	1.82	0.41
1:L:22:ARG:NH1	6:L:2034:HOH:O	2.53	0.40
1:M:105:VAL:HG21	1:M:113:ARG:NH2	2.36	0.40
1:O:96:MSE:HE3	1:O:96:MSE:HB3	1.77	0.40
1:Q:40:ALA:HB3	1:Q:48:VAL:HB	2.03	0.40
1:R:68:ARG:NH1	6:R:4014:HOH:O	2.53	0.40
1:V:80:ILE:HG13	1:V:82:MSE:SE	2.71	0.40
1:E:98:LYS:NZ	1:E:98:LYS:CB	2.84	0.40
1:M:81:ASP:OD1	1:M:81:ASP:C	2.63	0.40
1:X:66:MSE:HE1	1:Y:45:LEU:CD2	2.52	0.40
1:B:47:ILE:CD1	1:B:73:ILE:HD13	2.52	0.40
1:C:79:ARG:HA	6:C:192:HOH:O	2.20	0.40
1:D:32:GLU:OE1	1:D:34:TYR:OH	2.40	0.40
1:H:46:ASN:HB3	1:I:12:PHE:CE1	2.57	0.40
1:I:92:ILE:HG22	1:I:93:PHE:CE1	2.56	0.40
1:L:66:MSE:HE1	1:M:45:LEU:HB3	2.04	0.40
1:X:85:PHE:CE1	1:X:132:LEU:HD13	2.56	0.40
1:A:78:ARG:HE	1:A:78:ARG:HB3	1.46	0.40
1:K:128:ARG:O	1:K:128:ARG:HD2	2.21	0.40
1:A:92:ILE:HG13	1:A:132:LEU:HD13	2.03	0.40
1:E:91:LYS:O	1:K:117:ILE:HD11	2.21	0.40
1:G:83:ARG:CD	6:G:4055:HOH:O	2.69	0.40
1:I:117:ILE:O	1:I:117:ILE:HG23	2.21	0.40
1:J:32:GLU:OE1	1:J:34:TYR:OH	2.39	0.40
1:K:17:ASN:O	1:K:20:LEU:HD22	2.22	0.40
1:T:117:ILE:HD12	1:T:117:ILE:HA	1.82	0.40
1:Z:96:MSE:O	1:Z:109:GLY:N	2.45	0.40
1:2:52:ALA:O	1:2:59:LYS:HD2	2.20	0.40

All (1) 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)
6:I:5051:HOH:O	6:V:5110:HOH:O[1_455]	2.01	0.19

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	1	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	2	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	A	124/130 (95%)	124 (100%)	0	0	100	100
1	B	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	C	125/130 (96%)	122 (98%)	1 (1%)	2 (2%)	7	3
1	D	125/130 (96%)	125 (100%)	0	0	100	100
1	E	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	F	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	G	125/130 (96%)	125 (100%)	0	0	100	100
1	H	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
1	I	126/130 (97%)	126 (100%)	0	0	100	100
1	J	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
1	K	126/130 (97%)	124 (98%)	1 (1%)	1 (1%)	16	11
1	L	125/130 (96%)	125 (100%)	0	0	100	100
1	M	126/130 (97%)	126 (100%)	0	0	100	100
1	N	126/130 (97%)	126 (100%)	0	0	100	100
1	O	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	P	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	Q	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	R	125/130 (96%)	122 (98%)	1 (1%)	2 (2%)	7	3
1	S	125/130 (96%)	124 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
1	U	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
1	V	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
1	W	126/130 (97%)	124 (98%)	2 (2%)	0	100	100
1	X	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
1	Y	126/130 (97%)	124 (98%)	1 (1%)	1 (1%)	16	11
1	Z	126/130 (97%)	126 (100%)	0	0	100	100
All	All	3510/3640 (96%)	3476 (99%)	28 (1%)	6 (0%)	43	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	79	ARG
1	C	78	ARG
1	R	137	LEU
1	C	79	ARG
1	K	92	ILE
1	Y	94	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	109/109 (100%)	104 (95%)	5 (5%)	24	22
1	2	109/109 (100%)	102 (94%)	7 (6%)	16	12
1	A	108/109 (99%)	103 (95%)	5 (5%)	24	22
1	B	109/109 (100%)	103 (94%)	6 (6%)	19	17
1	C	109/109 (100%)	102 (94%)	7 (6%)	16	12
1	D	109/109 (100%)	101 (93%)	8 (7%)	13	9
1	E	109/109 (100%)	99 (91%)	10 (9%)	8	5
1	F	109/109 (100%)	101 (93%)	8 (7%)	13	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	109/109 (100%)	107 (98%)	2 (2%)	51	58
1	H	110/109 (101%)	107 (97%)	3 (3%)	39	42
1	I	110/109 (101%)	103 (94%)	7 (6%)	16	12
1	J	110/109 (101%)	103 (94%)	7 (6%)	16	12
1	K	110/109 (101%)	100 (91%)	10 (9%)	9	6
1	L	109/109 (100%)	100 (92%)	9 (8%)	10	7
1	M	110/109 (101%)	104 (94%)	6 (6%)	19	17
1	N	110/109 (101%)	104 (94%)	6 (6%)	19	17
1	O	109/109 (100%)	106 (97%)	3 (3%)	38	41
1	P	109/109 (100%)	101 (93%)	8 (7%)	13	9
1	Q	109/109 (100%)	105 (96%)	4 (4%)	30	30
1	R	109/109 (100%)	103 (94%)	6 (6%)	19	17
1	S	109/109 (100%)	100 (92%)	9 (8%)	10	7
1	T	109/109 (100%)	105 (96%)	4 (4%)	30	30
1	U	109/109 (100%)	105 (96%)	4 (4%)	30	30
1	V	110/109 (101%)	103 (94%)	7 (6%)	16	12
1	W	110/109 (101%)	108 (98%)	2 (2%)	51	58
1	X	110/109 (101%)	101 (92%)	9 (8%)	10	7
1	Y	110/109 (101%)	101 (92%)	9 (8%)	10	7
1	Z	110/109 (101%)	99 (90%)	11 (10%)	7	4
All	All	3062/3052 (100%)	2880 (94%)	182 (6%)	18	14

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	78	ARG
1	A	79	ARG
1	A	98	LYS
1	A	105	VAL
1	B	20	LEU
1	B	38	LEU
1	B	45	LEU
1	B	84	GLU
1	B	105	VAL

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Mol	Chain	Res	Type
1	B	138	LYS
1	C	15	GLU
1	C	41	VAL
1	C	45	LEU
1	C	80	ILE
1	C	100	ILE
1	C	105	VAL
1	C	117	ILE
1	D	38	LEU
1	D	45	LEU
1	D	66	MSE
1	D	78	ARG
1	D	91	LYS
1	D	96	MSE
1	D	127	GLU
1	D	131	ARG
1	E	38	LEU
1	E	45	LEU
1	E	54	ASN
1	E	79	ARG
1	E	96	MSE
1	E	98	LYS
1	E	105	VAL
1	E	110	ASP
1	E	113	ARG
1	E	114	VAL
1	F	35	LYS
1	F	38	LEU
1	F	45	LEU
1	F	74	ASP
1	F	79	ARG
1	F	96	MSE
1	F	127	GLU
1	F	138	LYS
1	G	38	LEU
1	G	105	VAL
1	H	25	GLN
1	H	45	LEU
1	H	132	LEU
1	I	45	LEU
1	I	74	ASP
1	I	91	LYS

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Mol	Chain	Res	Type
1	I	92	ILE
1	I	117	ILE
1	I	122	VAL
1	I	132	LEU
1	J	25	GLN
1	J	45	LEU
1	J	68	ARG
1	J	87	LYS
1	J	125	VAL
1	J	127	GLU
1	J	132	LEU
1	K	20	LEU
1	K	22	ARG
1	K	37	VAL
1	K	41	VAL
1	K	83	ARG
1	K	91	LYS
1	K	101	GLU
1	K	122	VAL
1	K	128	ARG
1	K	132	LEU
1	L	20	LEU
1	L	77	GLU
1	L	78	ARG
1	L	84	GLU
1	L	100	ILE
1	L	101	GLU
1	L	128	ARG
1	L	132	LEU
1	L	135	GLU
1	M	15	GLU
1	M	35	LYS
1	M	45	LEU
1	M	74	ASP
1	M	117	ILE
1	M	132	LEU
1	N	20	LEU
1	N	22	ARG
1	N	101	GLU
1	N	117	ILE
1	N	128	ARG
1	N	132	LEU

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Mol	Chain	Res	Type
1	O	45	LEU
1	O	105	VAL
1	O	112	VAL
1	P	15	GLU
1	P	38	LEU
1	P	45	LEU
1	P	54	ASN
1	P	59	LYS
1	P	84	GLU
1	P	105	VAL
1	P	117	ILE
1	Q	45	LEU
1	Q	79	ARG
1	Q	116	GLU
1	Q	127	GLU
1	R	38	LEU
1	R	45	LEU
1	R	78	ARG
1	R	80	ILE
1	R	131	ARG
1	R	134	GLU
1	S	17	ASN
1	S	20	LEU
1	S	30	ASN
1	S	38	LEU
1	S	45	LEU
1	S	54	ASN
1	S	79	ARG
1	S	96	MSE
1	S	135	GLU
1	T	20	LEU
1	T	38	LEU
1	T	78	ARG
1	T	117	ILE
1	U	38	LEU
1	U	45	LEU
1	U	83	ARG
1	U	138	LYS
1	V	20	LEU
1	V	35	LYS
1	V	62	ARG
1	V	68	ARG

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Mol	Chain	Res	Type
1	V	117	ILE
1	V	128	ARG
1	V	132	LEU
1	W	38	LEU
1	W	132	LEU
1	X	20	LEU
1	X	30	ASN
1	X	45	LEU
1	X	66	MSE
1	X	74	ASP
1	X	75	SER
1	X	90	GLU
1	X	132	LEU
1	X	139	ARG
1	Y	25	GLN
1	Y	35	LYS
1	Y	45	LEU
1	Y	66	MSE
1	Y	80	ILE
1	Y	84	GLU
1	Y	90	GLU
1	Y	91	LYS
1	Y	132	LEU
1	Z	16	LEU
1	Z	17	ASN
1	Z	19	LEU
1	Z	38	LEU
1	Z	45	LEU
1	Z	91	LYS
1	Z	103	THR
1	Z	111	LYS
1	Z	117	ILE
1	Z	132	LEU
1	Z	139	ARG
1	1	41	VAL
1	1	45	LEU
1	1	117	ILE
1	1	128	ARG
1	1	132	LEU
1	2	23	GLU
1	2	38	LEU
1	2	45	LEU

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Mol	Chain	Res	Type
1	2	105	VAL
1	2	117	ILE
1	2	122	VAL
1	2	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	72	HIS
1	A	104	ASN
1	B	25	GLN
1	B	72	HIS
1	C	43	ASN
1	C	72	HIS
1	C	88	GLN
1	C	104	ASN
1	D	18	ASN
1	D	61	ASN
1	D	72	HIS
1	D	104	ASN
1	E	25	GLN
1	E	54	ASN
1	E	72	HIS
1	E	104	ASN
1	F	25	GLN
1	F	72	HIS
1	F	104	ASN
1	G	61	ASN
1	G	72	HIS
1	H	25	GLN
1	H	72	HIS
1	I	61	ASN
1	I	72	HIS
1	I	88	GLN
1	J	25	GLN
1	J	72	HIS
1	K	51	ASN
1	K	72	HIS
1	L	25	GLN
1	L	44	GLN
1	L	51	ASN

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Mol	Chain	Res	Type
1	L	72	HIS
1	M	46	ASN
1	M	72	HIS
1	N	17	ASN
1	N	51	ASN
1	N	72	HIS
1	O	18	ASN
1	O	51	ASN
1	O	61	ASN
1	O	72	HIS
1	P	54	ASN
1	P	61	ASN
1	P	72	HIS
1	P	88	GLN
1	P	104	ASN
1	Q	72	HIS
1	Q	88	GLN
1	R	18	ASN
1	R	25	GLN
1	R	51	ASN
1	R	61	ASN
1	R	72	HIS
1	R	104	ASN
1	S	18	ASN
1	S	30	ASN
1	S	51	ASN
1	S	54	ASN
1	S	72	HIS
1	S	88	GLN
1	S	104	ASN
1	T	25	GLN
1	T	72	HIS
1	T	104	ASN
1	U	72	HIS
1	V	17	ASN
1	V	46	ASN
1	V	51	ASN
1	W	25	GLN
1	W	72	HIS
1	X	17	ASN
1	X	25	GLN
1	X	30	ASN

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Mol	Chain	Res	Type
1	X	44	GLN
1	X	72	HIS
1	Y	17	ASN
1	Y	25	GLN
1	Y	51	ASN
1	Y	61	ASN
1	Y	72	HIS
1	Z	25	GLN
1	Z	72	HIS
1	Z	104	ASN
1	1	25	GLN
1	1	44	GLN
1	1	46	ASN
1	1	72	HIS
1	2	25	GLN
1	2	72	HIS
1	2	104	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 33 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACY	Y	5008	-	3,3,3	1.24	1 (33%)	3,3,3	1.70	1 (33%)
4	GOL	H	4011	-	5,5,5	4.56	5 (100%)	5,5,5	5.90	3 (60%)
5	ACY	I	5010	-	3,3,3	1.31	1 (33%)	3,3,3	1.69	1 (33%)
5	ACY	X	5002	-	3,3,3	1.39	1 (33%)	3,3,3	1.81	1 (33%)
4	GOL	V	4008	-	5,5,5	5.13	5 (100%)	5,5,5	6.26	3 (60%)
5	ACY	2	5005	-	3,3,3	1.21	1 (33%)	3,3,3	1.90	1 (33%)
5	ACY	I	5004	-	3,3,3	1.48	1 (33%)	3,3,3	1.86	1 (33%)
4	GOL	1	4010	-	5,5,5	4.77	5 (100%)	5,5,5	6.28	3 (60%)
4	GOL	M	4003	-	5,5,5	4.68	5 (100%)	5,5,5	6.00	3 (60%)
5	ACY	W	5011	-	3,3,3	1.96	1 (33%)	3,3,3	1.95	1 (33%)
5	ACY	V	5007	-	3,3,3	1.21	1 (33%)	3,3,3	1.83	1 (33%)
4	GOL	X	4004	-	5,5,5	4.71	5 (100%)	5,5,5	6.33	3 (60%)
5	ACY	F	5015	-	3,3,3	1.70	1 (33%)	3,3,3	1.73	1 (33%)
4	GOL	R	4007	-	5,5,5	4.79	5 (100%)	5,5,5	6.07	3 (60%)
5	ACY	K	5013	-	3,3,3	1.45	1 (33%)	3,3,3	1.70	1 (33%)
5	ACY	W	5001	-	3,3,3	1.38	0	3,3,3	1.84	1 (33%)
5	ACY	M	5003	-	3,3,3	0.91	0	3,3,3	1.80	1 (33%)
4	GOL	W	4006	-	5,5,5	4.89	5 (100%)	5,5,5	6.20	3 (60%)
4	GOL	2	4009	-	5,5,5	4.92	5 (100%)	5,5,5	5.90	3 (60%)
4	GOL	A	4012	-	5,5,5	4.86	5 (100%)	5,5,5	5.86	3 (60%)
5	ACY	Z	5006	-	3,3,3	1.35	1 (33%)	3,3,3	1.70	1 (33%)
5	ACY	1	5014	-	3,3,3	1.22	0	3,3,3	1.94	1 (33%)
4	GOL	G	4001	-	5,5,5	4.95	5 (100%)	5,5,5	6.01	3 (60%)
5	ACY	H	5012	-	3,3,3	1.43	1 (33%)	3,3,3	1.76	1 (33%)
5	ACY	N	5009	-	3,3,3	1.91	1 (33%)	3,3,3	1.94	1 (33%)
4	GOL	H	4002	2	5,5,5	4.61	5 (100%)	5,5,5	6.17	3 (60%)
4	GOL	J	4005	-	5,5,5	4.82	5 (100%)	5,5,5	5.87	3 (60%)

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
4	GOL	W	4006	-	-	3/4/4/4	-
4	GOL	2	4009	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	4012	-	-	3/4/4/4	-
4	GOL	M	4003	-	-	3/4/4/4	-
4	GOL	1	4010	-	-	3/4/4/4	-
4	GOL	H	4011	-	-	3/4/4/4	-
4	GOL	X	4004	-	-	3/4/4/4	-
4	GOL	V	4008	-	-	3/4/4/4	-
4	GOL	R	4007	-	-	3/4/4/4	-
4	GOL	G	4001	-	-	3/4/4/4	-
4	GOL	H	4002	2	-	4/4/4/4	-
4	GOL	J	4005	-	-	3/4/4/4	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	4009	GOL	C3-C2	-8.85	1.18	1.51
4	V	4008	GOL	C3-C2	-8.59	1.19	1.51
4	W	4006	GOL	C3-C2	-8.39	1.19	1.51
4	R	4007	GOL	C3-C2	-8.35	1.20	1.51
4	1	4010	GOL	C3-C2	-8.21	1.20	1.51
4	M	4003	GOL	C3-C2	-8.19	1.20	1.51
4	A	4012	GOL	C3-C2	-8.18	1.20	1.51
4	J	4005	GOL	C3-C2	-8.16	1.20	1.51
4	X	4004	GOL	C3-C2	-8.05	1.21	1.51
4	G	4001	GOL	C3-C2	-7.92	1.21	1.51
4	H	4011	GOL	C3-C2	-7.88	1.21	1.51
4	H	4002	GOL	C3-C2	-7.77	1.22	1.51
4	W	4006	GOL	O1-C1	5.08	1.63	1.42
4	1	4010	GOL	O1-C1	4.81	1.62	1.42
4	A	4012	GOL	O1-C1	4.75	1.62	1.42
4	2	4009	GOL	O1-C1	4.69	1.62	1.42
4	V	4008	GOL	O1-C1	4.62	1.61	1.42
4	G	4001	GOL	O1-C1	4.49	1.61	1.42
4	J	4005	GOL	O1-C1	4.31	1.60	1.42
4	X	4004	GOL	O1-C1	4.28	1.60	1.42
4	R	4007	GOL	O1-C1	4.10	1.59	1.42
4	H	4011	GOL	O1-C1	4.07	1.59	1.42
4	H	4002	GOL	O1-C1	4.05	1.59	1.42
4	V	4008	GOL	C1-C2	-4.04	1.36	1.51
4	V	4008	GOL	O2-C2	-3.93	1.31	1.43
4	G	4001	GOL	O2-C2	-3.90	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	4003	GOL	O1-C1	3.68	1.57	1.42
4	H	4002	GOL	C1-C2	-3.63	1.37	1.51
4	G	4001	GOL	O3-C3	3.50	1.57	1.42
4	M	4003	GOL	C1-C2	-3.50	1.38	1.51
4	G	4001	GOL	C1-C2	-3.49	1.38	1.51
4	J	4005	GOL	C1-C2	-3.47	1.38	1.51
4	H	4011	GOL	O3-C3	3.36	1.56	1.42
4	X	4004	GOL	C1-C2	-3.30	1.39	1.51
4	H	4002	GOL	O3-C3	3.29	1.56	1.42
4	R	4007	GOL	O3-C3	3.27	1.56	1.42
4	W	4006	GOL	C1-C2	-3.26	1.39	1.51
4	A	4012	GOL	O2-C2	-3.21	1.34	1.43
4	J	4005	GOL	O2-C2	-3.19	1.34	1.43
4	H	4011	GOL	C1-C2	-3.17	1.39	1.51
5	W	5011	ACY	O-C	3.16	1.36	1.22
4	A	4012	GOL	O3-C3	3.16	1.55	1.42
4	1	4010	GOL	C1-C2	-3.13	1.39	1.51
4	R	4007	GOL	C1-C2	-3.07	1.40	1.51
4	X	4004	GOL	O3-C3	3.05	1.55	1.42
4	M	4003	GOL	O2-C2	-3.00	1.34	1.43
4	J	4005	GOL	O3-C3	2.94	1.54	1.42
4	A	4012	GOL	C1-C2	-2.91	1.40	1.51
4	R	4007	GOL	O2-C2	-2.89	1.35	1.43
4	1	4010	GOL	O3-C3	2.89	1.54	1.42
4	2	4009	GOL	C1-C2	-2.87	1.40	1.51
4	W	4006	GOL	O3-C3	2.86	1.54	1.42
4	X	4004	GOL	O2-C2	-2.81	1.35	1.43
4	M	4003	GOL	O3-C3	2.80	1.54	1.42
5	F	5015	ACY	O-C	2.77	1.34	1.22
5	N	5009	ACY	O-C	2.76	1.34	1.22
4	2	4009	GOL	O3-C3	2.61	1.53	1.42
5	K	5013	ACY	O-C	2.46	1.33	1.22
5	H	5012	ACY	O-C	2.44	1.32	1.22
4	2	4009	GOL	O2-C2	-2.37	1.36	1.43
4	H	4002	GOL	O2-C2	-2.35	1.36	1.43
5	I	5004	ACY	O-C	2.33	1.32	1.22
5	X	5002	ACY	O-C	2.31	1.32	1.22
5	Z	5006	ACY	O-C	2.29	1.32	1.22
4	1	4010	GOL	O2-C2	-2.22	1.36	1.43
4	V	4008	GOL	O3-C3	2.19	1.51	1.42
4	W	4006	GOL	O2-C2	-2.16	1.37	1.43
5	I	5010	ACY	O-C	2.13	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	5007	ACY	O-C	2.08	1.31	1.22
5	2	5005	ACY	O-C	2.07	1.31	1.22
5	Y	5008	ACY	O-C	2.05	1.31	1.22
4	H	4011	GOL	O2-C2	-2.01	1.37	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	4010	GOL	O3-C3-C2	11.53	162.30	110.38
4	X	4004	GOL	O3-C3-C2	11.52	162.22	110.38
4	V	4008	GOL	O3-C3-C2	11.39	161.66	110.38
4	W	4006	GOL	O3-C3-C2	11.37	161.55	110.38
4	H	4002	GOL	O3-C3-C2	11.29	161.21	110.38
4	R	4007	GOL	O3-C3-C2	11.15	160.59	110.38
4	G	4001	GOL	O3-C3-C2	10.95	159.66	110.38
4	M	4003	GOL	O3-C3-C2	10.89	159.39	110.38
4	2	4009	GOL	O3-C3-C2	10.81	159.03	110.38
4	J	4005	GOL	O3-C3-C2	10.76	158.83	110.38
4	H	4011	GOL	O3-C3-C2	10.74	158.73	110.38
4	A	4012	GOL	O3-C3-C2	10.69	158.51	110.38
4	X	4004	GOL	O2-C2-C3	7.52	140.31	109.18
4	V	4008	GOL	O2-C2-C3	7.32	139.51	109.18
4	H	4002	GOL	O2-C2-C3	7.32	139.47	109.18
4	1	4010	GOL	O2-C2-C3	7.24	139.17	109.18
4	M	4003	GOL	O2-C2-C3	7.13	138.71	109.18
4	R	4007	GOL	O2-C2-C3	7.07	138.46	109.18
4	W	4006	GOL	O2-C2-C3	7.02	138.26	109.18
4	G	4001	GOL	O2-C2-C3	7.01	138.22	109.18
4	H	4011	GOL	O2-C2-C3	6.96	137.98	109.18
4	J	4005	GOL	O2-C2-C3	6.92	137.83	109.18
4	A	4012	GOL	O2-C2-C3	6.80	137.33	109.18
4	2	4009	GOL	O2-C2-C3	6.60	136.51	109.18
4	2	4009	GOL	O1-C1-C2	3.44	125.86	110.38
4	V	4008	GOL	O1-C1-C2	3.31	125.28	110.38
4	G	4001	GOL	O1-C1-C2	3.30	125.24	110.38
4	W	4006	GOL	O1-C1-C2	3.28	125.16	110.38
4	A	4012	GOL	O1-C1-C2	3.25	125.00	110.38
4	M	4003	GOL	O1-C1-C2	3.11	124.36	110.38
4	H	4011	GOL	O1-C1-C2	3.04	124.07	110.38
4	H	4002	GOL	O1-C1-C2	2.99	123.84	110.38
4	X	4004	GOL	O1-C1-C2	2.98	123.80	110.38
4	R	4007	GOL	O1-C1-C2	2.97	123.76	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1	4010	GOL	O1-C1-C2	2.95	123.64	110.38
4	J	4005	GOL	O1-C1-C2	2.88	123.34	110.38
5	1	5014	ACY	O-C-CH3	-2.65	111.65	122.53
5	N	5009	ACY	O-C-CH3	-2.62	111.79	122.53
5	W	5011	ACY	O-C-CH3	-2.60	111.85	122.53
5	2	5005	ACY	O-C-CH3	-2.55	112.07	122.53
5	W	5001	ACY	O-C-CH3	-2.53	112.16	122.53
5	V	5007	ACY	O-C-CH3	-2.50	112.28	122.53
5	I	5004	ACY	O-C-CH3	-2.48	112.35	122.53
5	M	5003	ACY	O-C-CH3	-2.46	112.44	122.53
5	X	5002	ACY	O-C-CH3	-2.44	112.52	122.53
5	H	5012	ACY	O-C-CH3	-2.41	112.66	122.53
5	F	5015	ACY	O-C-CH3	-2.35	112.89	122.53
5	Y	5008	ACY	O-C-CH3	-2.33	112.97	122.53
5	Z	5006	ACY	O-C-CH3	-2.30	113.08	122.53
5	K	5013	ACY	O-C-CH3	-2.30	113.11	122.53
5	I	5010	ACY	O-C-CH3	-2.29	113.12	122.53

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	4001	GOL	O1-C1-C2-C3
4	H	4002	GOL	O1-C1-C2-C3
4	R	4007	GOL	O1-C1-C2-C3
4	V	4008	GOL	O1-C1-C2-C3
4	W	4006	GOL	O1-C1-C2-C3
4	1	4010	GOL	O1-C1-C2-C3
4	H	4002	GOL	C1-C2-C3-O3
4	M	4003	GOL	C1-C2-C3-O3
4	R	4007	GOL	C1-C2-C3-O3
4	V	4008	GOL	C1-C2-C3-O3
4	W	4006	GOL	C1-C2-C3-O3
4	X	4004	GOL	C1-C2-C3-O3
4	1	4010	GOL	C1-C2-C3-O3
4	X	4004	GOL	O1-C1-C2-O2
4	2	4009	GOL	O1-C1-C2-O2
4	A	4012	GOL	O1-C1-C2-O2
4	H	4011	GOL	O1-C1-C2-O2
4	J	4005	GOL	O1-C1-C2-O2
4	M	4003	GOL	O1-C1-C2-O2
4	A	4012	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	G	4001	GOL	O2-C2-C3-O3
4	H	4002	GOL	O1-C1-C2-O2
4	H	4002	GOL	O2-C2-C3-O3
4	H	4011	GOL	O2-C2-C3-O3
4	J	4005	GOL	O2-C2-C3-O3
4	M	4003	GOL	O2-C2-C3-O3
4	R	4007	GOL	O2-C2-C3-O3
4	V	4008	GOL	O2-C2-C3-O3
4	W	4006	GOL	O2-C2-C3-O3
4	X	4004	GOL	O2-C2-C3-O3
4	1	4010	GOL	O2-C2-C3-O3
4	2	4009	GOL	O2-C2-C3-O3
4	A	4012	GOL	C1-C2-C3-O3
4	G	4001	GOL	C1-C2-C3-O3
4	H	4011	GOL	C1-C2-C3-O3
4	2	4009	GOL	C1-C2-C3-O3
4	J	4005	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	5005	ACY	1	0
5	W	5011	ACY	7	0
4	X	4004	GOL	2	0
5	K	5013	ACY	4	0
4	W	4006	GOL	2	0
4	A	4012	GOL	1	0
4	H	4002	GOL	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	1	124/130 (95%)	-1.37	0 100 100	15, 34, 48, 53	0
1	2	124/130 (95%)	-1.42	0 100 100	16, 29, 51, 56	0
1	A	123/130 (94%)	-1.47	0 100 100	20, 26, 41, 53	0
1	B	124/130 (95%)	-1.47	0 100 100	18, 27, 39, 56	0
1	C	124/130 (95%)	-1.42	0 100 100	21, 30, 44, 60	0
1	D	124/130 (95%)	-1.33	0 100 100	22, 34, 54, 66	0
1	E	124/130 (95%)	-1.36	0 100 100	19, 33, 50, 64	0
1	F	124/130 (95%)	-1.41	0 100 100	19, 30, 47, 61	0
1	G	124/130 (95%)	-1.49	0 100 100	19, 26, 40, 55	0
1	H	125/130 (96%)	-1.51	0 100 100	16, 26, 40, 56	0
1	I	125/130 (96%)	-1.44	0 100 100	17, 28, 47, 69	0
1	J	125/130 (96%)	-1.31	0 100 100	18, 34, 55, 71	0
1	K	125/130 (96%)	-1.25	0 100 100	20, 39, 62, 72	0
1	L	124/130 (95%)	-1.32	0 100 100	18, 35, 54, 63	0
1	M	125/130 (96%)	-1.53	0 100 100	16, 25, 37, 53	0
1	N	125/130 (96%)	-1.51	0 100 100	16, 24, 37, 54	0
1	O	124/130 (95%)	-1.45	0 100 100	21, 28, 45, 60	0
1	P	124/130 (95%)	-1.45	0 100 100	20, 27, 45, 59	0
1	Q	124/130 (95%)	-1.43	0 100 100	17, 29, 44, 62	0
1	R	124/130 (95%)	-1.39	0 100 100	22, 33, 51, 65	0
1	S	124/130 (95%)	-1.37	0 100 100	21, 31, 50, 63	0
1	T	124/130 (95%)	-1.42	0 100 100	21, 30, 45, 64	0
1	U	124/130 (95%)	-1.45	0 100 100	20, 27, 42, 60	0
1	V	125/130 (96%)	-1.58	0 100 100	15, 23, 33, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9		
1	W	125/130 (96%)	-1.50	0	100	100	14, 26, 39, 56	0
1	X	125/130 (96%)	-1.52	0	100	100	14, 26, 40, 63	0
1	Y	125/130 (96%)	-1.48	0	100	100	14, 26, 47, 70	0
1	Z	125/130 (96%)	-1.39	0	100	100	16, 31, 54, 65	0
All	All	3482/3640 (95%)	-1.43	0	100	100	14, 29, 50, 72	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	A	3004	1/1	0.98	0.14	65,65,65,65	0
3	NA	B	3001	1/1	0.98	0.14	76,76,76,76	0
3	NA	R	3005	1/1	0.98	0.11	82,82,82,82	0
3	NA	S	3002	1/1	0.98	0.10	59,59,59,59	0
3	NA	V	3003	1/1	0.98	0.09	67,67,67,67	0
4	GOL	A	4012	6/6	0.98	0.05	56,56,57,59	0
4	GOL	H	4011	6/6	0.98	0.05	46,50,51,52	0
4	GOL	M	4003	6/6	0.98	0.05	43,49,50,51	0
4	GOL	R	4007	6/6	0.98	0.06	49,53,53,54	0
4	GOL	X	4004	6/6	0.98	0.06	45,48,50,50	0
4	GOL	1	4010	6/6	0.98	0.04	42,44,45,47	0
4	GOL	2	4009	6/6	0.98	0.05	47,47,48,49	0
5	ACY	W	5011	4/4	0.98	0.06	32,35,37,38	0
4	GOL	W	4006	6/6	0.99	0.03	34,37,40,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	J	4005	6/6	0.99	0.04	46,46,48,49	0
4	GOL	H	4002	6/6	0.99	0.05	52,54,56,57	0
4	GOL	G	4001	6/6	0.99	0.06	31,42,44,45	0
5	ACY	F	5015	4/4	0.99	0.05	41,44,44,44	0
5	ACY	H	5012	4/4	0.99	0.04	27,28,28,29	0
5	ACY	I	5004	4/4	0.99	0.05	36,39,40,40	0
5	ACY	I	5010	4/4	0.99	0.03	19,25,25,26	0
5	ACY	K	5013	4/4	0.99	0.06	46,47,47,48	0
5	ACY	M	5003	4/4	0.99	0.04	25,27,27,28	0
5	ACY	N	5009	4/4	0.99	0.03	29,30,30,31	0
4	GOL	V	4008	6/6	0.99	0.05	47,49,51,53	0
5	ACY	X	5002	4/4	0.99	0.04	25,27,27,28	0
5	ACY	Z	5006	4/4	0.99	0.04	30,32,32,34	0
5	ACY	1	5014	4/4	0.99	0.04	34,35,36,36	0
2	CD	A	2001	1/1	1.00	0.02	35,35,35,35	0
2	CD	A	2007	1/1	1.00	0.02	37,37,37,37	0
2	CD	B	2002	1/1	1.00	0.02	38,38,38,38	0
2	CD	D	2003	1/1	1.00	0.02	44,44,44,44	0
2	CD	D	2004	1/1	1.00	0.03	44,44,44,44	0
2	CD	E	2005	1/1	1.00	0.02	40,40,40,40	0
2	CD	F	2006	1/1	1.00	0.03	37,37,37,37	0
2	CD	H	2008	1/1	1.00	0.02	38,38,38,38	0
2	CD	H	2014	1/1	1.00	0.02	40,40,40,40	0
2	CD	I	2009	1/1	1.00	0.02	46,46,46,46	0
2	CD	J	2010	1/1	1.00	0.03	47,47,47,47	0
2	CD	K	2011	1/1	1.00	0.03	44,44,44,44	0
2	CD	L	2012	1/1	1.00	0.02	39,39,39,39	0
2	CD	M	2013	1/1	1.00	0.02	36,36,36,36	0
2	CD	O	2021	1/1	1.00	0.01	39,39,39,39	0
2	CD	P	2015	1/1	1.00	0.02	42,42,42,42	0
2	CD	P	2016	1/1	1.00	0.01	37,37,37,37	1
2	CD	Q	2017	1/1	1.00	0.02	43,43,43,43	0
2	CD	R	2018	1/1	1.00	0.02	41,41,41,41	0
2	CD	S	2019	1/1	1.00	0.01	39,39,39,39	0
2	CD	U	2020	1/1	1.00	0.02	41,41,41,41	0
2	CD	V	2022	1/1	1.00	0.02	34,34,34,34	0
2	CD	W	2023	1/1	1.00	0.03	37,37,37,37	0
2	CD	X	2024	1/1	1.00	0.03	37,37,37,37	0
5	ACY	V	5007	4/4	1.00	0.03	23,24,24,27	0
5	ACY	W	5001	4/4	1.00	0.02	23,23,26,27	0
2	CD	Y	2025	1/1	1.00	0.02	34,34,34,34	1
2	CD	Z	2026	1/1	1.00	0.02	40,40,40,40	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACY	Y	5008	4/4	1.00	0.02	21,24,24,28	0
2	CD	1	2027	1/1	1.00	0.02	42,42,42,42	0
2	CD	2	2028	1/1	1.00	0.02	36,36,36,36	1
5	ACY	2	5005	4/4	1.00	0.04	30,31,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.