



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:04 pm BST

PDB ID : 3U5P  
Title : Crystal structure of the complex of TRIM33 PHD-Bromo and H3(1-28)K9me  
3K14acK18acK23ac histone peptide  
Authors : Wang, Z.; Patel, D.J.  
Deposited on : 2011-10-11  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

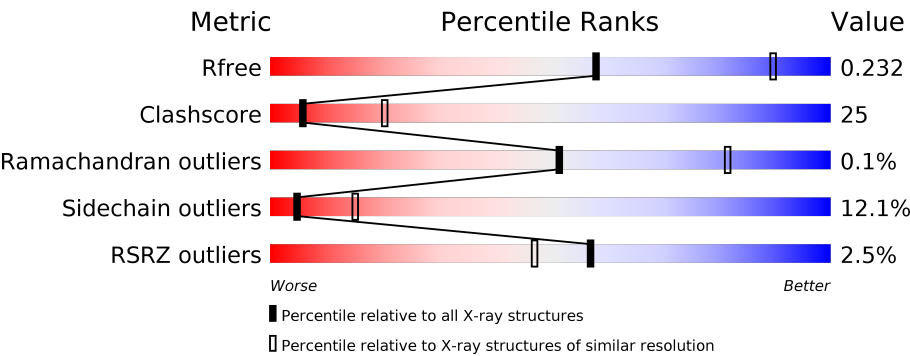
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	A	207	<div><div></div><div>53%30%7%9%</div></div>
1	B	207	<div><div>%</div><div>53%32%6%9%</div></div>
1	C	207	<div><div>%</div><div>49%34%7%9%</div></div>
1	D	207	<div><div>2%</div><div>56%27%8%9%</div></div>
1	E	207	<div><div>%</div><div>57%28%6%9%</div></div>
1	F	207	<div><div></div><div>56%26%9%9%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	207	
1	H	207	
2	I	28	
2	J	28	
2	K	28	
2	L	28	
2	M	28	
2	N	28	
2	O	28	
2	P	28	

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	ALY	L	14	-	-	-	X
2	ALY	O	14	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13261 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 E3 ubiquitin-protein ligase TRIM33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			
1	B	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			
1	C	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			
1	D	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			
1	E	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			
1	F	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			
1	G	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			
1	H	188	Total	C	N	O	S	0	0	0
			1522	973	252	282	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
B	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
C	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
D	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
E	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
F	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
G	881	SER	-	EXPRESSION TAG	UNP Q9UPN9
H	881	SER	-	EXPRESSION TAG	UNP Q9UPN9

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	18	Total	C	N	O	0	0	0
			137	82	31	24			
2	J	16	Total	C	N	O	0	0	0
			128	77	29	22			
2	K	16	Total	C	N	O	0	0	0
			128	77	29	22			
2	L	18	Total	C	N	O	0	0	0
			137	82	31	24			
2	M	19	Total	C	N	O	0	0	0
			146	87	33	26			
2	N	16	Total	C	N	O	0	0	0
			128	77	29	22			
2	O	18	Total	C	N	O	0	0	0
			137	82	31	24			
2	P	16	Total	C	N	O	0	0	0
			128	77	29	22			

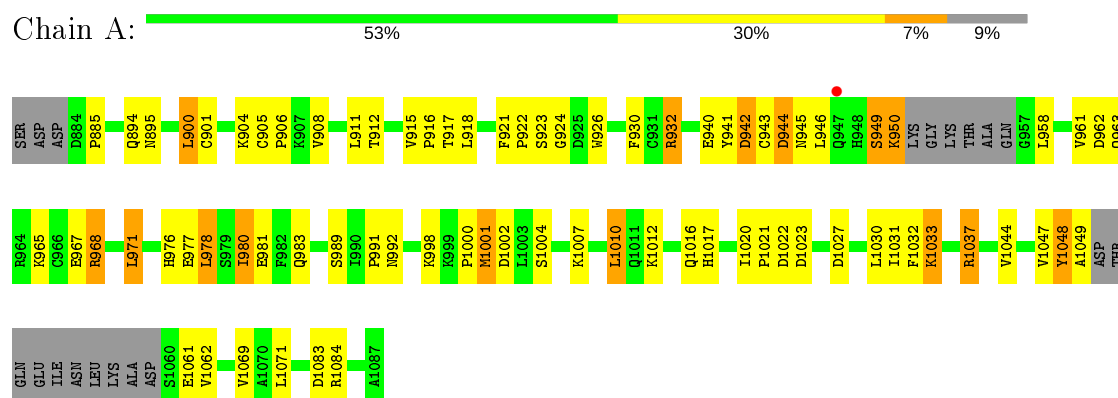
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		
3	H	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		

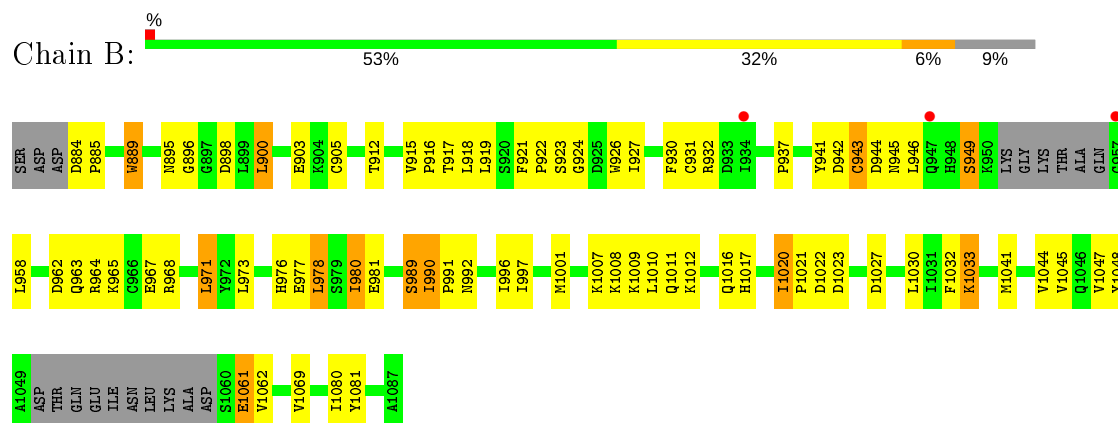
### 3 Residue-property plots [i](#)

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

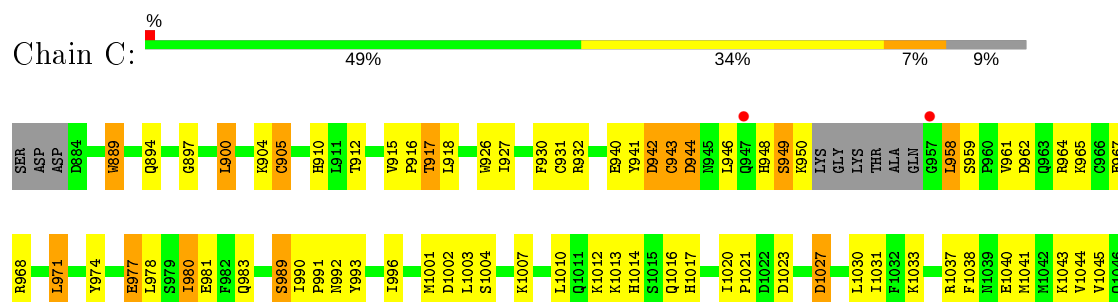
#### • Molecule 1: E3 ubiquitin-protein ligase TRIM33



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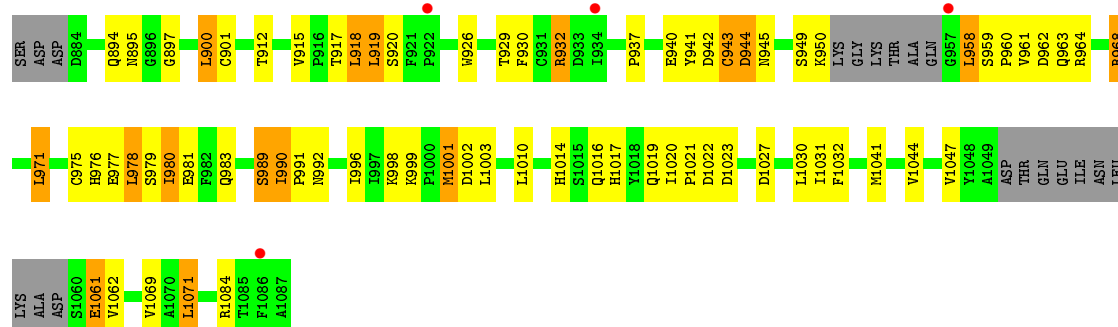


#### • Molecule 1: E3 ubiquitin-protein ligase TRIM33

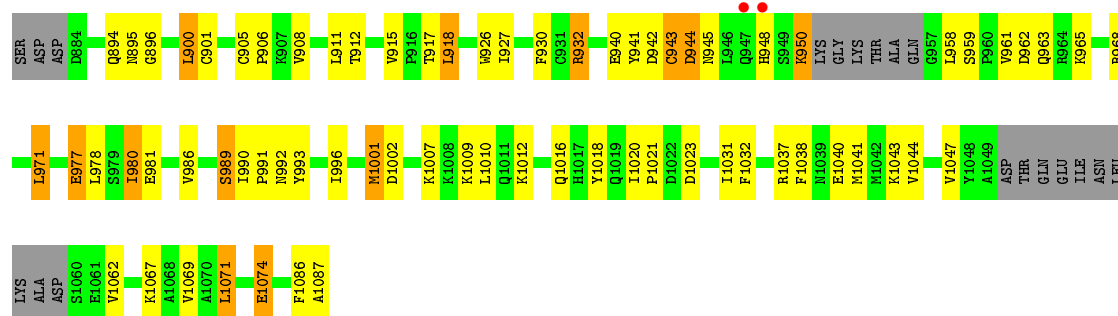




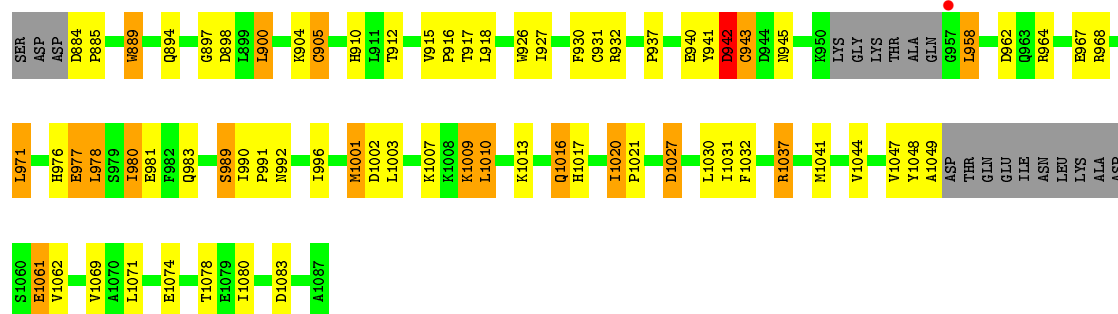
• Molecule 1: E3 ubiquitin-protein ligase TRIM33



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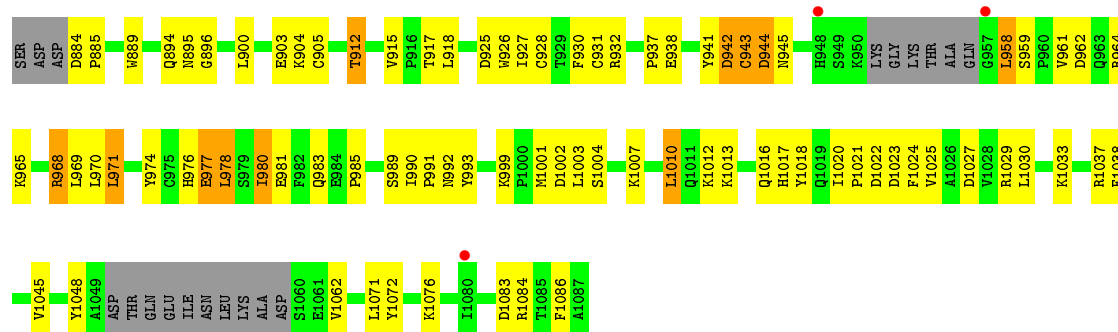


• Molecule 1: E3 ubiquitin-protein ligase TRIM33



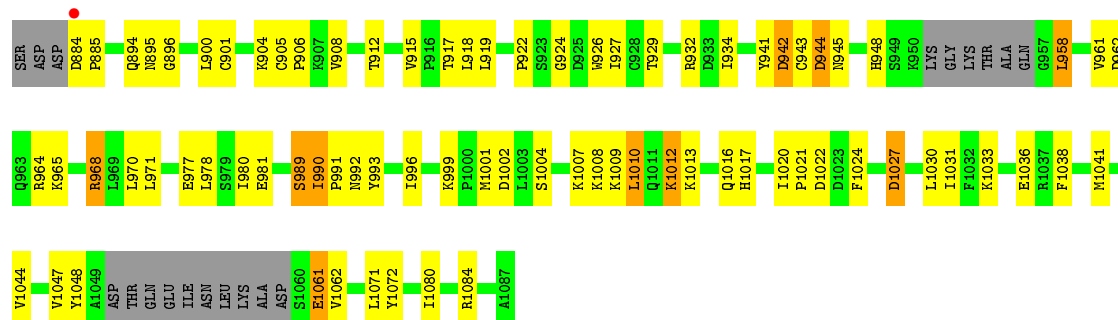
• Molecule 1: E3 ubiquitin-protein ligase TRIM33





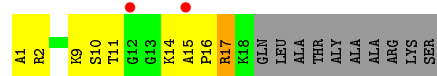
• Molecule 1: E3 ubiquitin-protein ligase TRIM33

Chain H: 53% 33% 5% 9%



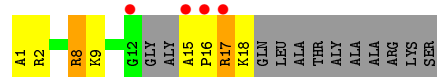
• Molecule 2: Histone H3.1

Chain I: 7% 32% 29% 36%



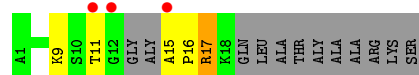
• Molecule 2: Histone H3.1

Chain J: 14% 29% 21% 7% 43%



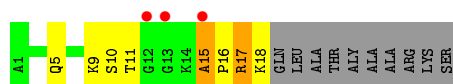
• Molecule 2: Histone H3.1

Chain K: 11% 39% 14% 43%

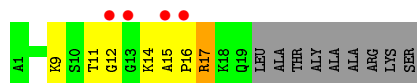
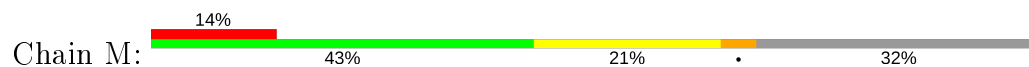


• Molecule 2: Histone H3.1

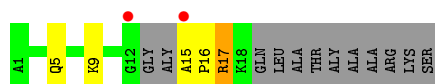
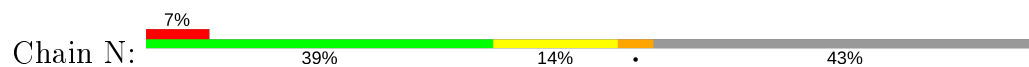
Chain L: 11% 36% 21% 7% 36%



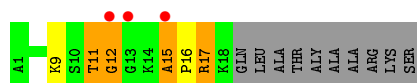
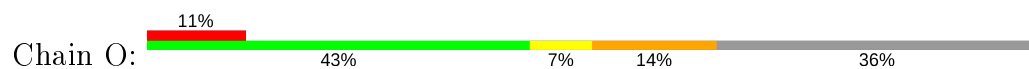
- Molecule 2: Histone H3.1



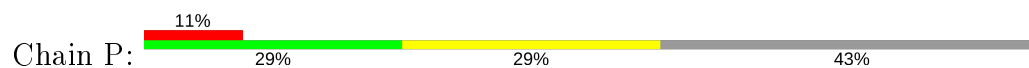
- Molecule 2: Histone H3.1



- Molecule 2: Histone H3.1



- Molecule 2: Histone H3.1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.43Å 63.61Å 124.61Å 90.01° 90.04° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 28.43 – 2.79	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.00-2.80) 93.7 (28.43-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.210 , 0.265 0.212 , 0.232	Depositor DCC
$R_{free}$ test set	2397 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 32.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for k,-h,l 0.478 for -k,h,l 0.480 for h,-k,-l 0.480 for -h,k,-l 0.487 for -h,-k,l 0.479 for k,h,-l 0.480 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M3L, ALY

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	0.68	0/1558	0.76	0/2105
1	B	0.69	1/1558 (0.1%)	0.73	0/2105
1	C	0.72	2/1558 (0.1%)	0.78	2/2105 (0.1%)
1	D	0.72	1/1558 (0.1%)	0.76	1/2105 (0.0%)
1	E	0.70	0/1558	0.75	0/2105
1	F	0.71	2/1558 (0.1%)	0.75	2/2105 (0.1%)
1	G	0.69	0/1558	0.77	1/2105 (0.0%)
1	H	0.70	0/1558	0.76	1/2105 (0.0%)
2	I	0.47	0/107	0.80	0/140
2	J	0.52	0/103	0.87	0/135
2	K	0.53	0/103	0.61	0/135
2	L	0.49	0/107	0.74	0/140
2	M	0.46	0/115	0.63	0/149
2	N	0.53	0/103	0.67	0/135
2	O	0.50	0/107	0.77	1/140 (0.7%)
2	P	0.50	0/103	0.63	0/135
All	All	0.69	6/13312 (0.0%)	0.75	8/17949 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1013	LYS	CE-NZ	5.95	1.64	1.49
1	D	950	LYS	CE-NZ	5.41	1.62	1.49
1	B	889	TRP	CD2-CE2	5.31	1.47	1.41
1	F	889	TRP	CD2-CE2	5.23	1.47	1.41
1	C	889	TRP	CD2-CE2	5.20	1.47	1.41
1	C	948	HIS	CG-CD2	5.04	1.44	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	958	LEU	CA-CB-CG	6.03	129.18	115.30
1	F	942	ASP	N-CA-C	-5.97	94.87	111.00
1	G	958	LEU	CA-CB-CG	5.95	129.00	115.30
2	O	12	GLY	N-CA-C	-5.52	99.29	113.10
1	H	958	LEU	CA-CB-CG	5.28	127.44	115.30
1	F	958	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	958	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	1077	LEU	CA-CB-CG	-5.19	103.35	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	932	ARG	Sidechain
1	D	932	ARG	Sidechain
1	E	932	ARG	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	A	1522	0	1486	72	0
1	B	1522	0	1486	84	0
1	C	1522	0	1487	75	0
1	D	1522	0	1486	69	0
1	E	1522	0	1486	70	0
1	F	1522	0	1487	66	0
1	G	1522	0	1486	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1522	0	1486	69	0
2	I	137	0	149	20	0
2	J	128	0	143	18	0
2	K	128	0	143	10	0
2	L	137	0	149	14	0
2	M	146	0	157	14	0
2	N	128	0	144	9	0
2	O	137	0	150	14	0
2	P	128	0	144	11	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
All	All	13261	0	13069	664	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 25.

All (664) 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)
2:L:15:ALA:HB1	2:L:16:PRO:CD	1.64	1.25
2:J:15:ALA:CB	2:J:16:PRO:HD3	1.64	1.25
2:I:16:PRO:O	2:I:17:ARG:HD3	1.35	1.24
2:O:15:ALA:HB1	2:O:16:PRO:CD	1.69	1.22
2:O:15:ALA:HB1	2:O:16:PRO:HD3	1.19	1.17
2:K:16:PRO:O	2:K:17:ARG:HD2	1.43	1.16
2:L:15:ALA:CB	2:L:16:PRO:HD2	1.75	1.14
1:C:1077:LEU:HD12	1:C:1077:LEU:O	1.47	1.11
2:J:15:ALA:HB3	2:J:16:PRO:CD	1.83	1.08
2:J:15:ALA:HB1	2:J:16:PRO:HD3	1.36	1.07
2:J:16:PRO:O	2:J:17:ARG:HD2	1.55	1.07
2:I:17:ARG:HG3	2:I:17:ARG:HH11	1.20	1.06
2:J:15:ALA:CB	2:J:16:PRO:CD	2.33	1.05
2:O:15:ALA:CB	2:O:16:PRO:CD	2.31	1.04
1:G:943:CYS:SG	1:G:945:ASN:N	2.31	1.02
1:E:1074:GLU:HA	1:E:1074:GLU:OE1	1.62	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:943:CYS:SG	1:G:945:ASN:HB2	2.03	0.99
1:H:990:ILE:N	1:H:990:ILE:HD13	1.73	0.99
2:L:16:PRO:O	2:L:17:ARG:HD2	1.64	0.98
1:D:932:ARG:CZ	1:D:941:TYR:HE2	1.77	0.97
1:D:932:ARG:CZ	1:D:941:TYR:CE2	2.47	0.97
2:J:15:ALA:HB3	2:J:16:PRO:HD3	1.45	0.96
2:P:16:PRO:O	2:P:17:ARG:HD3	1.65	0.95
1:A:980:ILE:H	1:A:980:ILE:HD13	1.29	0.95
2:I:14:ALY:C	2:I:16:PRO:HD2	1.96	0.94
2:N:15:ALA:N	2:N:16:PRO:CD	2.30	0.94
2:P:15:ALA:N	2:P:16:PRO:CD	2.31	0.94
2:L:10:SER:O	2:L:11:THR:HG22	1.68	0.94
1:B:932:ARG:NH2	1:B:964:ARG:CD	2.32	0.93
2:L:15:ALA:HB1	2:L:16:PRO:HD2	0.94	0.93
2:K:15:ALA:N	2:K:16:PRO:CD	2.31	0.93
1:F:915:VAL:HG22	1:F:1007:LYS:HE3	1.49	0.93
1:F:981:GLU:OE2	2:N:17:ARG:HD2	1.66	0.93
1:B:912:THR:HA	1:B:917:THR:HG23	1.50	0.92
1:B:932:ARG:HD3	1:B:941:TYR:OH	1.70	0.92
1:B:932:ARG:HD3	1:B:941:TYR:CE2	2.05	0.92
1:B:932:ARG:HD3	1:B:941:TYR:CZ	2.06	0.91
1:C:989:SER:O	1:C:991:PRO:HD3	1.69	0.91
2:I:17:ARG:CG	2:I:17:ARG:HH11	1.84	0.91
1:E:926:TRP:NE1	1:E:941:TYR:HE1	1.68	0.91
1:H:989:SER:O	1:H:991:PRO:HD3	1.71	0.91
1:D:990:ILE:HD13	1:D:990:ILE:N	1.83	0.90
2:I:10:SER:O	2:I:11:THR:HG23	1.70	0.90
1:A:932:ARG:CZ	1:A:941:TYR:CE2	2.55	0.89
1:D:989:SER:O	1:D:991:PRO:HD3	1.71	0.89
1:C:932:ARG:NH1	1:C:941:TYR:CD2	2.41	0.89
1:F:912:THR:HA	1:F:917:THR:HG23	1.53	0.89
2:I:16:PRO:O	2:I:17:ARG:CD	2.21	0.89
1:D:991:PRO:O	1:D:992:ASN:HB2	1.73	0.89
1:H:1020:ILE:HD12	1:H:1021:PRO:HD2	1.55	0.88
1:A:932:ARG:CZ	1:A:941:TYR:HE2	1.86	0.88
1:E:926:TRP:NE1	1:E:941:TYR:CE1	2.41	0.88
1:B:932:ARG:CZ	1:B:941:TYR:HE2	1.87	0.88
2:I:15:ALA:N	2:I:16:PRO:CD	2.37	0.87
2:K:15:ALA:N	2:K:16:PRO:HD3	1.90	0.86
1:B:1045:VAL:HG13	1:G:1048:TYR:HE1	1.41	0.86
1:G:932:ARG:NH1	1:G:941:TYR:CD2	2.44	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1077:LEU:C	1:C:1077:LEU:HD12	1.89	0.86
1:F:989:SER:O	1:F:991:PRO:HD3	1.76	0.85
2:I:14:ALY:C	2:I:16:PRO:CD	2.54	0.85
1:A:912:THR:HA	1:A:917:THR:HG23	1.57	0.84
1:B:932:ARG:NH2	1:B:964:ARG:HD3	1.92	0.84
1:C:977:GLU:H	1:C:977:GLU:CD	1.79	0.84
1:H:990:ILE:H	1:H:990:ILE:HD13	1.35	0.84
1:B:989:SER:O	1:B:991:PRO:HD3	1.77	0.84
2:I:15:ALA:N	2:I:16:PRO:HD3	1.92	0.84
2:M:14:ALY:C	2:M:16:PRO:CD	2.56	0.83
1:H:912:THR:HA	1:H:917:THR:HG23	1.61	0.82
1:F:990:ILE:N	1:F:990:ILE:HD13	1.93	0.82
1:F:932:ARG:NH1	1:F:941:TYR:CD2	2.47	0.82
2:M:14:ALY:C	2:M:16:PRO:HD2	2.09	0.81
1:B:932:ARG:NH1	1:B:941:TYR:CE2	2.49	0.81
1:G:912:THR:HA	1:G:917:THR:HG23	1.63	0.81
1:G:943:CYS:SG	1:G:945:ASN:CB	2.68	0.81
1:C:894:GLN:O	2:K:9:M3L:HM23	1.81	0.80
1:B:1020:ILE:HG22	1:B:1023:ASP:OD2	1.80	0.80
1:B:1045:VAL:HG13	1:G:1048:TYR:CE1	2.17	0.80
2:M:15:ALA:N	2:M:16:PRO:HD3	1.97	0.79
1:E:912:THR:HA	1:E:917:THR:HG23	1.65	0.79
2:J:8:ARG:HH11	2:J:8:ARG:CG	1.95	0.79
1:G:980:ILE:H	1:G:980:ILE:HD13	1.47	0.79
1:E:932:ARG:CZ	1:E:941:TYR:CE2	2.66	0.78
1:H:990:ILE:N	1:H:990:ILE:CD1	2.46	0.78
1:B:991:PRO:O	1:B:992:ASN:HB2	1.81	0.78
2:K:16:PRO:O	2:K:17:ARG:CD	2.31	0.78
2:L:16:PRO:O	2:L:17:ARG:CD	2.32	0.78
1:A:932:ARG:HD3	1:A:941:TYR:CE2	2.19	0.77
1:A:943:CYS:SG	1:A:945:ASN:HB2	2.23	0.77
1:G:977:GLU:CD	1:G:977:GLU:H	1.86	0.77
1:C:915:VAL:HG22	1:C:1007:LYS:HE3	1.66	0.77
1:H:894:GLN:O	2:P:9:M3L:HM23	1.84	0.77
1:H:932:ARG:NH1	1:H:941:TYR:CD2	2.53	0.77
1:B:932:ARG:CD	1:B:941:TYR:CE2	2.68	0.77
1:C:991:PRO:O	1:C:992:ASN:HB2	1.83	0.76
2:M:15:ALA:N	2:M:16:PRO:CD	2.48	0.76
1:E:943:CYS:SG	1:E:945:ASN:HB2	2.26	0.76
1:F:1020:ILE:HD13	1:F:1021:PRO:HD2	1.67	0.75
2:J:15:ALA:HB3	2:J:16:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ARG:NE	1:A:941:TYR:HE2	1.85	0.74
1:E:977:GLU:H	1:E:977:GLU:CD	1.88	0.74
1:G:1020:ILE:HG13	1:G:1021:PRO:HD2	1.70	0.74
1:E:1020:ILE:HG22	1:E:1023:ASP:OD2	1.87	0.74
1:A:943:CYS:SG	1:A:945:ASN:N	2.59	0.74
1:D:990:ILE:HD13	1:D:990:ILE:H	1.49	0.74
1:B:980:ILE:HD13	1:B:980:ILE:H	1.51	0.73
1:B:932:ARG:NH2	1:B:964:ARG:HG2	2.02	0.73
1:D:977:GLU:CD	1:D:977:GLU:H	1.89	0.73
1:E:1074:GLU:CA	1:E:1074:GLU:OE1	2.36	0.73
1:A:894:GLN:O	2:I:9:M3L:HM23	1.89	0.72
1:C:926:TRP:NE1	1:C:941:TYR:HE1	1.88	0.72
1:G:926:TRP:NE1	1:G:941:TYR:CE1	2.58	0.72
1:H:932:ARG:NH1	1:H:941:TYR:CE2	2.58	0.72
2:J:16:PRO:O	2:J:17:ARG:CD	2.37	0.71
1:G:961:VAL:HG12	1:G:965:LYS:HE2	1.72	0.71
2:P:15:ALA:N	2:P:16:PRO:HD3	2.03	0.71
1:B:932:ARG:NH1	1:B:941:TYR:HE2	1.88	0.71
1:E:932:ARG:HD3	1:E:941:TYR:CE2	2.26	0.71
1:C:1061:GLU:OE1	1:C:1061:GLU:N	2.24	0.70
1:E:894:GLN:HG3	2:M:9:M3L:CM2	2.21	0.70
2:O:15:ALA:HB1	2:O:16:PRO:HD2	1.66	0.70
1:F:942:ASP:OD1	1:F:942:ASP:C	2.30	0.70
1:F:977:GLU:OE1	1:F:977:GLU:N	2.23	0.70
1:G:989:SER:O	1:G:991:PRO:HD3	1.92	0.70
1:E:944:ASP:C	1:E:944:ASP:OD1	2.30	0.70
1:E:932:ARG:NH1	1:E:941:TYR:CD2	2.59	0.70
1:B:932:ARG:CD	1:B:941:TYR:HE2	2.05	0.69
1:H:942:ASP:OD1	1:H:942:ASP:C	2.29	0.69
1:D:943:CYS:SG	1:D:945:ASN:HB2	2.32	0.69
1:D:944:ASP:C	1:D:944:ASP:OD1	2.30	0.69
1:G:1020:ILE:HG22	1:G:1023:ASP:OD2	1.92	0.69
2:O:15:ALA:CB	2:O:16:PRO:HD2	2.21	0.69
1:C:944:ASP:C	1:C:944:ASP:OD1	2.31	0.69
1:D:932:ARG:NH2	1:D:941:TYR:HE2	1.90	0.69
2:I:14:ALY:CB	2:I:16:PRO:HD2	2.24	0.68
1:H:932:ARG:CZ	1:H:941:TYR:HE2	2.07	0.68
2:N:15:ALA:N	2:N:16:PRO:HD3	2.08	0.68
2:M:16:PRO:O	2:M:17:ARG:HD3	1.94	0.68
1:B:932:ARG:NH2	1:B:964:ARG:CG	2.56	0.68
1:E:943:CYS:SG	1:E:945:ASN:N	2.67	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1061:GLU:CD	1:D:1061:GLU:H	1.98	0.68
1:E:932:ARG:CZ	1:E:941:TYR:CD2	2.76	0.68
1:G:926:TRP:NE1	1:G:941:TYR:HE1	1.92	0.68
1:A:980:ILE:HD13	1:A:980:ILE:N	2.05	0.67
1:B:977:GLU:H	1:B:977:GLU:CD	1.97	0.67
1:A:932:ARG:CD	1:A:941:TYR:CE2	2.76	0.67
1:C:926:TRP:NE1	1:C:941:TYR:CE1	2.62	0.67
1:A:924:GLY:O	2:I:1:ALA:HB2	1.95	0.67
1:G:970:LEU:HD22	1:G:1010:LEU:HD23	1.77	0.67
2:P:15:ALA:N	2:P:16:PRO:HD2	2.10	0.67
1:F:916:PRO:HG3	1:F:967:GLU:OE2	1.94	0.67
1:C:1044:VAL:O	1:C:1047:VAL:HG12	1.95	0.66
1:C:942:ASP:O	1:C:942:ASP:CG	2.32	0.66
1:H:977:GLU:H	1:H:977:GLU:CD	1.99	0.66
1:E:945:ASN:OD1	1:E:1012:LYS:HB2	1.95	0.66
1:F:991:PRO:O	1:F:992:ASN:HB2	1.94	0.66
2:I:17:ARG:NH1	2:I:17:ARG:CG	2.52	0.66
1:B:942:ASP:O	1:B:942:ASP:CG	2.32	0.66
1:C:905:CYS:HB3	1:C:931:CYS:SG	2.36	0.66
1:B:958:LEU:HD23	1:B:963:GLN:OE1	1.94	0.65
2:N:15:ALA:N	2:N:16:PRO:HD2	2.12	0.65
1:A:962:ASP:HB3	1:A:1021:PRO:HG3	1.76	0.65
1:G:1020:ILE:CG1	1:G:1021:PRO:HD2	2.25	0.65
1:D:932:ARG:NH2	1:D:941:TYR:CE2	2.64	0.65
1:B:932:ARG:CZ	1:B:941:TYR:CE2	2.75	0.65
1:C:930:PHE:CZ	1:C:971:LEU:HD12	2.31	0.65
1:B:915:VAL:HG22	1:B:1007:LYS:HE3	1.78	0.64
1:D:894:GLN:O	2:L:9:M3L:HM23	1.97	0.64
1:D:919:LEU:HD12	1:D:942:ASP:O	1.97	0.64
1:C:932:ARG:NH1	1:C:941:TYR:CE2	2.66	0.64
1:C:958:LEU:HB2	1:C:1017:HIS:CE1	2.33	0.64
1:D:1044:VAL:O	1:D:1047:VAL:HG12	1.98	0.64
1:G:930:PHE:CZ	1:G:971:LEU:HD13	2.32	0.64
1:G:991:PRO:O	1:G:992:ASN:HB2	1.96	0.64
1:D:932:ARG:HD3	1:D:941:TYR:CZ	2.33	0.64
1:D:943:CYS:SG	1:D:945:ASN:N	2.70	0.64
1:C:932:ARG:CZ	1:C:941:TYR:CE2	2.81	0.63
1:C:989:SER:O	1:C:991:PRO:CD	2.43	0.63
1:B:924:GLY:O	2:J:1:ALA:HB2	1.98	0.63
1:G:894:GLN:O	2:O:9:M3L:HM23	1.98	0.63
1:G:943:CYS:SG	1:G:945:ASN:CA	2.86	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:932:ARG:CZ	1:E:941:TYR:HE2	2.12	0.63
1:B:932:ARG:NH1	1:B:941:TYR:CD2	2.66	0.63
1:F:1020:ILE:HD13	1:F:1021:PRO:CD	2.29	0.62
1:E:943:CYS:SG	1:E:945:ASN:CB	2.87	0.62
1:H:1044:VAL:O	1:H:1047:VAL:HG12	1.99	0.62
2:O:16:PRO:O	2:O:17:ARG:HD2	1.98	0.62
1:F:1002:ASP:OD2	1:F:1002:ASP:C	2.37	0.62
1:G:1022:ASP:OD2	1:G:1084:ARG:NH2	2.33	0.62
1:D:930:PHE:CZ	1:D:971:LEU:HD12	2.35	0.62
1:H:1020:ILE:CD1	1:H:1021:PRO:HD2	2.29	0.62
2:I:10:SER:O	2:I:11:THR:CG2	2.45	0.62
1:B:1080:ILE:HG22	1:B:1081:TYR:CD2	2.35	0.62
1:F:943:CYS:SG	1:F:945:ASN:N	2.73	0.62
2:J:8:ARG:HH11	2:J:8:ARG:HG3	1.64	0.62
1:H:991:PRO:O	1:H:992:ASN:HB2	2.00	0.62
1:A:1048:TYR:O	1:A:1049:ALA:HB2	2.00	0.62
1:C:981:GLU:HG3	1:C:1062:VAL:HG22	1.81	0.62
1:B:1009:LYS:NZ	1:B:1027:ASP:OD2	2.33	0.61
2:M:16:PRO:O	2:M:17:ARG:CD	2.48	0.61
1:A:1020:ILE:HD12	1:A:1021:PRO:HD2	1.83	0.61
1:A:932:ARG:HD3	1:A:941:TYR:CZ	2.34	0.61
1:F:904:LYS:HG3	1:F:927:ILE:HG21	1.83	0.61
1:B:932:ARG:NE	1:B:941:TYR:HE2	1.98	0.61
1:E:941:TYR:O	1:E:943:CYS:N	2.31	0.61
1:E:989:SER:O	1:E:991:PRO:HD3	2.00	0.61
2:M:14:ALY:C	2:M:16:PRO:HD3	2.29	0.61
1:B:932:ARG:HH21	1:B:964:ARG:CD	2.09	0.61
1:B:980:ILE:N	1:B:980:ILE:HD13	2.16	0.61
1:D:990:ILE:N	1:D:990:ILE:CD1	2.55	0.61
1:H:932:ARG:CZ	1:H:941:TYR:CE2	2.84	0.61
1:D:989:SER:O	1:D:991:PRO:CD	2.48	0.60
1:F:937:PRO:HG3	1:F:964:ARG:CZ	2.31	0.60
2:P:16:PRO:O	2:P:17:ARG:CD	2.43	0.60
1:D:941:TYR:C	1:D:943:CYS:H	2.04	0.60
1:E:1040:GLU:OE2	1:E:1043:LYS:NZ	2.34	0.60
1:F:989:SER:O	1:F:991:PRO:CD	2.49	0.60
1:D:932:ARG:HD3	1:D:941:TYR:OH	2.01	0.60
1:G:1012:LYS:HG3	1:G:1017:HIS:NE2	2.16	0.60
1:F:905:CYS:HB3	1:F:931:CYS:SG	2.41	0.60
1:B:943:CYS:HB2	1:B:945:ASN:H	1.67	0.60
1:F:926:TRP:NE1	1:F:941:TYR:CE1	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1045:VAL:CG1	1:G:1048:TYR:HE1	2.14	0.60
1:G:942:ASP:CG	1:G:942:ASP:O	2.38	0.59
1:B:976:HIS:CE1	1:B:978:LEU:HB2	2.37	0.59
1:D:941:TYR:O	1:D:943:CYS:N	2.31	0.59
1:E:932:ARG:NE	1:E:941:TYR:HE2	2.00	0.59
1:H:919:LEU:HD12	1:H:942:ASP:OD1	2.01	0.59
1:E:990:ILE:HD13	1:E:990:ILE:N	2.16	0.59
1:A:941:TYR:O	1:A:943:CYS:N	2.31	0.59
1:F:1032:PHE:CZ	1:F:1069:VAL:HG12	2.38	0.59
1:C:932:ARG:NH2	1:C:964:ARG:HD3	2.17	0.59
1:E:1071:LEU:O	1:E:1074:GLU:HB2	2.03	0.59
1:D:1032:PHE:CZ	1:D:1069:VAL:HG12	2.38	0.59
1:C:1080:ILE:HG22	1:C:1081:TYR:CD2	2.37	0.59
1:F:930:PHE:CZ	1:F:971:LEU:HD13	2.38	0.59
1:G:1020:ILE:CD1	1:G:1021:PRO:HD2	2.33	0.58
1:H:942:ASP:O	1:H:942:ASP:CG	2.40	0.58
1:D:1020:ILE:HG22	1:D:1023:ASP:OD2	2.04	0.58
1:C:1020:ILE:CD1	1:C:1021:PRO:HD2	2.34	0.58
1:E:932:ARG:CD	1:E:941:TYR:CE2	2.86	0.58
1:A:932:ARG:CZ	1:A:941:TYR:CD2	2.86	0.58
1:C:1020:ILE:HG22	1:C:1023:ASP:OD2	2.03	0.58
1:F:962:ASP:HB3	1:F:1021:PRO:HG3	1.85	0.58
1:G:905:CYS:HB3	1:G:931:CYS:SG	2.43	0.58
1:B:1020:ILE:HD12	1:B:1022:ASP:OD1	2.04	0.58
1:C:946:LEU:O	1:C:949:SER:HB2	2.04	0.58
1:E:961:VAL:HG12	1:E:965:LYS:HE3	1.85	0.58
1:A:1037:ARG:HA	1:A:1037:ARG:HH11	1.69	0.58
1:H:989:SER:O	1:H:991:PRO:CD	2.48	0.58
1:A:916:PRO:HG3	1:A:967:GLU:OE2	2.04	0.57
1:D:930:PHE:CE2	1:D:971:LEU:HD12	2.39	0.57
1:E:981:GLU:HG3	1:E:1062:VAL:HG22	1.86	0.57
2:K:17:ARG:HG2	2:K:17:ARG:HH11	1.67	0.57
2:L:10:SER:O	2:L:11:THR:CG2	2.47	0.57
1:A:912:THR:HG22	1:A:917:THR:CG2	2.35	0.57
1:D:1002:ASP:HA	1:D:1031:ILE:HD13	1.86	0.57
1:F:927:ILE:HD11	1:F:932:ARG:HA	1.86	0.57
1:H:929:THR:O	1:H:968:ARG:NH1	2.36	0.57
1:G:932:ARG:CZ	1:G:941:TYR:CE2	2.88	0.57
1:D:915:VAL:HB	1:D:971:LEU:HD23	1.85	0.57
1:G:932:ARG:HD3	1:G:941:TYR:CE2	2.40	0.57
1:F:932:ARG:CZ	1:F:941:TYR:CE2	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:961:VAL:HG12	1:H:965:LYS:HE3	1.87	0.57
1:G:894:GLN:HG3	2:O:9:M3L:HM21	1.85	0.57
1:A:885:PRO:HG2	2:I:2:ARG:HH12	1.70	0.57
2:J:8:ARG:HH11	2:J:8:ARG:HG2	1.68	0.56
1:F:990:ILE:HD13	1:F:990:ILE:H	1.66	0.56
1:H:1002:ASP:HA	1:H:1031:ILE:HD13	1.87	0.56
1:A:930:PHE:CE2	1:A:971:LEU:HD13	2.40	0.56
1:H:904:LYS:HB2	1:H:927:ILE:CG2	2.35	0.56
2:I:17:ARG:NH1	2:I:17:ARG:HG3	2.02	0.56
1:A:1020:ILE:CD1	1:A:1021:PRO:HD2	2.36	0.56
1:G:932:ARG:HD3	1:G:941:TYR:CZ	2.40	0.56
1:F:1044:VAL:O	1:F:1047:VAL:HG12	2.06	0.56
1:B:915:VAL:HB	1:B:971:LEU:HD23	1.87	0.56
1:C:1020:ILE:HG13	1:C:1021:PRO:HD2	1.87	0.56
1:E:1020:ILE:HG13	1:E:1021:PRO:HD2	1.88	0.56
2:P:16:PRO:C	2:P:17:ARG:HD3	2.26	0.56
1:A:1048:TYR:O	1:A:1049:ALA:CB	2.54	0.56
1:D:941:TYR:C	1:D:943:CYS:N	2.59	0.56
1:E:962:ASP:HB3	1:E:1021:PRO:HG3	1.87	0.56
1:B:989:SER:O	1:B:991:PRO:CD	2.50	0.56
1:G:927:ILE:HD11	1:G:932:ARG:HA	1.88	0.56
1:B:937:PRO:HG3	1:B:964:ARG:CZ	2.36	0.55
1:C:1002:ASP:HA	1:C:1031:ILE:HD13	1.88	0.55
1:D:912:THR:HA	1:D:917:THR:HG23	1.87	0.55
1:E:915:VAL:HB	1:E:971:LEU:HD23	1.88	0.55
1:A:915:VAL:HG22	1:A:1007:LYS:HE3	1.87	0.55
1:A:1001:MET:HB3	1:A:1031:ILE:HG12	1.88	0.55
1:A:977:GLU:CD	1:A:977:GLU:H	2.10	0.55
1:E:941:TYR:C	1:E:943:CYS:H	2.09	0.55
1:G:930:PHE:CE2	1:G:971:LEU:HD13	2.42	0.55
1:H:924:GLY:O	2:P:1:ALA:HB2	2.06	0.55
1:A:981:GLU:HG3	1:A:1062:VAL:HG22	1.88	0.55
1:B:962:ASP:HB3	1:B:1021:PRO:HG3	1.88	0.55
1:F:926:TRP:NE1	1:F:941:TYR:HE1	2.05	0.54
1:G:980:ILE:N	1:G:980:ILE:HD13	2.18	0.54
1:H:1004:SER:O	1:H:1008:LYS:HG3	2.08	0.54
1:A:1044:VAL:O	1:A:1047:VAL:HG12	2.08	0.54
1:D:929:THR:O	1:D:968:ARG:NH1	2.40	0.54
1:A:1002:ASP:C	1:A:1002:ASP:OD2	2.46	0.54
1:B:1020:ILE:HD13	1:B:1021:PRO:HD2	1.89	0.54
1:C:912:THR:HA	1:C:917:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1048:TYR:O	1:F:1049:ALA:HB2	2.08	0.54
1:F:932:ARG:HD3	1:F:941:TYR:CE2	2.42	0.54
1:G:937:PRO:HG3	1:G:964:ARG:CZ	2.37	0.54
1:F:884:ASP:OD1	1:F:885:PRO:HD2	2.08	0.54
1:G:1001:MET:HB2	1:G:1030:LEU:HD23	1.90	0.54
1:G:981:GLU:HG3	1:G:1062:VAL:HG22	1.90	0.54
1:A:942:ASP:CG	1:A:942:ASP:O	2.46	0.54
1:B:1048:TYR:CE2	1:G:1045:VAL:HG13	2.43	0.54
1:D:926:TRP:NE1	1:D:941:TYR:HE1	2.06	0.54
1:G:1002:ASP:OD2	1:G:1002:ASP:C	2.46	0.53
1:H:915:VAL:HG22	1:H:1007:LYS:HE3	1.90	0.53
1:B:1012:LYS:HG2	1:B:1017:HIS:NE2	2.23	0.53
1:H:958:LEU:HB2	1:H:1017:HIS:NE2	2.23	0.53
1:E:900:LEU:HD22	1:E:901:CYS:O	2.08	0.53
1:E:1002:ASP:OD1	1:E:1002:ASP:N	2.41	0.53
2:I:14:ALY:CB	2:I:16:PRO:CD	2.86	0.53
1:D:1014:HIS:HB3	1:D:1017:HIS:HB2	1.91	0.53
1:D:937:PRO:HG3	1:D:964:ARG:NE	2.24	0.53
1:G:1027:ASP:O	1:G:1030:LEU:HB3	2.09	0.53
1:C:904:LYS:HB2	1:C:927:ILE:HG21	1.91	0.53
1:F:932:ARG:NH1	1:F:941:TYR:CE2	2.76	0.53
1:F:996:ILE:HD13	1:F:1041:MET:HB3	1.91	0.53
1:C:1014:HIS:HB3	1:C:1017:HIS:HB2	1.91	0.52
1:E:991:PRO:O	1:E:992:ASN:HB2	2.09	0.52
1:A:941:TYR:C	1:A:943:CYS:N	2.62	0.52
1:C:1020:ILE:HD12	1:C:1021:PRO:HD2	1.91	0.52
1:D:926:TRP:NE1	1:D:941:TYR:CE1	2.77	0.52
1:G:945:ASN:ND2	1:G:1012:LYS:HD3	2.24	0.52
1:B:1045:VAL:CG1	1:G:1048:TYR:CE1	2.91	0.52
1:E:932:ARG:NE	1:E:941:TYR:CE2	2.77	0.52
1:D:937:PRO:HG3	1:D:964:ARG:CZ	2.39	0.52
1:F:932:ARG:HD3	1:F:941:TYR:CZ	2.45	0.52
1:H:944:ASP:O	1:H:948:HIS:HB2	2.09	0.52
1:A:941:TYR:C	1:A:943:CYS:H	2.13	0.52
1:B:981:GLU:HG3	1:B:1062:VAL:HG22	1.92	0.52
1:A:911:LEU:HD11	1:A:921:PHE:CE2	2.45	0.51
2:M:14:ALY:O	2:M:16:PRO:HD2	2.10	0.51
1:B:1020:ILE:HD13	1:B:1021:PRO:CD	2.40	0.51
1:A:912:THR:HG22	1:A:917:THR:HG21	1.92	0.51
1:G:1003:LEU:O	1:G:1004:SER:C	2.47	0.51
1:E:941:TYR:C	1:E:943:CYS:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:976:HIS:CE1	1:F:978:LEU:HB2	2.45	0.51
1:H:1061:GLU:H	1:H:1061:GLU:CD	2.14	0.51
1:F:977:GLU:CD	1:F:977:GLU:H	2.07	0.51
1:E:894:GLN:HG3	2:M:9:M3L:HM22	1.93	0.51
1:B:937:PRO:HG3	1:B:964:ARG:NE	2.26	0.51
1:C:894:GLN:O	2:K:9:M3L:CM2	2.56	0.51
1:E:1009:LYS:HD2	1:E:1018:TYR:CE1	2.46	0.51
1:G:932:ARG:NH2	1:G:964:ARG:HD3	2.26	0.51
1:G:959:SER:HB3	1:G:962:ASP:HB2	1.93	0.51
1:A:943:CYS:SG	1:A:945:ASN:CB	2.98	0.51
1:G:1020:ILE:HD12	1:G:1021:PRO:HD2	1.93	0.51
1:G:990:ILE:N	1:G:990:ILE:HD13	2.26	0.51
1:B:1061:GLU:CD	1:B:1061:GLU:H	2.15	0.51
1:B:1044:VAL:O	1:B:1047:VAL:HG12	2.11	0.50
1:G:1010:LEU:HD21	1:G:1024:PHE:HE1	1.76	0.50
1:H:1013:LYS:O	1:H:1013:LYS:HG2	2.11	0.50
1:H:945:ASN:OD1	1:H:1012:LYS:HB2	2.11	0.50
1:A:942:ASP:OD1	1:A:942:ASP:O	2.29	0.50
1:F:1002:ASP:O	1:F:1002:ASP:OD2	2.29	0.50
1:H:981:GLU:HG3	1:H:1062:VAL:HG22	1.92	0.50
1:B:930:PHE:CZ	1:B:971:LEU:HD12	2.46	0.50
1:G:915:VAL:HG22	1:G:1007:LYS:HE3	1.92	0.50
1:F:942:ASP:OD1	1:F:942:ASP:O	2.29	0.50
1:G:993:TYR:HA	1:G:1038:PHE:CE1	2.46	0.50
1:A:930:PHE:CZ	1:A:971:LEU:HD13	2.46	0.50
1:B:1001:MET:HB2	1:B:1030:LEU:HD23	1.94	0.50
1:D:962:ASP:HB3	1:D:1021:PRO:HG3	1.94	0.50
1:E:894:GLN:HG3	2:M:9:M3L:HM23	1.93	0.50
1:F:1048:TYR:O	1:F:1049:ALA:CB	2.59	0.50
1:C:1074:GLU:O	1:C:1078:THR:HG23	2.12	0.50
1:D:958:LEU:HB2	1:D:1017:HIS:CE1	2.47	0.50
1:E:944:ASP:O	1:E:944:ASP:OD1	2.30	0.50
1:G:1012:LYS:HA	1:G:1017:HIS:CD2	2.47	0.50
1:C:1012:LYS:HA	1:C:1017:HIS:CD2	2.47	0.50
1:F:1027:ASP:O	1:F:1030:LEU:HB3	2.12	0.49
1:G:981:GLU:HG2	2:O:17:ARG:HD2	1.93	0.49
1:A:944:ASP:N	1:A:944:ASP:OD1	2.31	0.49
1:C:930:PHE:CE2	1:C:971:LEU:HD12	2.47	0.49
1:D:932:ARG:NE	1:D:941:TYR:HE2	2.08	0.49
1:E:912:THR:HG22	1:E:917:THR:CG2	2.41	0.49
1:C:1013:LYS:HG2	1:C:1013:LYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:942:ASP:O	1:G:942:ASP:OD2	2.30	0.49
1:B:932:ARG:HH22	1:B:964:ARG:HG2	1.72	0.49
1:C:977:GLU:N	1:C:977:GLU:OE2	2.45	0.49
1:F:930:PHE:CE2	1:F:971:LEU:HD13	2.48	0.49
1:C:1020:ILE:CG1	1:C:1021:PRO:HD2	2.42	0.49
2:K:17:ARG:HG2	2:K:17:ARG:NH1	2.27	0.49
1:E:915:VAL:HG22	1:E:1007:LYS:HE3	1.94	0.49
1:F:1020:ILE:CD1	1:F:1021:PRO:HD2	2.41	0.49
1:A:1022:ASP:OD2	1:A:1084:ARG:NH2	2.46	0.49
1:E:905:CYS:HB2	1:E:906:PRO:HD2	1.94	0.49
1:F:1061:GLU:CD	1:F:1061:GLU:H	2.15	0.49
1:G:1002:ASP:O	1:G:1002:ASP:OD2	2.30	0.49
1:C:1037:ARG:NH2	1:H:996:ILE:O	2.45	0.49
1:G:943:CYS:SG	1:G:944:ASP:N	2.86	0.49
1:C:942:ASP:O	1:C:942:ASP:OD1	2.31	0.49
1:E:932:ARG:HD3	1:E:941:TYR:CZ	2.47	0.49
1:H:970:LEU:HD22	1:H:1010:LEU:HD23	1.94	0.49
1:A:1002:ASP:OD2	1:A:1002:ASP:O	2.31	0.48
1:D:1019:GLN:OE1	1:D:1019:GLN:HA	2.13	0.48
1:D:932:ARG:HD3	1:D:941:TYR:CE2	2.47	0.48
1:H:1001:MET:HB2	1:H:1030:LEU:HD23	1.95	0.48
1:F:1009:LYS:HE2	1:F:1016:GLN:HB3	1.96	0.48
1:H:1080:ILE:O	1:H:1080:ILE:HG22	2.12	0.48
1:B:932:ARG:HH21	1:B:964:ARG:CG	2.25	0.48
1:E:977:GLU:N	1:E:977:GLU:CD	2.63	0.48
1:F:941:TYR:O	1:F:942:ASP:C	2.51	0.48
1:D:981:GLU:HG2	2:L:17:ARG:HD2	1.95	0.48
1:G:889:TRP:CE2	2:O:9:M3L:HM32	2.48	0.48
1:H:932:ARG:HD3	1:H:941:TYR:CE2	2.47	0.48
1:F:894:GLN:O	2:N:9:M3L:HM23	2.13	0.48
1:C:915:VAL:HG23	1:C:971:LEU:HD23	1.95	0.48
1:G:932:ARG:NH1	1:G:941:TYR:CE2	2.81	0.48
1:C:897:GLY:HA3	1:C:910:HIS:HE2	1.79	0.48
1:G:976:HIS:CE1	1:G:978:LEU:HB2	2.48	0.48
2:M:11:THR:HG22	2:M:12:GLY:H	1.78	0.48
1:A:900:LEU:HD22	1:A:901:CYS:O	2.13	0.48
1:A:950:LYS:HA	1:A:950:LYS:HD3	1.60	0.48
1:G:930:PHE:HA	1:G:968:ARG:HD2	1.95	0.48
1:D:959:SER:HB3	1:D:962:ASP:HB2	1.95	0.48
1:G:983:GLN:HG2	1:G:1003:LEU:HD12	1.96	0.48
1:G:932:ARG:CZ	1:G:941:TYR:CD2	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1061:GLU:CD	1:H:1061:GLU:N	2.67	0.48
1:D:981:GLU:HG3	1:D:1062:VAL:HG22	1.96	0.48
1:C:961:VAL:HG22	1:C:965:LYS:HE3	1.96	0.48
1:H:993:TYR:HA	1:H:1038:PHE:CE1	2.49	0.48
2:P:18:ALY:HE3	2:P:18:ALY:HH31	1.51	0.47
1:D:1071:LEU:HD13	1:D:1071:LEU:HA	1.69	0.47
1:B:1020:ILE:CD1	1:B:1021:PRO:HD2	2.44	0.47
2:J:2:ARG:NH1	2:J:2:ARG:HB3	2.29	0.47
2:O:16:PRO:O	2:O:17:ARG:CD	2.61	0.47
1:A:1033:LYS:HB2	1:A:1033:LYS:HE2	1.54	0.47
1:G:1083:ASP:OD2	1:G:1083:ASP:N	2.47	0.47
1:C:900:LEU:HD22	1:C:926:TRP:CE3	2.48	0.47
1:C:930:PHE:CZ	1:C:971:LEU:CD1	2.97	0.47
1:E:942:ASP:CG	1:E:942:ASP:O	2.50	0.47
1:F:983:GLN:HG2	1:F:1003:LEU:HD12	1.97	0.47
1:G:1086:PHE:CD1	1:G:1086:PHE:N	2.82	0.47
1:B:942:ASP:OD1	1:B:942:ASP:O	2.32	0.47
1:E:901:CYS:HA	1:E:908:VAL:HG12	1.96	0.47
1:G:1010:LEU:HD21	1:G:1024:PHE:CE1	2.50	0.47
1:G:912:THR:HA	1:G:917:THR:CG2	2.40	0.47
1:F:980:ILE:HG12	1:F:980:ILE:H	1.46	0.47
1:A:1048:TYR:CD2	1:A:1048:TYR:N	2.83	0.47
1:E:980:ILE:HG12	1:E:980:ILE:H	1.47	0.47
2:P:11:THR:HG22	2:P:12:GLY:H	1.80	0.47
1:C:1021:PRO:HB2	1:C:1086:PHE:HE2	1.80	0.47
1:F:900:LEU:HD22	1:F:926:TRP:CE3	2.50	0.47
1:F:981:GLU:OE2	2:N:17:ARG:CD	2.52	0.47
2:K:15:ALA:N	2:K:16:PRO:HD2	2.27	0.47
1:E:926:TRP:CE2	1:E:941:TYR:HE1	2.31	0.46
1:F:1001:MET:HB3	1:F:1031:ILE:HG12	1.96	0.46
1:H:1048:TYR:N	1:H:1048:TYR:CD2	2.83	0.46
2:O:11:THR:O	2:O:12:GLY:C	2.51	0.46
1:C:932:ARG:CZ	1:C:941:TYR:HE2	2.28	0.46
1:D:900:LEU:HD22	1:D:901:CYS:O	2.15	0.46
1:B:930:PHE:CE2	1:B:971:LEU:HD12	2.51	0.46
1:B:965:LYS:HD3	1:B:1080:ILE:HG23	1.97	0.46
1:C:932:ARG:HD3	1:C:941:TYR:CE2	2.50	0.46
1:D:1027:ASP:O	1:D:1030:LEU:HB3	2.15	0.46
1:H:1002:ASP:CA	1:H:1031:ILE:HD13	2.45	0.46
1:H:901:CYS:HA	1:H:908:VAL:HG12	1.96	0.46
1:C:904:LYS:HB2	1:C:927:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:944:ASP:O	1:C:944:ASP:OD1	2.33	0.46
1:H:943:CYS:SG	1:H:945:ASN:HB2	2.56	0.46
1:D:971:LEU:HD13	1:D:975:CYS:SG	2.55	0.46
1:E:958:LEU:HD12	1:E:963:GLN:OE1	2.15	0.46
1:H:1012:LYS:HD3	1:H:1017:HIS:CE1	2.50	0.46
1:B:905:CYS:HB3	1:B:931:CYS:SG	2.55	0.46
1:D:958:LEU:HB2	1:D:1017:HIS:NE2	2.30	0.46
1:D:1020:ILE:HD12	1:D:1021:PRO:HD2	1.96	0.46
1:H:942:ASP:OD1	1:H:942:ASP:O	2.32	0.46
1:C:1027:ASP:O	1:C:1030:LEU:HB3	2.16	0.46
1:H:912:THR:HA	1:H:917:THR:CG2	2.41	0.46
1:A:958:LEU:HD12	1:A:963:GLN:OE1	2.16	0.46
1:B:927:ILE:HD11	1:B:932:ARG:HA	1.97	0.46
1:C:1045:VAL:CG1	1:H:1048:TYR:CE1	2.98	0.46
1:C:980:ILE:HG12	1:C:980:ILE:H	1.43	0.46
1:D:1061:GLU:CD	1:D:1061:GLU:N	2.68	0.46
1:B:980:ILE:CD1	1:B:980:ILE:H	2.18	0.46
1:G:1020:ILE:HG13	1:G:1021:PRO:CD	2.44	0.46
1:H:1010:LEU:HD21	1:H:1024:PHE:CE1	2.51	0.46
1:B:884:ASP:OD1	1:B:885:PRO:HD2	2.16	0.46
1:E:930:PHE:CZ	1:E:971:LEU:HD12	2.51	0.46
1:F:1080:ILE:O	1:F:1080:ILE:HG22	2.15	0.46
1:H:884:ASP:OD2	1:H:885:PRO:HD2	2.16	0.46
1:B:1061:GLU:N	1:B:1061:GLU:OE2	2.34	0.45
1:B:981:GLU:HG2	2:J:16:PRO:O	2.16	0.45
1:G:941:TYR:O	1:G:943:CYS:N	2.40	0.45
1:A:1083:ASP:N	1:A:1083:ASP:OD2	2.49	0.45
1:C:983:GLN:O	1:C:1004:SER:HB3	2.16	0.45
1:E:959:SER:O	1:E:963:GLN:HB2	2.17	0.45
2:I:9:M3L:HD2	2:I:9:M3L:HM22	1.62	0.45
1:A:1061:GLU:CD	1:A:1061:GLU:H	2.18	0.45
1:A:961:VAL:HG12	1:A:965:LYS:HE3	1.98	0.45
1:B:996:ILE:HD13	1:B:1041:MET:HB3	1.97	0.45
1:A:932:ARG:NE	1:A:941:TYR:CE2	2.71	0.45
1:C:916:PRO:HD3	1:C:967:GLU:OE1	2.17	0.45
1:C:977:GLU:N	1:C:977:GLU:CD	2.60	0.45
1:D:1001:MET:HB3	1:D:1031:ILE:HG12	1.99	0.45
1:G:1025:VAL:O	1:G:1029:ARG:HG3	2.17	0.45
1:A:991:PRO:O	1:A:992:ASN:HB2	2.15	0.45
1:B:996:ILE:HG22	1:B:997:ILE:HD13	1.99	0.45
1:G:884:ASP:OD1	1:G:885:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:LEU:O	1:A:949:SER:HB2	2.17	0.45
1:B:963:GLN:HG3	1:B:967:GLU:OE1	2.16	0.45
1:C:983:GLN:HG2	1:C:1003:LEU:HD12	1.99	0.45
1:D:980:ILE:H	1:D:980:ILE:HG12	1.39	0.45
1:H:904:LYS:HB2	1:H:927:ILE:HG22	1.97	0.45
1:H:932:ARG:NH2	1:H:964:ARG:HD3	2.32	0.45
1:D:932:ARG:NE	1:D:941:TYR:CE2	2.84	0.45
1:E:950:LYS:HD3	1:E:950:LYS:HA	1.74	0.45
1:H:932:ARG:NH1	1:H:941:TYR:HD2	2.08	0.45
1:F:915:VAL:CG2	1:F:1007:LYS:HE3	2.34	0.45
1:H:905:CYS:HB2	1:H:906:PRO:CD	2.47	0.45
2:L:9:M3L:HM32	2:L:9:M3L:HD3	1.73	0.45
1:B:932:ARG:HH21	1:B:964:ARG:HD2	1.80	0.44
1:B:932:ARG:HH21	1:B:964:ARG:HG2	1.82	0.44
1:H:904:LYS:HB2	1:H:927:ILE:HG21	1.99	0.44
1:D:932:ARG:CZ	1:D:941:TYR:CD2	2.97	0.44
1:A:922:PRO:HG2	1:A:926:TRP:CD1	2.53	0.44
1:B:1008:LYS:O	1:B:1011:GLN:HB2	2.18	0.44
1:E:1044:VAL:O	1:E:1047:VAL:HG12	2.17	0.44
1:A:932:ARG:NH1	1:A:941:TYR:CD2	2.86	0.44
1:E:930:PHE:CE2	1:E:971:LEU:HD12	2.52	0.44
1:C:1071:LEU:HA	1:C:1071:LEU:HD13	1.89	0.44
1:D:959:SER:OG	1:D:960:PRO:HD2	2.17	0.44
1:G:903:GLU:OE2	1:G:925:ASP:HB3	2.17	0.44
2:L:15:ALA:CB	2:L:16:PRO:CD	2.44	0.44
2:L:18:ALY:HH31	2:L:18:ALY:HE3	1.75	0.44
1:D:989:SER:O	1:D:990:ILE:C	2.56	0.44
1:F:1010:LEU:HD12	1:F:1010:LEU:HA	1.75	0.44
1:G:928:CYS:C	1:G:941:TYR:OH	2.56	0.44
1:H:1022:ASP:OD2	1:H:1084:ARG:NH2	2.50	0.44
1:A:1027:ASP:O	1:A:1030:LEU:HB3	2.18	0.44
1:B:943:CYS:HB2	1:B:945:ASN:N	2.32	0.44
1:C:1040:GLU:OE2	1:C:1043:LYS:NZ	2.51	0.44
1:G:958:LEU:HD23	1:G:1018:TYR:O	2.17	0.44
1:D:1020:ILE:CD1	1:D:1021:PRO:HD2	2.47	0.44
1:F:958:LEU:HB2	1:F:1017:HIS:CE1	2.52	0.44
1:G:894:GLN:O	2:O:9:M3L:CM2	2.64	0.44
2:J:9:M3L:HD3	2:J:9:M3L:HM23	1.55	0.44
2:O:9:M3L:HM23	2:O:9:M3L:HD3	1.72	0.44
1:B:946:LEU:O	1:B:949:SER:HB2	2.18	0.44
1:F:937:PRO:HG3	1:F:964:ARG:NE	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:977:GLU:CD	1:G:977:GLU:N	2.65	0.44
1:H:996:ILE:HD13	1:H:1041:MET:HB3	2.00	0.44
1:A:1027:ASP:O	1:A:1030:LEU:N	2.50	0.43
1:C:1078:THR:OG1	1:C:1079:GLU:N	2.51	0.43
1:F:1061:GLU:CD	1:F:1061:GLU:N	2.72	0.43
1:F:1083:ASP:OD2	1:F:1083:ASP:N	2.52	0.43
1:D:958:LEU:HD12	1:D:963:GLN:OE1	2.18	0.43
1:G:980:ILE:CD1	1:G:980:ILE:H	2.16	0.43
1:E:996:ILE:HD13	1:E:1041:MET:HG2	2.01	0.43
1:E:996:ILE:HD13	1:E:1041:MET:HB3	1.99	0.43
1:G:1076:LYS:HD3	1:G:1076:LYS:HA	1.61	0.43
1:H:962:ASP:HB3	1:H:1021:PRO:HG3	2.00	0.43
1:E:1020:ILE:CG1	1:E:1021:PRO:HD2	2.48	0.43
1:H:932:ARG:NE	1:H:941:TYR:HE2	2.15	0.43
1:H:927:ILE:HD11	1:H:932:ARG:HA	2.01	0.43
2:N:9:M3L:HM32	2:N:9:M3L:HD3	1.84	0.43
1:A:932:ARG:HD3	1:A:941:TYR:OH	2.19	0.43
1:B:916:PRO:HD3	1:B:967:GLU:OE2	2.18	0.43
1:A:981:GLU:HG2	2:I:17:ARG:HD2	2.01	0.43
1:E:993:TYR:HA	1:E:1038:PHE:CE1	2.53	0.43
1:B:996:ILE:HD13	1:B:1041:MET:CG	2.49	0.43
1:C:1076:LYS:HD3	1:C:1076:LYS:HA	1.77	0.43
1:F:889:TRP:CD2	2:N:9:M3L:HM32	2.54	0.43
1:G:941:TYR:C	1:G:943:CYS:N	2.72	0.43
1:A:1012:LYS:HG2	1:A:1017:HIS:NE2	2.34	0.42
1:A:1020:ILE:O	1:A:1023:ASP:HB2	2.19	0.42
2:M:9:M3L:HM32	2:M:9:M3L:HD3	1.69	0.42
1:B:945:ASN:OD1	1:B:1012:LYS:HB2	2.18	0.42
1:C:993:TYR:HA	1:C:1038:PHE:CE1	2.54	0.42
1:H:927:ILE:CD1	1:H:932:ARG:HA	2.49	0.42
1:C:996:ILE:HD13	1:C:1041:MET:HB3	2.02	0.42
1:D:1022:ASP:OD2	1:D:1084:ARG:NH2	2.47	0.42
1:D:932:ARG:CD	1:D:941:TYR:CE2	3.02	0.42
1:A:905:CYS:HB2	1:A:906:PRO:CD	2.50	0.42
1:B:990:ILE:N	1:B:990:ILE:CD1	2.83	0.42
1:E:1001:MET:HB3	1:E:1031:ILE:HG12	2.00	0.42
1:A:998:LYS:C	1:A:1000:PRO:HD3	2.39	0.42
1:A:901:CYS:HA	1:A:908:VAL:HG12	2.01	0.42
1:B:889:TRP:CD2	2:J:9:M3L:HM22	2.55	0.42
1:G:974:TYR:OH	1:G:1004:SER:HA	2.20	0.42
1:E:1086:PHE:O	1:E:1087:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1074:GLU:O	1:F:1078:THR:HG23	2.19	0.42
1:F:898:ASP:OD2	2:N:5:GLN:NE2	2.52	0.42
1:G:989:SER:O	1:G:991:PRO:CD	2.65	0.42
1:G:983:GLN:O	1:G:1004:SER:HB3	2.19	0.42
2:P:9:M3L:HM22	2:P:9:M3L:HD2	1.74	0.42
1:B:937:PRO:CG	1:B:964:ARG:CZ	2.97	0.42
1:E:895:ASN:OD1	1:E:896:GLY:N	2.47	0.42
1:F:897:GLY:HA3	1:F:910:HIS:HE2	1.85	0.42
1:A:983:GLN:O	1:A:1004:SER:HB3	2.20	0.42
1:A:976:HIS:CE1	1:A:978:LEU:HB2	2.55	0.42
1:F:927:ILE:CD1	1:F:932:ARG:HA	2.49	0.42
1:H:895:ASN:OD1	1:H:896:GLY:N	2.50	0.42
2:L:15:ALA:HB1	2:L:16:PRO:HD3	1.83	0.42
1:E:932:ARG:NH1	1:E:941:TYR:HD2	2.13	0.41
1:H:934:ILE:HD13	1:H:965:LYS:HG2	2.01	0.41
1:C:1048:TYR:CD2	1:C:1048:TYR:N	2.88	0.41
1:C:912:THR:HA	1:C:917:THR:CG2	2.50	0.41
1:E:911:LEU:HB3	1:E:918:LEU:O	2.19	0.41
1:E:992:ASN:O	1:E:996:ILE:HG13	2.19	0.41
1:F:981:GLU:HG3	1:F:1062:VAL:HG22	2.02	0.41
1:G:895:ASN:OD1	1:G:896:GLY:N	2.49	0.41
1:H:945:ASN:OD1	1:H:1012:LYS:N	2.45	0.41
1:B:921:PHE:HA	1:B:922:PRO:HD3	1.94	0.41
1:E:932:ARG:CZ	1:E:941:TYR:HD2	2.33	0.41
1:E:986:VAL:HG11	1:E:993:TYR:CD1	2.56	0.41
1:A:1032:PHE:CZ	1:A:1069:VAL:HG12	2.54	0.41
1:D:998:LYS:HA	1:D:998:LYS:HD3	1.85	0.41
1:H:1033:LYS:HB2	1:H:1033:LYS:HE2	1.66	0.41
2:I:17:ARG:HA	2:I:17:ARG:HD2	1.67	0.41
2:J:16:PRO:C	2:J:17:ARG:HD2	2.34	0.41
1:C:932:ARG:HD3	1:C:941:TYR:CZ	2.55	0.41
1:C:950:LYS:HD2	1:C:950:LYS:HA	1.93	0.41
1:F:1037:ARG:HA	1:F:1037:ARG:HH11	1.85	0.41
1:G:932:ARG:HH21	1:G:964:ARG:CD	2.33	0.41
1:H:1047:VAL:C	1:H:1048:TYR:HD2	2.24	0.41
1:H:1047:VAL:HG13	1:H:1048:TYR:CD2	2.55	0.41
1:C:932:ARG:NH1	1:C:941:TYR:HD2	2.12	0.41
1:C:989:SER:O	1:C:990:ILE:C	2.56	0.41
1:D:918:LEU:HD12	1:D:918:LEU:HA	1.93	0.41
1:D:976:HIS:CE1	1:D:978:LEU:HB2	2.56	0.41
1:E:1032:PHE:CZ	1:E:1069:VAL:HG12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:VAL:HG13	1:A:1048:TYR:CD2	2.56	0.41
1:B:990:ILE:HA	1:B:991:PRO:HD2	1.93	0.41
1:F:1001:MET:HG2	1:F:1030:LEU:HD23	2.02	0.41
1:H:1009:LYS:NZ	1:H:1027:ASP:OD2	2.52	0.41
1:H:990:ILE:HA	1:H:991:PRO:HD2	1.92	0.41
1:A:1048:TYR:HD2	1:A:1048:TYR:N	2.19	0.41
1:C:1001:MET:HB2	1:C:1030:LEU:HD23	2.02	0.41
1:D:930:PHE:CZ	1:D:971:LEU:CD1	3.03	0.41
1:A:1020:ILE:CG1	1:A:1021:PRO:HD2	2.50	0.41
1:A:930:PHE:HA	1:A:968:ARG:HD2	2.02	0.41
1:B:903:GLU:CD	1:B:926:TRP:H	2.24	0.41
1:D:983:GLN:HG2	1:D:1003:LEU:HD12	2.03	0.41
1:B:1033:LYS:HE2	1:B:1033:LYS:HB2	1.73	0.40
2:M:16:PRO:O	2:M:17:ARG:HD2	2.20	0.40
1:C:941:TYR:O	1:C:943:CYS:N	2.53	0.40
1:D:979:SER:O	1:D:983:GLN:HG3	2.21	0.40
1:G:969:LEU:HD23	1:G:969:LEU:HA	1.92	0.40
1:A:1010:LEU:HD12	1:A:1010:LEU:HA	1.89	0.40
1:B:900:LEU:HD13	1:B:926:TRP:CZ3	2.56	0.40
1:C:1012:LYS:HG3	1:C:1017:HIS:NE2	2.36	0.40
1:D:897:GLY:O	2:L:5:GLN:HA	2.22	0.40
1:H:922:PRO:HG3	1:H:926:TRP:CD1	2.57	0.40
2:J:18:ALY:HH31	2:J:18:ALY:HE3	1.72	0.40
1:C:889:TRP:CE2	2:K:9:M3L:HM32	2.56	0.40
1:E:927:ILE:HD11	1:E:932:ARG:HA	2.03	0.40
1:B:1032:PHE:CZ	1:B:1069:VAL:HG12	2.56	0.40
1:B:895:ASN:OD1	1:B:896:GLY:N	2.52	0.40
1:B:973:LEU:HD23	1:B:973:LEU:N	2.35	0.40
1:C:959:SER:HB3	1:C:962:ASP:HB2	2.03	0.40
1:D:996:ILE:HD13	1:D:1041:MET:CB	2.52	0.40
1:E:989:SER:O	1:E:990:ILE:C	2.60	0.40
1:F:1027:ASP:O	1:F:1030:LEU:N	2.52	0.40
1:G:985:PRO:HA	1:G:1002:ASP:OD1	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/207 (88%)	170 (93%)	12 (7%)	0	100	100
1	B	182/207 (88%)	174 (96%)	8 (4%)	0	100	100
1	C	182/207 (88%)	177 (97%)	5 (3%)	0	100	100
1	D	182/207 (88%)	174 (96%)	8 (4%)	0	100	100
1	E	182/207 (88%)	175 (96%)	7 (4%)	0	100	100
1	F	182/207 (88%)	177 (97%)	5 (3%)	0	100	100
1	G	182/207 (88%)	171 (94%)	11 (6%)	0	100	100
1	H	182/207 (88%)	170 (93%)	12 (7%)	0	100	100
2	I	14/28 (50%)	14 (100%)	0	0	100	100
2	J	11/28 (39%)	10 (91%)	1 (9%)	0	100	100
2	K	11/28 (39%)	10 (91%)	1 (9%)	0	100	100
2	L	14/28 (50%)	13 (93%)	0	1 (7%)	1	2
2	M	14/28 (50%)	13 (93%)	1 (7%)	0	100	100
2	N	11/28 (39%)	10 (91%)	1 (9%)	0	100	100
2	O	14/28 (50%)	13 (93%)	0	1 (7%)	1	2
2	P	11/28 (39%)	11 (100%)	0	0	100	100
All	All	1556/1880 (83%)	1482 (95%)	72 (5%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	15	ALA
2	L	15	ALA

### 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	173/189 (92%)	151 (87%)	22 (13%)	4	14
1	B	173/189 (92%)	154 (89%)	19 (11%)	6	19
1	C	173/189 (92%)	150 (87%)	23 (13%)	4	12
1	D	173/189 (92%)	151 (87%)	22 (13%)	4	14
1	E	173/189 (92%)	153 (88%)	20 (12%)	5	17
1	F	173/189 (92%)	152 (88%)	21 (12%)	5	15
1	G	173/189 (92%)	152 (88%)	21 (12%)	5	15
1	H	173/189 (92%)	154 (89%)	19 (11%)	6	19
2	I	10/16 (62%)	9 (90%)	1 (10%)	7	22
2	J	10/16 (62%)	8 (80%)	2 (20%)	1	4
2	K	10/16 (62%)	8 (80%)	2 (20%)	1	4
2	L	10/16 (62%)	9 (90%)	1 (10%)	7	22
2	M	11/16 (69%)	10 (91%)	1 (9%)	9	27
2	N	10/16 (62%)	9 (90%)	1 (10%)	7	22
2	O	10/16 (62%)	8 (80%)	2 (20%)	1	4
2	P	10/16 (62%)	10 (100%)	0	100	100
All	All	1465/1640 (89%)	1288 (88%)	177 (12%)	5	15

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	895	ASN
1	A	900	LEU
1	A	904	LYS
1	A	918	LEU
1	A	923	SER
1	A	940	GLU
1	A	942	ASP
1	A	944	ASP

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Mol	Chain	Res	Type
1	A	949	SER
1	A	950	LYS
1	A	968	ARG
1	A	971	LEU
1	A	978	LEU
1	A	980	ILE
1	A	989	SER
1	A	1001	MET
1	A	1010	LEU
1	A	1016	GLN
1	A	1033	LYS
1	A	1037	ARG
1	A	1048	TYR
1	A	1071	LEU
2	I	17	ARG
1	B	898	ASP
1	B	900	LEU
1	B	918	LEU
1	B	919	LEU
1	B	923	SER
1	B	943	CYS
1	B	944	ASP
1	B	949	SER
1	B	968	ARG
1	B	971	LEU
1	B	978	LEU
1	B	980	ILE
1	B	989	SER
1	B	990	ILE
1	B	1010	LEU
1	B	1016	GLN
1	B	1020	ILE
1	B	1033	LYS
1	B	1061	GLU
2	J	8	ARG
2	J	17	ARG
1	C	900	LEU
1	C	905	CYS
1	C	917	THR
1	C	918	LEU
1	C	940	GLU
1	C	942	ASP

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Mol	Chain	Res	Type
1	C	943	CYS
1	C	944	ASP
1	C	949	SER
1	C	968	ARG
1	C	971	LEU
1	C	974	TYR
1	C	977	GLU
1	C	978	LEU
1	C	980	ILE
1	C	989	SER
1	C	1010	LEU
1	C	1016	GLN
1	C	1027	ASP
1	C	1033	LYS
1	C	1071	LEU
1	C	1077	LEU
1	C	1082	SER
2	K	11	THR
2	K	17	ARG
1	D	895	ASN
1	D	900	LEU
1	D	918	LEU
1	D	919	LEU
1	D	920	SER
1	D	940	GLU
1	D	943	CYS
1	D	944	ASP
1	D	949	SER
1	D	961	VAL
1	D	968	ARG
1	D	971	LEU
1	D	978	LEU
1	D	980	ILE
1	D	989	SER
1	D	990	ILE
1	D	999	LYS
1	D	1001	MET
1	D	1010	LEU
1	D	1016	GLN
1	D	1061	GLU
1	D	1071	LEU
2	L	17	ARG

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Mol	Chain	Res	Type
1	E	900	LEU
1	E	918	LEU
1	E	940	GLU
1	E	943	CYS
1	E	944	ASP
1	E	948	HIS
1	E	950	LYS
1	E	968	ARG
1	E	971	LEU
1	E	977	GLU
1	E	978	LEU
1	E	980	ILE
1	E	989	SER
1	E	1001	MET
1	E	1010	LEU
1	E	1016	GLN
1	E	1037	ARG
1	E	1067	LYS
1	E	1071	LEU
1	E	1074	GLU
2	M	17	ARG
1	F	900	LEU
1	F	905	CYS
1	F	918	LEU
1	F	940	GLU
1	F	942	ASP
1	F	943	CYS
1	F	968	ARG
1	F	971	LEU
1	F	977	GLU
1	F	978	LEU
1	F	980	ILE
1	F	989	SER
1	F	1001	MET
1	F	1009	LYS
1	F	1010	LEU
1	F	1016	GLN
1	F	1020	ILE
1	F	1027	ASP
1	F	1037	ARG
1	F	1061	GLU
1	F	1071	LEU

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Mol	Chain	Res	Type
2	N	17	ARG
1	G	900	LEU
1	G	904	LYS
1	G	912	THR
1	G	918	LEU
1	G	938	GLU
1	G	942	ASP
1	G	943	CYS
1	G	944	ASP
1	G	968	ARG
1	G	971	LEU
1	G	977	GLU
1	G	978	LEU
1	G	980	ILE
1	G	999	LYS
1	G	1010	LEU
1	G	1013	LYS
1	G	1016	GLN
1	G	1033	LYS
1	G	1037	ARG
1	G	1071	LEU
1	G	1072	TYR
2	O	11	THR
2	O	17	ARG
1	H	900	LEU
1	H	918	LEU
1	H	942	ASP
1	H	944	ASP
1	H	968	ARG
1	H	971	LEU
1	H	978	LEU
1	H	980	ILE
1	H	989	SER
1	H	990	ILE
1	H	999	LYS
1	H	1010	LEU
1	H	1012	LYS
1	H	1016	GLN
1	H	1027	ASP
1	H	1036	GLU
1	H	1061	GLU
1	H	1071	LEU

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Mol	Chain	Res	Type
1	H	1072	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	5	GLN
1	C	1017	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

20 non-standard protein/DNA/RNA residues 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	M3L	M	9	2	10,11,12	0.75	0	9,14,16	0.86	0
2	ALY	L	14	2	3,4,12	0.60	0	2,4,14	0.88	0
2	M3L	N	9	2	10,11,12	0.79	0	9,14,16	0.57	0
2	ALY	L	18	2	10,11,12	0.64	0	7,12,14	1.15	1 (14%)
2	ALY	O	18	2	10,11,12	0.63	0	7,12,14	0.98	0
2	ALY	N	18	2	10,11,12	0.55	0	7,12,14	1.35	2 (28%)
2	ALY	I	18	2	10,11,12	0.47	0	7,12,14	0.91	0
2	ALY	K	18	2	10,11,12	0.47	0	7,12,14	1.55	3 (42%)
2	ALY	J	18	2	10,11,12	0.49	0	7,12,14	0.75	0
2	M3L	P	9	2	10,11,12	0.76	0	9,14,16	1.01	0
2	M3L	I	9	2	10,11,12	0.70	0	9,14,16	1.22	1 (11%)
2	M3L	K	9	2	10,11,12	0.77	0	9,14,16	0.70	0
2	ALY	M	14	2	3,4,12	0.61	0	2,4,14	0.69	0
2	ALY	P	18	2	10,11,12	0.68	0	7,12,14	1.29	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ALY	O	14	2	3,4,12	0.67	0	2,4,14	0.85	0
2	M3L	O	9	2	10,11,12	0.92	0	9,14,16	1.04	1 (11%)
2	ALY	M	18	2	10,11,12	0.56	0	7,12,14	1.03	1 (14%)
2	M3L	L	9	2	10,11,12	0.65	0	9,14,16	0.74	0
2	ALY	I	14	2	3,4,12	0.66	0	2,4,14	0.70	0
2	M3L	J	9	2	10,11,12	0.78	0	9,14,16	0.80	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	M3L	M	9	2	-	4/9/10/12	-
2	ALY	L	14	2	-	0/0/2/12	-
2	M3L	N	9	2	-	1/9/10/12	-
2	ALY	L	18	2	-	4/9/10/12	-
2	ALY	O	18	2	-	4/9/10/12	-
2	ALY	N	18	2	-	4/9/10/12	-
2	ALY	I	18	2	-	5/9/10/12	-
2	ALY	K	18	2	-	5/9/10/12	-
2	ALY	J	18	2	-	4/9/10/12	-
2	M3L	P	9	2	-	5/9/10/12	-
2	M3L	I	9	2	-	4/9/10/12	-
2	M3L	K	9	2	-	1/9/10/12	-
2	ALY	M	14	2	-	0/0/2/12	-
2	ALY	P	18	2	-	7/9/10/12	-
2	ALY	O	14	2	-	0/0/2/12	-
2	M3L	O	9	2	-	4/9/10/12	-
2	ALY	M	18	2	-	5/9/10/12	-
2	M3L	L	9	2	-	2/9/10/12	-
2	ALY	I	14	2	-	0/0/2/12	-
2	M3L	J	9	2	-	7/9/10/12	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	18	ALY	CH3-CH-NZ	2.50	120.51	116.09
2	P	18	ALY	CE-NZ-CH	-2.49	118.72	122.56
2	K	18	ALY	OH-CH-CH3	-2.29	117.81	122.06
2	M	18	ALY	CE-NZ-CH	2.28	126.06	122.56
2	N	18	ALY	OH-CH-CH3	-2.18	118.00	122.06
2	K	18	ALY	CE-NZ-CH	2.16	125.88	122.56
2	L	18	ALY	OH-CH-CH3	-2.12	118.11	122.06
2	O	9	M3L	CD-CE-NZ	-2.10	107.29	116.03
2	I	9	M3L	CD-CE-NZ	-2.08	107.38	116.03
2	N	18	ALY	CH3-CH-NZ	2.02	119.67	116.09

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	18	ALY	O-C-CA-CB
2	K	18	ALY	N-CA-CB-CG
2	K	18	ALY	C-CA-CB-CG
2	P	18	ALY	N-CA-CB-CG
2	P	18	ALY	C-CA-CB-CG
2	J	9	M3L	N-CA-CB-CG
2	J	9	M3L	C-CA-CB-CG
2	K	18	ALY	CG-CD-CE-NZ
2	J	18	ALY	CG-CD-CE-NZ
2	L	18	ALY	OH-CH-NZ-CE
2	L	18	ALY	CH3-CH-NZ-CE
2	O	18	ALY	OH-CH-NZ-CE
2	O	18	ALY	CH3-CH-NZ-CE
2	N	18	ALY	OH-CH-NZ-CE
2	N	18	ALY	CH3-CH-NZ-CE
2	I	18	ALY	OH-CH-NZ-CE
2	I	18	ALY	CH3-CH-NZ-CE
2	K	18	ALY	OH-CH-NZ-CE
2	K	18	ALY	CH3-CH-NZ-CE
2	J	18	ALY	OH-CH-NZ-CE
2	J	18	ALY	CH3-CH-NZ-CE
2	P	18	ALY	OH-CH-NZ-CE
2	P	18	ALY	CH3-CH-NZ-CE
2	M	18	ALY	OH-CH-NZ-CE
2	M	18	ALY	CH3-CH-NZ-CE
2	L	18	ALY	CG-CD-CE-NZ
2	M	18	ALY	CG-CD-CE-NZ
2	O	18	ALY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
2	I	18	ALY	CG-CD-CE-NZ
2	N	18	ALY	CG-CD-CE-NZ
2	M	9	M3L	CG-CD-CE-NZ
2	I	9	M3L	CD-CE-NZ-CM2
2	I	9	M3L	CD-CE-NZ-CM3
2	P	18	ALY	CG-CD-CE-NZ
2	M	9	M3L	CD-CE-NZ-CM1
2	M	9	M3L	CD-CE-NZ-CM3
2	I	9	M3L	CD-CE-NZ-CM1
2	M	9	M3L	CD-CE-NZ-CM2
2	O	18	ALY	CE-CD-CG-CB
2	P	18	ALY	CA-CB-CG-CD
2	K	9	M3L	CE-CD-CG-CB
2	P	18	ALY	CE-CD-CG-CB
2	N	18	ALY	CE-CD-CG-CB
2	I	9	M3L	CE-CD-CG-CB
2	J	9	M3L	CG-CD-CE-NZ
2	I	18	ALY	CE-CD-CG-CB
2	J	18	ALY	CE-CD-CG-CB
2	M	18	ALY	CE-CD-CG-CB
2	P	9	M3L	CD-CE-NZ-CM3
2	L	18	ALY	CE-CD-CG-CB
2	O	9	M3L	CD-CE-NZ-CM2
2	J	9	M3L	CD-CE-NZ-CM1
2	P	9	M3L	CD-CE-NZ-CM2
2	J	9	M3L	CD-CE-NZ-CM2
2	P	9	M3L	CD-CE-NZ-CM1
2	J	9	M3L	CD-CE-NZ-CM3
2	N	9	M3L	CE-CD-CG-CB
2	O	9	M3L	CD-CE-NZ-CM1
2	O	9	M3L	CD-CE-NZ-CM3
2	L	9	M3L	CG-CD-CE-NZ
2	P	9	M3L	CG-CD-CE-NZ
2	L	9	M3L	CE-CD-CG-CB
2	O	9	M3L	CE-CD-CG-CB
2	P	9	M3L	C-CA-CB-CG
2	J	9	M3L	CA-CB-CG-CD
2	M	18	ALY	N-CA-CB-CG

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	9	M3L	4	0
2	N	9	M3L	3	0
2	L	18	ALY	1	0
2	J	18	ALY	1	0
2	P	9	M3L	2	0
2	I	9	M3L	2	0
2	K	9	M3L	3	0
2	M	14	ALY	4	0
2	P	18	ALY	1	0
2	O	9	M3L	5	0
2	L	9	M3L	2	0
2	I	14	ALY	4	0
2	J	9	M3L	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	188/207 (90%)	-0.20	1 (0%) 91 88	48, 85, 143, 190	0
1	B	188/207 (90%)	-0.22	3 (1%) 72 66	49, 86, 148, 215	0
1	C	188/207 (90%)	-0.24	2 (1%) 80 75	49, 85, 141, 188	0
1	D	188/207 (90%)	-0.28	4 (2%) 63 54	52, 84, 138, 184	0
1	E	188/207 (90%)	-0.22	2 (1%) 80 75	49, 86, 144, 206	0
1	F	188/207 (90%)	-0.25	1 (0%) 91 88	49, 85, 141, 183	0
1	G	188/207 (90%)	-0.27	3 (1%) 72 66	49, 85, 140, 180	0
1	H	188/207 (90%)	-0.23	1 (0%) 91 88	50, 85, 141, 189	0
2	I	15/28 (53%)	0.59	2 (13%) 3 2	84, 108, 188, 190	0
2	J	14/28 (50%)	1.53	4 (28%) 0 0	77, 97, 170, 189	0
2	K	14/28 (50%)	1.08	3 (21%) 0 0	77, 108, 155, 171	0
2	L	15/28 (53%)	0.57	3 (20%) 1 0	76, 101, 169, 188	0
2	M	16/28 (57%)	1.23	4 (25%) 0 0	83, 120, 186, 198	0
2	N	14/28 (50%)	1.34	2 (14%) 2 1	74, 109, 148, 176	0
2	O	15/28 (53%)	0.60	3 (20%) 1 0	80, 105, 187, 190	0
2	P	14/28 (50%)	0.94	3 (21%) 0 0	76, 112, 171, 179	0
All	All	1621/1880 (86%)	-0.15	41 (2%) 57 47	48, 87, 150, 215	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	12	GLY	14.1
2	J	12	GLY	12.1
2	K	12	GLY	11.6
2	M	12	GLY	9.0
2	P	12	GLY	7.4

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Mol	Chain	Res	Type	RSRZ
1	E	948	HIS	6.1
2	J	16	PRO	4.9
1	B	947	GLN	4.5
2	L	15	ALA	4.5
2	I	12	GLY	4.5
1	E	947	GLN	4.5
2	O	12	GLY	4.4
2	L	13	GLY	4.3
2	M	13	GLY	4.0
2	P	11	THR	3.7
2	J	15	ALA	3.7
2	N	15	ALA	3.3
2	K	15	ALA	3.1
2	O	15	ALA	3.0
2	M	16	PRO	2.9
2	I	15	ALA	2.8
2	P	15	ALA	2.7
1	B	957	GLY	2.7
2	M	15	ALA	2.7
1	B	934	ILE	2.7
1	C	947	GLN	2.7
1	G	957	GLY	2.7
2	K	11	THR	2.5
1	D	957	GLY	2.5
1	G	1080	ILE	2.5
2	L	12	GLY	2.5
1	A	947	GLN	2.4
1	C	957	GLY	2.4
2	O	13	GLY	2.3
1	F	957	GLY	2.2
1	H	884	ASP	2.2
1	D	934	ILE	2.2
1	G	948	HIS	2.2
2	J	17	ARG	2.1
1	D	1086	PHE	2.1
1	D	922	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ALY	M	14	5/13	0.71	0.28	167,190,192,198	0
2	ALY	L	14	5/13	0.74	0.69	169,184,191,193	0
2	ALY	O	14	5/13	0.76	0.78	165,190,197,205	0
2	ALY	I	14	5/13	0.79	0.30	169,189,194,194	0
2	ALY	K	18	12/13	0.84	0.26	49,89,120,127	0
2	ALY	J	18	12/13	0.86	0.19	48,90,118,123	0
2	ALY	P	18	12/13	0.86	0.24	50,93,127,130	0
2	ALY	O	18	12/13	0.89	0.20	42,93,128,131	0
2	ALY	L	18	12/13	0.91	0.19	38,83,116,117	0
2	ALY	I	18	12/13	0.91	0.21	44,82,129,131	0
2	ALY	N	18	12/13	0.93	0.21	44,83,126,131	0
2	M3L	M	9	12/13	0.93	0.20	62,83,117,119	0
2	ALY	M	18	12/13	0.94	0.20	44,84,140,145	0
2	M3L	K	9	12/13	0.94	0.25	69,83,108,111	0
2	M3L	O	9	12/13	0.95	0.23	68,79,124,127	0
2	M3L	N	9	12/13	0.95	0.24	63,77,107,109	0
2	M3L	P	9	12/13	0.95	0.18	72,82,119,125	0
2	M3L	L	9	12/13	0.96	0.15	62,83,119,121	0
2	M3L	I	9	12/13	0.96	0.23	63,78,113,123	0
2	M3L	J	9	12/13	0.96	0.21	61,78,119,128	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	E	2	1/1	0.98	0.15	92,92,92,92	0
3	ZN	H	2	1/1	0.98	0.16	92,92,92,92	0
3	ZN	C	2	1/1	0.99	0.16	89,89,89,89	0
3	ZN	D	2	1/1	0.99	0.15	86,86,86,86	0
3	ZN	B	1	1/1	0.99	0.15	61,61,61,61	0
3	ZN	G	2	1/1	0.99	0.15	88,88,88,88	0
3	ZN	F	1	1/1	0.99	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	H	1	1/1	0.99	0.12	68,68,68,68	0
3	ZN	A	1	1/1	0.99	0.17	66,66,66,66	0
3	ZN	C	1	1/1	0.99	0.13	67,67,67,67	0
3	ZN	F	2	1/1	0.99	0.20	88,88,88,88	0
3	ZN	G	1	1/1	0.99	0.18	69,69,69,69	0
3	ZN	A	2	1/1	0.99	0.16	87,87,87,87	0
3	ZN	B	2	1/1	0.99	0.17	89,89,89,89	0
3	ZN	E	1	1/1	1.00	0.15	69,69,69,69	0
3	ZN	D	1	1/1	1.00	0.15	68,68,68,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.