



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:51 AM GMT

PDB ID : 3MQ9  
Title : Crystal Structure of Ectodomain Mutant of BST-2/Tetherin/CD317 Fused to MBP  
Authors : Xiong, Y.; Yang, H.; Wang, J.; Meng, W.  
Deposited on : 2010-04-27  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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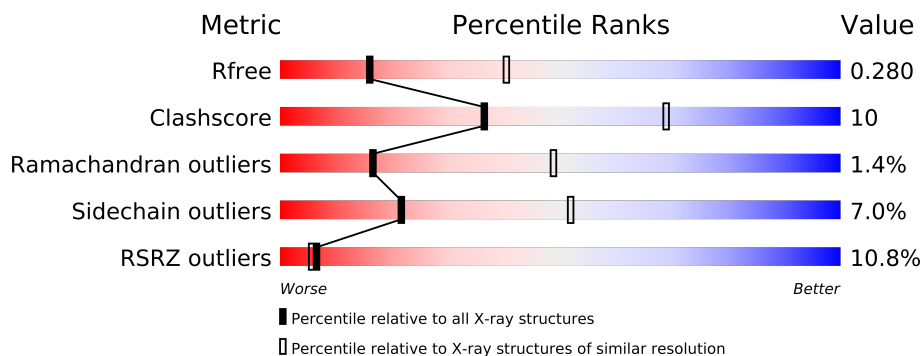
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	
1	C	471	
1	D	471	
1	E	471	
1	F	471	
1	G	471	
1	H	471	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28225 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	B	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	C	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	D	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	E	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	F	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	G	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			
1	H	454	Total	C	N	O	S	Se	0	0	0
			3520	2240	591	680	6	3			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	ALA	-	EXPRESSION TAG	UNP Q10589
A	371	ALA	-	EXPRESSION TAG	UNP Q10589
A	372	ARG	-	EXPRESSION TAG	UNP Q10589
A	373	ASP	-	EXPRESSION TAG	UNP Q10589
A	374	GLY	-	EXPRESSION TAG	UNP Q10589
A	375	LEU	-	EXPRESSION TAG	UNP Q10589
A	376	ARG	-	EXPRESSION TAG	UNP Q10589
A	377	ALA	-	EXPRESSION TAG	UNP Q10589
A	378	VAL	-	EXPRESSION TAG	UNP Q10589
A	379	MSE	-	EXPRESSION TAG	UNP Q10589
A	380	GLU	-	EXPRESSION TAG	UNP Q10589
A	381	ALA	-	EXPRESSION TAG	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ARG	-	EXPRESSION TAG	UNP Q10589
A	383	ASN	-	EXPRESSION TAG	UNP Q10589
A	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
B	370	ALA	-	EXPRESSION TAG	UNP Q10589
B	371	ALA	-	EXPRESSION TAG	UNP Q10589
B	372	ARG	-	EXPRESSION TAG	UNP Q10589
B	373	ASP	-	EXPRESSION TAG	UNP Q10589
B	374	GLY	-	EXPRESSION TAG	UNP Q10589
B	375	LEU	-	EXPRESSION TAG	UNP Q10589
B	376	ARG	-	EXPRESSION TAG	UNP Q10589
B	377	ALA	-	EXPRESSION TAG	UNP Q10589
B	378	VAL	-	EXPRESSION TAG	UNP Q10589
B	379	MSE	-	EXPRESSION TAG	UNP Q10589
B	380	GLU	-	EXPRESSION TAG	UNP Q10589
B	381	ALA	-	EXPRESSION TAG	UNP Q10589
B	382	ARG	-	EXPRESSION TAG	UNP Q10589
B	383	ASN	-	EXPRESSION TAG	UNP Q10589
B	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
C	370	ALA	-	EXPRESSION TAG	UNP Q10589
C	371	ALA	-	EXPRESSION TAG	UNP Q10589
C	372	ARG	-	EXPRESSION TAG	UNP Q10589
C	373	ASP	-	EXPRESSION TAG	UNP Q10589
C	374	GLY	-	EXPRESSION TAG	UNP Q10589
C	375	LEU	-	EXPRESSION TAG	UNP Q10589
C	376	ARG	-	EXPRESSION TAG	UNP Q10589
C	377	ALA	-	EXPRESSION TAG	UNP Q10589
C	378	VAL	-	EXPRESSION TAG	UNP Q10589
C	379	MSE	-	EXPRESSION TAG	UNP Q10589
C	380	GLU	-	EXPRESSION TAG	UNP Q10589
C	381	ALA	-	EXPRESSION TAG	UNP Q10589
C	382	ARG	-	EXPRESSION TAG	UNP Q10589
C	383	ASN	-	EXPRESSION TAG	UNP Q10589
C	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
D	370	ALA	-	EXPRESSION TAG	UNP Q10589
D	371	ALA	-	EXPRESSION TAG	UNP Q10589
D	372	ARG	-	EXPRESSION TAG	UNP Q10589
D	373	ASP	-	EXPRESSION TAG	UNP Q10589
D	374	GLY	-	EXPRESSION TAG	UNP Q10589
D	375	LEU	-	EXPRESSION TAG	UNP Q10589
D	376	ARG	-	EXPRESSION TAG	UNP Q10589
D	377	ALA	-	EXPRESSION TAG	UNP Q10589
D	378	VAL	-	EXPRESSION TAG	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
D	379	MSE	-	EXPRESSION TAG	UNP Q10589
D	380	GLU	-	EXPRESSION TAG	UNP Q10589
D	381	ALA	-	EXPRESSION TAG	UNP Q10589
D	382	ARG	-	EXPRESSION TAG	UNP Q10589
D	383	ASN	-	EXPRESSION TAG	UNP Q10589
D	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
E	370	ALA	-	EXPRESSION TAG	UNP Q10589
E	371	ALA	-	EXPRESSION TAG	UNP Q10589
E	372	ARG	-	EXPRESSION TAG	UNP Q10589
E	373	ASP	-	EXPRESSION TAG	UNP Q10589
E	374	GLY	-	EXPRESSION TAG	UNP Q10589
E	375	LEU	-	EXPRESSION TAG	UNP Q10589
E	376	ARG	-	EXPRESSION TAG	UNP Q10589
E	377	ALA	-	EXPRESSION TAG	UNP Q10589
E	378	VAL	-	EXPRESSION TAG	UNP Q10589
E	379	MSE	-	EXPRESSION TAG	UNP Q10589
E	380	GLU	-	EXPRESSION TAG	UNP Q10589
E	381	ALA	-	EXPRESSION TAG	UNP Q10589
E	382	ARG	-	EXPRESSION TAG	UNP Q10589
E	383	ASN	-	EXPRESSION TAG	UNP Q10589
E	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
F	370	ALA	-	EXPRESSION TAG	UNP Q10589
F	371	ALA	-	EXPRESSION TAG	UNP Q10589
F	372	ARG	-	EXPRESSION TAG	UNP Q10589
F	373	ASP	-	EXPRESSION TAG	UNP Q10589
F	374	GLY	-	EXPRESSION TAG	UNP Q10589
F	375	LEU	-	EXPRESSION TAG	UNP Q10589
F	376	ARG	-	EXPRESSION TAG	UNP Q10589
F	377	ALA	-	EXPRESSION TAG	UNP Q10589
F	378	VAL	-	EXPRESSION TAG	UNP Q10589
F	379	MSE	-	EXPRESSION TAG	UNP Q10589
F	380	GLU	-	EXPRESSION TAG	UNP Q10589
F	381	ALA	-	EXPRESSION TAG	UNP Q10589
F	382	ARG	-	EXPRESSION TAG	UNP Q10589
F	383	ASN	-	EXPRESSION TAG	UNP Q10589
F	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
G	370	ALA	-	EXPRESSION TAG	UNP Q10589
G	371	ALA	-	EXPRESSION TAG	UNP Q10589
G	372	ARG	-	EXPRESSION TAG	UNP Q10589
G	373	ASP	-	EXPRESSION TAG	UNP Q10589
G	374	GLY	-	EXPRESSION TAG	UNP Q10589
G	375	LEU	-	EXPRESSION TAG	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
G	376	ARG	-	EXPRESSION TAG	UNP Q10589
G	377	ALA	-	EXPRESSION TAG	UNP Q10589
G	378	VAL	-	EXPRESSION TAG	UNP Q10589
G	379	MSE	-	EXPRESSION TAG	UNP Q10589
G	380	GLU	-	EXPRESSION TAG	UNP Q10589
G	381	ALA	-	EXPRESSION TAG	UNP Q10589
G	382	ARG	-	EXPRESSION TAG	UNP Q10589
G	383	ASN	-	EXPRESSION TAG	UNP Q10589
G	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
H	370	ALA	-	EXPRESSION TAG	UNP Q10589
H	371	ALA	-	EXPRESSION TAG	UNP Q10589
H	372	ARG	-	EXPRESSION TAG	UNP Q10589
H	373	ASP	-	EXPRESSION TAG	UNP Q10589
H	374	GLY	-	EXPRESSION TAG	UNP Q10589
H	375	LEU	-	EXPRESSION TAG	UNP Q10589
H	376	ARG	-	EXPRESSION TAG	UNP Q10589
H	377	ALA	-	EXPRESSION TAG	UNP Q10589
H	378	VAL	-	EXPRESSION TAG	UNP Q10589
H	379	MSE	-	EXPRESSION TAG	UNP Q10589
H	380	GLU	-	EXPRESSION TAG	UNP Q10589
H	381	ALA	-	EXPRESSION TAG	UNP Q10589
H	382	ARG	-	EXPRESSION TAG	UNP Q10589
H	383	ASN	-	EXPRESSION TAG	UNP Q10589
H	409	ALA	CYS	ENGINEERED MUTATION	UNP Q10589

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	19	Total O 19 19	0	0
2	C	2	Total O 2 2	0	0
2	D	6	Total O 6 6	0	0
2	E	11	Total O 11 11	0	0
2	F	5	Total O 5 5	0	0
2	G	1	Total O 1 1	0	0

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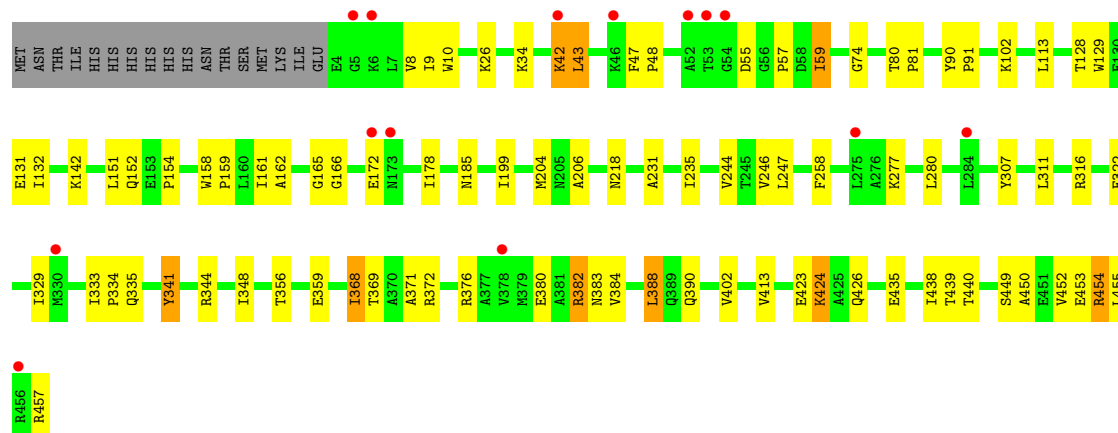
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	9	Total	O	0	0
			9	9		

### 3 Residue-property plots

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

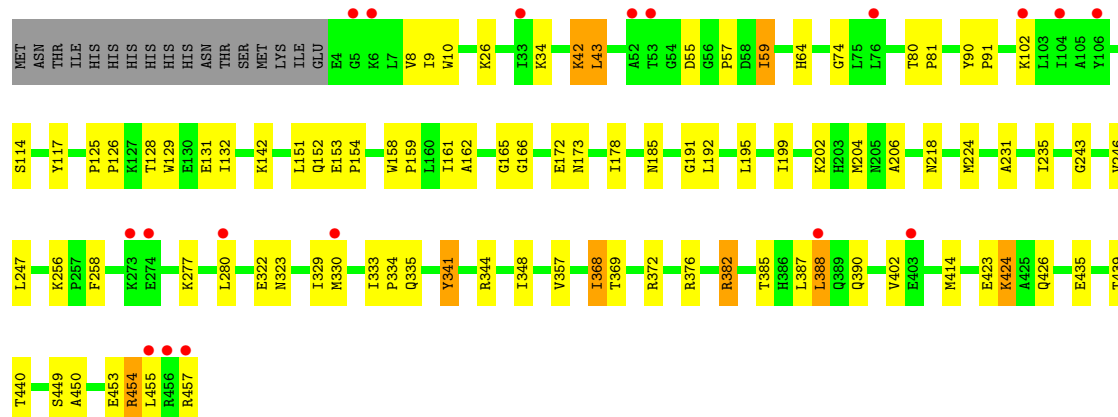
- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain A: 



- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain B: 

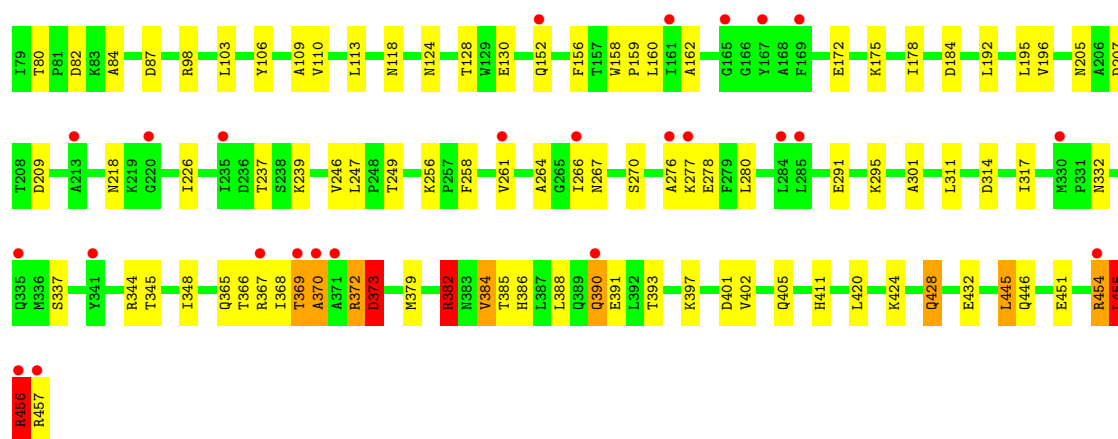


- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Chain C: 







- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

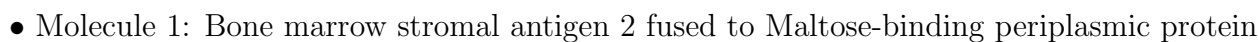
Chain D:

- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

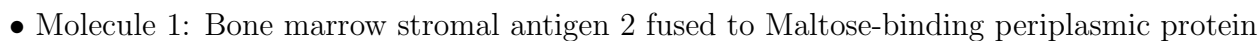
Chain E:

- Molecule 1: Bone marrow stromal antigen 2 fused to Maltose-binding periplasmic protein

Age Group	Percentage
18-24	~10%
25-34	~85%
35-44	~75%
45-54	~10%
55-64	~5%
65+	~1%

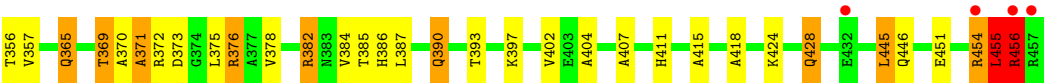


Responsibility	Percentage
Current government	85%
Opposition	10%
Both	5%



Age Group	Percentage
18-24	10%
25-34	75%
35-44	10%
45-54	3%
55-64	1%
65-74	1%
75-84	1%
85+	1%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.50Å 202.44Å 107.28Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	42.47 – 2.80 42.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.47-2.80) 93.8 (42.47-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.231 , 0.279 0.231 , 0.280	Depositor DCC
$R_{free}$ test set	4743 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , -20.0	EDS
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 94564 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28225	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.62	0/3590	0.65	0/4861
1	B	0.67	0/3590	0.70	0/4861
1	C	0.63	0/3590	0.69	1/4861 (0.0%)
1	D	0.55	0/3590	0.67	3/4861 (0.1%)
1	E	0.57	0/3590	0.63	0/4861
1	F	0.50	0/3590	0.63	0/4861
1	G	0.46	0/3590	0.58	1/4861 (0.0%)
1	H	0.61	0/3590	0.71	1/4861 (0.0%)
All	All	0.58	0/28720	0.66	6/38888 (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	C	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	236	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	G	382	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	D	382	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	D	456	ARG	CG-CD-NE	5.47	123.28	111.80
1	D	456	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	382	ARG	NE-CZ-NH1	5.23	122.91	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	372	ARG	Peptide
1	H	455	LEU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3520	0	3491	66	0
1	B	3520	0	3491	71	0
1	C	3520	0	3491	90	0
1	D	3520	0	3491	92	0
1	E	3520	0	3491	69	0
1	F	3520	0	3491	82	1
1	G	3520	0	3491	83	0
1	H	3520	0	3491	119	0
2	A	12	0	0	2	0
2	B	19	0	0	2	0
2	C	2	0	0	0	0
2	D	6	0	0	1	0
2	E	11	0	0	0	0
2	F	5	0	0	0	0
2	G	1	0	0	0	0
2	H	9	0	0	0	0
All	All	28225	0	27928	579	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (579) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:370:ALA:HB1	1:H:371:ALA:CB	1.36	1.50
1:D:456:ARG:NH1	1:D:456:ARG:HB3	1.25	1.49
1:D:456:ARG:CB	1:D:456:ARG:HH11	1.38	1.36
1:C:456:ARG:NH1	1:C:456:ARG:HB3	1.52	1.23
1:D:371:ALA:O	1:D:376:ARG:NH2	1.72	1.22

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:370:ALA:CB	1:H:371:ALA:CB	2.22	1.17
1:H:370:ALA:CB	1:H:371:ALA:HB2	1.75	1.15
1:H:456:ARG:NH1	1:H:456:ARG:HB2	1.61	1.14
1:H:456:ARG:CB	1:H:456:ARG:CZ	2.26	1.13
1:A:402:VAL:HG11	1:D:402:VAL:HG11	1.21	1.11
1:C:456:ARG:HB3	1:C:456:ARG:CZ	1.78	1.09
1:A:402:VAL:CG1	1:D:402:VAL:HG11	1.81	1.09
1:B:455:LEU:HD13	1:C:456:ARG:HH12	1.16	1.08
1:C:369:THR:HG22	1:C:370:ALA:H	1.09	1.07
1:A:455:LEU:HD13	1:D:456:ARG:NH1	1.69	1.06
1:H:456:ARG:HB3	1:H:456:ARG:CZ	1.81	1.05
1:B:455:LEU:HD13	1:C:456:ARG:NH1	1.71	1.04
1:G:456:ARG:HB2	1:G:456:ARG:NH1	1.72	1.04
1:H:370:ALA:HB1	1:H:371:ALA:HB3	1.38	1.03
1:E:455:LEU:HD13	1:H:456:ARG:NH2	1.74	1.02
1:G:456:ARG:HB3	1:G:456:ARG:CZ	1.89	1.00
1:G:456:ARG:CB	1:G:456:ARG:CZ	2.40	0.99
1:D:455:LEU:O	1:D:456:ARG:HB2	1.64	0.98
1:D:177:ASP:OD1	1:D:180:ASP:HB3	1.70	0.92
1:C:456:ARG:NH1	1:C:456:ARG:CB	2.33	0.90
1:E:450:ALA:HB1	1:E:454:ARG:HH21	1.38	0.89
1:H:370:ALA:CB	1:H:371:ALA:HB3	1.95	0.88
1:D:371:ALA:CB	1:D:372:ARG:HA	2.03	0.88
1:C:369:THR:CG2	1:C:370:ALA:H	1.87	0.88
1:H:456:ARG:HB2	1:H:456:ARG:CZ	1.99	0.88
1:H:370:ALA:HB1	1:H:371:ALA:HB2	0.87	0.86
1:F:387:LEU:HB2	1:H:341:TYR:CZ	2.10	0.86
1:H:82:ASP:OD1	1:H:84:ALA:HB3	1.76	0.86
1:E:402:VAL:HG11	1:H:402:VAL:HG11	1.56	0.86
1:E:455:LEU:HB3	1:H:456:ARG:CZ	2.06	0.86
1:F:450:ALA:HB1	1:F:454:ARG:HH21	1.40	0.86
1:A:455:LEU:HD13	1:D:456:ARG:HH12	1.33	0.86
1:A:450:ALA:HB1	1:A:454:ARG:HH21	1.39	0.86
1:E:455:LEU:HD13	1:H:456:ARG:HH22	1.40	0.85
1:C:369:THR:HG22	1:C:370:ALA:N	1.91	0.84
1:F:455:LEU:HB3	1:G:456:ARG:CZ	2.06	0.84
1:H:456:ARG:CB	1:H:456:ARG:NH1	2.39	0.83
1:D:371:ALA:HB3	1:D:372:ARG:HA	1.60	0.82
1:B:173:ASN:HD22	1:D:143:GLY:HA3	1.43	0.82
1:A:384:VAL:HG23	1:C:49:GLN:HG2	1.62	0.81
1:G:456:ARG:CB	1:G:456:ARG:NH1	2.43	0.81
1:B:450:ALA:HB1	1:B:454:ARG:HH21	1.43	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:455:LEU:HD13	1:G:456:ARG:NH2	1.96	0.81
1:E:402:VAL:CG1	1:H:402:VAL:HG11	2.10	0.81
1:B:256:LYS:HE3	2:B:473:HOH:O	1.80	0.81
1:F:402:VAL:HG11	1:G:402:VAL:HG11	1.63	0.80
1:D:455:LEU:O	1:D:456:ARG:CB	2.31	0.79
1:E:455:LEU:HD13	1:H:456:ARG:CZ	2.12	0.79
1:F:388:LEU:HB2	1:H:384:VAL:HG11	1.65	0.79
1:D:456:ARG:NH1	1:D:456:ARG:CB	2.16	0.79
1:D:445:LEU:C	1:D:445:LEU:HD23	2.03	0.79
1:F:387:LEU:HB2	1:H:341:TYR:CE2	2.18	0.78
1:A:341:TYR:HB3	1:C:405:GLN:HE21	1.49	0.78
1:C:455:LEU:O	1:C:456:ARG:HB2	1.83	0.77
1:F:402:VAL:CG1	1:G:402:VAL:HG11	2.14	0.77
1:E:344:ARG:O	1:E:348:ILE:HD13	1.84	0.77
1:B:344:ARG:O	1:B:348:ILE:HD13	1.85	0.76
1:B:59:ILE:HD12	1:B:280:LEU:HD11	1.67	0.76
1:B:173:ASN:ND2	1:D:143:GLY:HA3	2.02	0.75
1:E:9:ILE:HG12	1:E:59:ILE:HG23	1.69	0.75
1:B:9:ILE:HG12	1:B:59:ILE:HG23	1.68	0.74
1:G:368:ILE:O	1:G:369:THR:HG22	1.87	0.74
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.53	0.74
1:D:61:PHE:CE2	1:D:264:ALA:HB2	2.24	0.73
1:B:341:TYR:HB3	1:D:405:GLN:HE21	1.53	0.73
1:H:371:ALA:HB3	1:H:376:ARG:NH1	2.04	0.73
1:F:455:LEU:HD13	1:G:456:ARG:HH22	1.53	0.73
1:A:9:ILE:HG12	1:A:59:ILE:HG23	1.71	0.73
1:D:59:ILE:HD12	1:D:60:ILE:N	2.03	0.73
1:A:368:ILE:HG22	1:A:369:THR:HG23	1.71	0.72
1:G:338:ALA:HB3	1:G:368:ILE:HD12	1.71	0.72
1:D:382:ARG:HH11	1:D:382:ARG:HG2	1.55	0.72
1:E:59:ILE:HD12	1:E:280:LEU:HD11	1.72	0.71
1:B:455:LEU:CD1	1:C:456:ARG:NH1	2.51	0.71
1:A:59:ILE:HD12	1:A:280:LEU:HD11	1.73	0.71
1:D:113:LEU:HD13	1:D:226:ILE:HG22	1.71	0.71
1:D:366:THR:HG21	1:F:359:GLU:HB3	1.72	0.71
1:H:61:PHE:CE2	1:H:264:ALA:HB2	2.25	0.70
1:F:9:ILE:HG12	1:F:59:ILE:HG23	1.72	0.70
1:C:456:ARG:HH11	1:C:456:ARG:CB	2.04	0.70
1:E:455:LEU:HB3	1:H:456:ARG:NE	2.06	0.69
1:H:382:ARG:HG2	1:H:382:ARG:HH11	1.58	0.69
1:H:454:ARG:O	1:H:456:ARG:N	2.26	0.69
1:F:455:LEU:HD13	1:G:456:ARG:CZ	2.22	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:371:ALA:CB	1:D:372:ARG:CA	2.71	0.69
1:H:456:ARG:HB2	1:H:456:ARG:HH11	1.58	0.68
1:A:151:LEU:HD21	1:A:204:MET:HE1	1.75	0.68
1:F:455:LEU:HD13	1:G:456:ARG:NH1	2.08	0.68
1:D:454:ARG:O	1:D:456:ARG:N	2.26	0.68
1:C:128:THR:HG22	1:C:249:THR:OG1	1.93	0.68
1:F:453:GLU:O	1:F:457:ARG:HG3	1.94	0.68
1:G:382:ARG:HG2	1:G:382:ARG:HH11	1.59	0.68
1:F:344:ARG:O	1:F:348:ILE:HD13	1.95	0.67
1:D:9:ILE:HG23	1:D:59:ILE:HG13	1.75	0.67
1:E:151:LEU:HD21	1:E:204:MET:HE1	1.76	0.67
1:D:445:LEU:HD23	1:D:446:GLN:N	2.10	0.66
1:F:59:ILE:HD12	1:F:280:LEU:HD11	1.77	0.66
1:F:455:LEU:CD1	1:G:456:ARG:NH1	2.59	0.66
1:C:98:ARG:HG2	1:C:103:LEU:HD23	1.78	0.66
1:F:450:ALA:HB1	1:F:454:ARG:NH2	2.11	0.66
1:H:80:THR:O	1:H:277:LYS:NZ	2.30	0.65
1:H:445:LEU:C	1:H:445:LEU:HD23	2.17	0.65
1:G:98:ARG:HG2	1:G:103:LEU:HD23	1.77	0.65
1:F:387:LEU:HD22	1:H:341:TYR:CD2	2.32	0.65
1:A:450:ALA:HB1	1:A:454:ARG:NH2	2.11	0.64
1:E:450:ALA:HB1	1:E:454:ARG:NH2	2.11	0.64
1:C:455:LEU:O	1:C:456:ARG:CB	2.44	0.64
1:C:454:ARG:O	1:C:456:ARG:N	2.31	0.64
1:C:369:THR:CG2	1:C:370:ALA:N	2.55	0.64
1:E:453:GLU:O	1:E:457:ARG:HG3	1.97	0.63
1:D:113:LEU:HD13	1:D:226:ILE:CG2	2.27	0.63
1:H:64:HIS:CD2	1:H:261:VAL:H	2.17	0.63
1:E:455:LEU:CD1	1:H:456:ARG:NH1	2.62	0.63
1:H:64:HIS:HD2	1:H:261:VAL:H	1.44	0.63
1:A:380:GLU:OE1	1:C:391:GLU:OE2	2.17	0.63
1:G:456:ARG:HB2	1:G:456:ARG:HH11	1.63	0.62
1:G:373:ASP:OD2	1:G:377:ALA:HB2	1.99	0.62
1:B:453:GLU:O	1:B:457:ARG:HG3	1.99	0.62
1:F:399:PHE:CE2	1:G:399:PHE:CE2	2.87	0.62
1:C:366:THR:O	1:C:368:ILE:N	2.32	0.62
1:A:388:LEU:HB2	1:C:384:VAL:HG11	1.81	0.62
1:A:368:ILE:HG22	1:A:369:THR:CG2	2.30	0.62
1:H:104:ILE:HD12	1:H:104:ILE:C	2.20	0.62
1:C:344:ARG:O	1:C:348:ILE:HD12	1.99	0.62
1:H:372:ARG:H	1:H:376:ARG:NH2	1.97	0.62
1:D:98:ARG:HG2	1:D:103:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:80:THR:O	1:G:277:LYS:NZ	2.33	0.61
1:D:439:THR:HG23	2:D:463:HOH:O	1.98	0.61
1:D:64:HIS:HD2	1:D:261:VAL:H	1.47	0.61
1:C:428:GLN:O	1:C:432:GLU:HG2	2.00	0.61
1:B:195:LEU:HD12	1:B:195:LEU:O	2.00	0.61
1:H:371:ALA:HB3	1:H:376:ARG:CZ	2.30	0.61
1:B:368:ILE:HG23	1:B:369:THR:HG23	1.83	0.61
1:A:402:VAL:HG13	1:D:402:VAL:HG11	1.81	0.60
1:A:453:GLU:O	1:A:457:ARG:HG3	2.01	0.60
1:B:192:LEU:HD23	1:B:357:VAL:HG13	1.82	0.60
1:A:344:ARG:O	1:A:348:ILE:HD13	2.00	0.60
1:H:59:ILE:HD11	1:H:61:PHE:CD1	2.36	0.60
1:C:246:VAL:HG12	1:C:247:LEU:O	2.02	0.60
1:F:455:LEU:CD1	1:G:456:ARG:HH12	2.15	0.60
1:H:370:ALA:HB3	1:H:376:ARG:NH1	2.17	0.59
1:B:246:VAL:CG2	1:B:322:GLU:OE1	2.51	0.59
1:A:383:ASN:HD21	1:C:53:THR:CG2	2.15	0.59
1:A:402:VAL:CG1	1:D:402:VAL:CG1	2.69	0.59
1:C:43:LEU:HD12	1:C:43:LEU:C	2.23	0.59
1:H:372:ARG:HA	1:H:376:ARG:HH21	1.66	0.59
1:G:454:ARG:O	1:G:456:ARG:N	2.35	0.59
1:H:370:ALA:CA	1:H:371:ALA:HB2	2.33	0.59
1:H:59:ILE:HD11	1:H:61:PHE:CE1	2.38	0.59
1:C:80:THR:O	1:C:277:LYS:NZ	2.36	0.59
1:H:158:TRP:CE2	1:H:162:ALA:HB2	2.37	0.59
1:C:372:ARG:HG2	1:C:372:ARG:HH11	1.68	0.59
1:C:456:ARG:CZ	1:C:456:ARG:CB	2.67	0.58
1:E:455:LEU:CD1	1:H:456:ARG:CZ	2.81	0.58
1:C:445:LEU:HD23	1:C:446:GLN:N	2.18	0.58
1:E:341:TYR:HB3	1:G:405:GLN:HE21	1.67	0.58
1:E:329:ILE:H	1:E:329:ILE:HD12	1.68	0.58
1:A:129:TRP:HA	1:A:132:ILE:HD12	1.84	0.58
1:C:445:LEU:HD23	1:C:445:LEU:C	2.23	0.58
1:A:423:GLU:O	1:A:424:LYS:HB2	2.03	0.58
1:D:64:HIS:HE1	1:D:330:MET:O	1.87	0.58
1:C:82:ASP:OD1	1:C:84:ALA:HB3	2.03	0.58
1:G:7:LEU:HB2	1:G:35:VAL:HG22	1.86	0.58
1:G:152:GLN:HE22	1:G:207:ASP:HA	1.69	0.58
1:G:158:TRP:CE2	1:G:162:ALA:HB2	2.39	0.57
1:D:371:ALA:HB1	1:D:372:ARG:HA	1.83	0.57
1:A:246:VAL:CG2	1:A:322:GLU:OE1	2.51	0.57
1:C:311:LEU:HB3	1:C:317:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:370:ALA:HB3	1:H:371:ALA:HB3	1.85	0.57
1:G:8:VAL:HG13	1:G:57:PRO:HA	1.86	0.57
1:A:113:LEU:HG	2:A:460:HOH:O	2.05	0.57
1:F:151:LEU:HD21	1:F:204:MET:HE1	1.85	0.57
1:F:384:VAL:HG21	1:H:387:LEU:HD23	1.86	0.57
1:B:329:ILE:H	1:B:329:ILE:HD12	1.68	0.57
1:B:387:LEU:HB2	1:D:341:TYR:CZ	2.39	0.57
1:B:151:LEU:HD21	1:B:204:MET:HE1	1.87	0.56
1:F:455:LEU:HD13	1:G:456:ARG:HH12	1.69	0.56
1:A:455:LEU:HB3	1:D:456:ARG:CZ	2.35	0.56
1:A:455:LEU:CD1	1:D:456:ARG:NH1	2.57	0.56
1:B:199:ILE:HG21	1:B:206:ALA:HB2	1.88	0.56
1:D:420:LEU:HD11	1:D:424:LYS:HE3	1.87	0.56
1:F:129:TRP:HA	1:F:132:ILE:HD12	1.88	0.56
1:D:104:ILE:HD12	1:D:105:ALA:N	2.21	0.56
1:H:370:ALA:CB	1:H:376:ARG:NH1	2.68	0.56
1:D:366:THR:CG2	1:F:359:GLU:HB3	2.35	0.56
1:G:445:LEU:HD23	1:G:446:GLN:N	2.21	0.56
1:B:450:ALA:HB1	1:B:454:ARG:NH2	2.16	0.56
1:A:59:ILE:HD11	1:A:280:LEU:HD21	1.88	0.56
1:A:356:THR:OG1	1:A:359:GLU:HG2	2.06	0.56
1:H:365:GLN:O	1:H:369:THR:OG1	2.24	0.56
1:H:372:ARG:H	1:H:376:ARG:CZ	2.19	0.55
1:B:8:VAL:HG13	1:B:57:PRO:HA	1.89	0.55
1:H:128:THR:HB	1:H:130:GLU:OE1	2.07	0.55
1:F:158:TRP:CE2	1:F:162:ALA:HB2	2.41	0.55
1:E:341:TYR:CE2	1:G:406:ALA:HA	2.42	0.55
1:B:59:ILE:CD1	1:B:280:LEU:HD11	2.36	0.55
1:A:154:PRO:HG3	1:A:344:ARG:HA	1.89	0.55
1:E:455:LEU:HD13	1:H:456:ARG:NH1	2.22	0.55
1:F:178:ILE:HG22	1:F:333:ILE:HD12	1.88	0.55
1:D:177:ASP:OD1	1:D:180:ASP:CB	2.51	0.55
1:B:59:ILE:CD1	1:B:280:LEU:HD21	2.37	0.55
1:F:154:PRO:HG3	1:F:344:ARG:HA	1.89	0.55
1:F:8:VAL:HG13	1:F:57:PRO:HA	1.89	0.55
1:E:128:THR:OG1	1:E:131:GLU:HG2	2.07	0.55
1:E:10:TRP:HB3	1:E:43:LEU:HD13	1.90	0.54
1:G:128:THR:HG22	1:G:249:THR:OG1	2.07	0.54
1:E:246:VAL:CG2	1:E:322:GLU:OE1	2.55	0.54
1:E:59:ILE:HD11	1:E:280:LEU:HD21	1.90	0.54
1:A:10:TRP:HB3	1:A:43:LEU:HD13	1.89	0.54
1:F:246:VAL:CG2	1:F:322:GLU:OE1	2.55	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:TRP:HA	1:B:132:ILE:HD12	1.89	0.54
1:H:59:ILE:HD12	1:H:60:ILE:N	2.22	0.54
1:H:255:SER:O	1:H:257:PRO:HD3	2.07	0.54
1:H:372:ARG:HA	1:H:376:ARG:NH2	2.22	0.54
1:D:371:ALA:HB1	1:D:372:ARG:CA	2.37	0.54
1:E:356:THR:OG1	1:E:359:GLU:HG2	2.07	0.54
1:E:9:ILE:CG1	1:E:59:ILE:HG23	2.38	0.54
1:G:388:LEU:HD23	1:H:385:THR:HG21	1.90	0.54
1:C:366:THR:C	1:C:368:ILE:H	2.11	0.54
1:E:341:TYR:CZ	1:G:406:ALA:HA	2.41	0.54
1:G:61:PHE:CE2	1:G:264:ALA:HB2	2.43	0.54
1:B:423:GLU:O	1:B:424:LYS:HB2	2.07	0.54
1:G:59:ILE:HD11	1:G:61:PHE:CE1	2.43	0.53
1:D:82:ASP:OD1	1:D:84:ALA:HB3	2.08	0.53
1:B:388:LEU:HB2	1:D:384:VAL:HG11	1.90	0.53
1:F:59:ILE:HD11	1:F:280:LEU:HD21	1.89	0.53
1:B:402:VAL:CG1	1:C:402:VAL:HG11	2.37	0.53
1:H:95:ASP:OD1	1:H:98:ARG:NH1	2.41	0.53
1:F:199:ILE:HG21	1:F:206:ALA:HB2	1.88	0.53
1:F:423:GLU:O	1:F:424:LYS:HB2	2.08	0.53
1:A:59:ILE:CD1	1:A:280:LEU:HD21	2.39	0.53
1:F:59:ILE:CD1	1:F:280:LEU:HD21	2.39	0.53
1:B:335:GLN:OE1	1:B:335:GLN:N	2.41	0.53
1:A:8:VAL:HG13	1:A:57:PRO:HA	1.90	0.53
1:C:59:ILE:HD11	1:C:61:PHE:CE1	2.44	0.53
1:G:445:LEU:C	1:G:445:LEU:HD23	2.29	0.53
1:G:372:ARG:O	1:G:373:ASP:C	2.46	0.53
1:B:246:VAL:HG12	1:B:247:LEU:O	2.08	0.53
1:B:59:ILE:HD11	1:B:280:LEU:HD21	1.89	0.53
1:D:130:GLU:N	1:D:130:GLU:OE1	2.38	0.53
1:E:455:LEU:HD12	1:H:456:ARG:NH1	2.24	0.53
1:E:199:ILE:HG21	1:E:206:ALA:HB2	1.91	0.53
1:G:393:THR:HG22	1:G:397:LYS:HE2	1.91	0.52
1:C:68:GLY:HA3	1:C:332:ASN:O	2.09	0.52
1:G:82:ASP:OD1	1:G:84:ALA:HB3	2.08	0.52
1:D:218:ASN:HD22	1:D:218:ASN:N	2.07	0.52
1:G:386:HIS:O	1:G:390:GLN:HG2	2.09	0.52
1:A:59:ILE:CD1	1:A:280:LEU:HD11	2.38	0.52
2:A:464:HOH:O	1:B:414:MSE:HE2	2.08	0.52
1:B:166:GLY:HA2	1:B:185:ASN:HD21	1.75	0.52
1:E:388:LEU:HD21	1:F:385:THR:CG2	2.39	0.52
1:H:205:ASN:ND2	1:H:207:ASP:OD1	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:9:ILE:CG1	1:B:59:ILE:HG23	2.37	0.52
1:B:154:PRO:HG3	1:B:344:ARG:HA	1.91	0.52
1:A:152:GLN:O	1:A:348:ILE:HD11	2.10	0.52
1:E:8:VAL:HG13	1:E:57:PRO:HA	1.91	0.52
1:E:129:TRP:HA	1:E:132:ILE:HD12	1.92	0.52
1:C:386:HIS:O	1:C:390:GLN:HG2	2.08	0.52
1:H:372:ARG:N	1:H:376:ARG:NH2	2.58	0.52
1:E:59:ILE:CD1	1:E:280:LEU:HD21	2.40	0.52
1:D:113:LEU:HD22	1:D:227:ASN:HA	1.92	0.52
1:H:64:HIS:HE1	1:H:330:MET:O	1.93	0.52
1:D:390:GLN:HA	1:D:390:GLN:HE21	1.74	0.52
1:H:370:ALA:CA	1:H:371:ALA:CB	2.88	0.51
1:E:341:TYR:HE2	1:G:406:ALA:HB2	1.74	0.51
1:F:335:GLN:N	1:F:335:GLN:OE1	2.43	0.51
1:B:128:THR:OG1	1:B:131:GLU:HG2	2.10	0.51
1:E:423:GLU:O	1:E:424:LYS:HB2	2.09	0.51
1:E:246:VAL:HG12	1:E:247:LEU:O	2.09	0.51
1:D:136:ASP:HA	1:D:146:ALA:HB2	1.93	0.51
1:D:371:ALA:O	1:D:376:ARG:CZ	2.50	0.51
1:F:128:THR:OG1	1:F:131:GLU:HG2	2.09	0.51
1:A:9:ILE:CG1	1:A:59:ILE:HG23	2.41	0.51
1:C:158:TRP:CE2	1:C:162:ALA:HB2	2.46	0.51
1:E:178:ILE:HG22	1:E:333:ILE:HD12	1.92	0.51
1:F:329:ILE:HD12	1:F:329:ILE:H	1.75	0.51
1:D:7:LEU:HB2	1:D:35:VAL:HG22	1.93	0.51
1:E:152:GLN:O	1:E:348:ILE:HD11	2.11	0.51
1:E:231:ALA:O	1:E:235:ILE:HG13	2.10	0.51
1:B:117:TYR:CZ	1:B:243:GLY:HA3	2.46	0.51
1:E:388:LEU:CD2	1:F:385:THR:HG21	2.40	0.51
1:D:293:VAL:CG1	1:D:299:LEU:HD21	2.41	0.51
1:D:115:LEU:HB2	1:D:247:LEU:HD23	1.93	0.50
1:E:59:ILE:CD1	1:E:280:LEU:HD11	2.41	0.50
1:E:307:TYR:CE2	1:E:311:LEU:HD11	2.46	0.50
1:B:195:LEU:HD12	1:B:195:LEU:C	2.31	0.50
1:A:329:ILE:HD12	1:A:329:ILE:H	1.75	0.50
1:D:80:THR:O	1:D:277:LYS:NZ	2.45	0.50
1:H:181:VAL:HG13	1:H:183:VAL:HG23	1.93	0.50
1:D:205:ASN:ND2	1:D:207:ASP:OD1	2.42	0.50
1:D:238:SER:OG	1:D:240:VAL:HG23	2.12	0.50
1:F:10:TRP:HB3	1:F:43:LEU:HD13	1.94	0.49
1:G:382:ARG:CG	1:G:382:ARG:HH11	2.24	0.49
1:G:336:MET:O	1:G:339:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:158:TRP:CD1	1:D:258:PHE:CE2	3.00	0.49
1:H:98:ARG:HG2	1:H:103:LEU:HD23	1.95	0.49
1:E:154:PRO:HG3	1:E:344:ARG:HA	1.93	0.49
1:F:9:ILE:CG1	1:F:59:ILE:HG23	2.40	0.49
1:B:382:ARG:CG	1:B:382:ARG:HH11	2.26	0.49
1:H:107:PRO:O	1:H:108:ILE:HD13	2.13	0.49
1:B:178:ILE:HG22	1:B:333:ILE:HD12	1.94	0.49
1:C:314:ASP:HB3	1:C:317:ILE:HD12	1.94	0.49
1:B:10:TRP:HB3	1:B:43:LEU:HD13	1.94	0.49
1:C:267:ASN:HB3	1:C:270:SER:HB2	1.95	0.49
1:A:178:ILE:HG22	1:A:333:ILE:HD12	1.94	0.49
1:G:205:ASN:ND2	1:G:207:ASP:OD1	2.45	0.49
1:D:336:MET:O	1:D:339:PHE:HB3	2.12	0.49
1:A:128:THR:OG1	1:A:131:GLU:HG2	2.13	0.49
1:F:152:GLN:O	1:F:348:ILE:HD11	2.13	0.49
1:F:399:PHE:CD2	1:G:399:PHE:CZ	3.01	0.49
1:F:382:ARG:HH11	1:F:382:ARG:CG	2.26	0.49
1:C:369:THR:O	1:C:370:ALA:HB3	2.13	0.48
1:F:455:LEU:HB3	1:G:456:ARG:NE	2.27	0.48
1:G:381:ALA:O	1:G:385:THR:HG23	2.13	0.48
1:B:158:TRP:N	1:B:159:PRO:HD2	2.28	0.48
1:B:158:TRP:HB3	1:B:159:PRO:HD3	1.94	0.48
1:D:344:ARG:O	1:D:348:ILE:HD12	2.14	0.48
1:E:344:ARG:O	1:E:348:ILE:CD1	2.59	0.48
1:A:388:LEU:HD21	1:B:385:THR:CG2	2.44	0.48
1:H:158:TRP:CD1	1:H:258:PHE:CE2	3.02	0.48
1:C:266:ILE:HD13	1:C:276:ALA:HB3	1.96	0.48
1:D:104:ILE:C	1:D:104:ILE:HD12	2.34	0.48
1:A:335:GLN:OE1	1:A:335:GLN:N	2.46	0.48
1:A:382:ARG:HH11	1:A:382:ARG:CG	2.26	0.48
1:C:128:THR:HB	1:C:130:GLU:OE1	2.14	0.48
1:H:404:ALA:O	1:H:407:ALA:HB3	2.14	0.48
1:B:117:TYR:CE1	1:B:125:PRO:HG3	2.49	0.48
1:H:267:ASN:HB3	1:H:270:SER:HB2	1.96	0.48
1:F:158:TRP:CD1	1:F:258:PHE:CE2	3.02	0.48
1:H:192:LEU:HD23	1:H:357:VAL:HG13	1.95	0.48
1:A:158:TRP:N	1:A:159:PRO:HD2	2.29	0.48
1:B:348:ILE:N	1:B:348:ILE:HD12	2.30	0.47
1:B:158:TRP:CD1	1:B:258:PHE:CE2	3.02	0.47
1:H:293:VAL:CG1	1:H:299:LEU:HD21	2.44	0.47
1:F:384:VAL:CG2	1:H:387:LEU:HD23	2.44	0.47
1:C:393:THR:HG22	1:C:397:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:399:PHE:CE2	1:G:399:PHE:CZ	3.02	0.47
1:G:390:GLN:HA	1:G:390:GLN:HE21	1.79	0.47
1:B:80:THR:O	1:B:277:LYS:NZ	2.47	0.47
1:D:401:ASP:O	1:D:405:GLN:HG2	2.14	0.47
1:B:341:TYR:CE2	1:D:406:ALA:HA	2.50	0.47
1:E:158:TRP:CE2	1:E:162:ALA:HB2	2.50	0.47
1:C:47:PHE:HA	1:C:50:VAL:HG22	1.97	0.47
1:B:455:LEU:HB3	1:C:456:ARG:NH1	2.29	0.47
1:E:385:THR:OG1	1:F:389:GLN:NE2	2.48	0.47
1:C:124:ASN:N	1:C:124:ASN:HD22	2.13	0.47
1:C:369:THR:HG23	1:C:373:ASP:OD1	2.15	0.47
1:G:59:ILE:HD13	1:G:264:ALA:HB1	1.96	0.47
1:C:420:LEU:HD11	1:C:424:LYS:HE3	1.95	0.47
1:B:152:GLN:O	1:B:348:ILE:HD11	2.15	0.47
1:A:158:TRP:CE2	1:A:162:ALA:HB2	2.50	0.47
1:D:454:ARG:O	1:D:455:LEU:C	2.53	0.47
1:H:113:LEU:HD11	1:H:156:PHE:HA	1.96	0.47
1:A:80:THR:O	1:A:277:LYS:NZ	2.48	0.47
1:H:386:HIS:O	1:H:390:GLN:HG2	2.15	0.47
1:B:231:ALA:O	1:B:235:ILE:HG13	2.15	0.47
1:H:79:ILE:HD12	1:H:106:TYR:CE1	2.50	0.47
1:F:440:THR:HG22	1:F:441:LEU:N	2.30	0.47
1:G:388:LEU:HD23	1:H:385:THR:CG2	2.44	0.46
1:E:382:ARG:HH11	1:E:382:ARG:CG	2.27	0.46
1:C:205:ASN:ND2	1:C:207:ASP:OD1	2.45	0.46
1:E:341:TYR:CE2	1:G:406:ALA:CA	2.98	0.46
1:B:158:TRP:CE2	1:B:162:ALA:HB2	2.50	0.46
1:H:154:PRO:HB3	1:H:343:VAL:HG12	1.97	0.46
1:G:64:HIS:CD2	1:G:261:VAL:H	2.33	0.46
1:E:80:THR:O	1:E:277:LYS:NZ	2.49	0.46
1:F:384:VAL:HG13	1:H:384:VAL:HG13	1.96	0.46
1:A:246:VAL:HG21	1:A:322:GLU:OE1	2.15	0.46
1:G:426:GLN:NE2	1:G:426:GLN:HA	2.29	0.46
1:C:109:ALA:O	1:C:261:VAL:HA	2.15	0.46
1:A:246:VAL:HG22	1:A:322:GLU:HG2	1.98	0.46
1:E:388:LEU:CD2	1:F:385:THR:CG2	2.94	0.46
1:G:314:ASP:HB3	1:G:317:ILE:HD12	1.98	0.46
1:F:387:LEU:HD22	1:H:341:TYR:CE2	2.51	0.46
1:F:80:THR:O	1:F:277:LYS:NZ	2.49	0.46
1:G:9:ILE:HG23	1:G:59:ILE:HG13	1.98	0.46
1:C:158:TRP:HB3	1:C:159:PRO:CD	2.46	0.46
1:H:336:MET:O	1:H:339:PHE:HB3	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:455:LEU:C	1:H:456:ARG:HG3	2.35	0.46
1:C:195:LEU:O	1:C:195:LEU:HD12	2.16	0.46
1:E:335:GLN:N	1:E:335:GLN:OE1	2.48	0.46
1:H:218:ASN:HD21	1:H:235:ILE:HG12	1.81	0.46
1:A:231:ALA:O	1:A:235:ILE:HG13	2.15	0.46
1:B:455:LEU:HB3	1:C:456:ARG:CZ	2.46	0.46
1:E:166:GLY:HA2	1:E:185:ASN:HD21	1.81	0.46
1:D:344:ARG:O	1:D:348:ILE:CD1	2.63	0.45
1:C:160:LEU:O	1:C:160:LEU:HD12	2.15	0.45
1:G:369:THR:O	1:G:370:ALA:HB2	2.15	0.45
1:C:59:ILE:HD11	1:C:61:PHE:CD1	2.52	0.45
1:H:415:ALA:O	1:H:418:ALA:HB3	2.16	0.45
1:H:344:ARG:O	1:H:348:ILE:HD12	2.15	0.45
1:A:158:TRP:CD1	1:A:258:PHE:CE2	3.04	0.45
1:A:166:GLY:HA2	1:A:185:ASN:HD21	1.81	0.45
1:H:217:PHE:HA	1:H:222:THR:HG22	1.98	0.45
1:H:371:ALA:O	1:H:372:ARG:HB2	2.15	0.45
1:H:376:ARG:HB3	1:H:376:ARG:HE	1.35	0.45
1:B:368:ILE:CG2	1:B:369:THR:HG23	2.46	0.45
1:A:244:VAL:HB	1:A:316:ARG:HG2	1.99	0.45
1:A:90:TYR:HA	1:A:91:PRO:HD2	1.79	0.45
1:F:166:GLY:HA2	1:F:185:ASN:HD21	1.81	0.45
1:D:371:ALA:C	1:D:376:ARG:NH2	2.60	0.45
1:A:158:TRP:HB3	1:A:159:PRO:HD3	1.98	0.45
1:F:59:ILE:CD1	1:F:280:LEU:HD11	2.46	0.45
1:H:445:LEU:HD23	1:H:446:GLN:N	2.31	0.45
1:E:246:VAL:HG21	1:E:322:GLU:OE1	2.17	0.45
1:G:59:ILE:HD12	1:G:60:ILE:N	2.32	0.45
1:C:118:ASN:OD1	1:C:118:ASN:C	2.55	0.45
1:G:393:THR:OG1	1:H:382:ARG:NH2	2.50	0.45
1:H:59:ILE:HD13	1:H:264:ALA:HB1	1.99	0.45
1:C:152:GLN:HE22	1:C:207:ASP:HA	1.82	0.45
1:E:450:ALA:CB	1:E:454:ARG:HH21	2.21	0.45
1:C:393:THR:HG23	1:D:382:ARG:NH2	2.32	0.45
1:G:345:THR:HG22	1:G:349:ASN:ND2	2.31	0.45
1:F:246:VAL:HG12	1:F:247:LEU:O	2.17	0.45
1:B:388:LEU:HD11	1:C:388:LEU:HD21	1.98	0.45
1:H:234:ASN:HA	1:H:234:ASN:HD22	1.61	0.45
1:A:402:VAL:HG13	1:D:402:VAL:CG1	2.43	0.44
1:H:382:ARG:CG	1:H:382:ARG:HH11	2.28	0.44
1:C:226:ILE:HD13	1:C:247:LEU:HD22	1.98	0.44
1:C:61:PHE:CE2	1:C:264:ALA:HB2	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:339:PHE:CZ	1:E:343:VAL:HG21	2.52	0.44
1:H:308:GLU:OE2	1:H:321:MET:HE2	2.17	0.44
1:E:64:HIS:CE1	1:E:330:MET:O	2.70	0.44
1:G:192:LEU:HD23	1:G:357:VAL:HG13	1.98	0.44
1:D:39:HIS:N	1:D:40:PRO:CD	2.80	0.44
1:D:445:LEU:C	1:D:445:LEU:CD2	2.78	0.44
1:F:158:TRP:HB3	1:F:159:PRO:HD3	1.98	0.44
1:C:291:GLU:O	1:C:295:LYS:HG3	2.17	0.44
1:H:152:GLN:HE22	1:H:207:ASP:HA	1.83	0.44
1:B:117:TYR:CE1	1:B:243:GLY:HA3	2.52	0.44
1:E:158:TRP:HB3	1:E:159:PRO:HD3	1.99	0.44
1:F:195:LEU:O	1:F:195:LEU:HD12	2.16	0.44
1:E:410:ASN:HD22	1:F:337:SER:HB2	1.83	0.44
1:D:386:HIS:O	1:D:390:GLN:HG2	2.18	0.44
1:E:90:TYR:HA	1:E:91:PRO:HD2	1.80	0.44
1:E:158:TRP:CD1	1:E:258:PHE:CE2	3.05	0.44
1:G:370:ALA:C	1:G:372:ARG:H	2.20	0.44
1:G:152:GLN:NE2	1:G:207:ASP:HA	2.33	0.44
1:C:158:TRP:CD1	1:C:258:PHE:CE2	3.06	0.44
1:A:438:ILE:CD1	1:D:434:LEU:HD22	2.48	0.44
1:D:456:ARG:HB3	1:D:456:ARG:HH11	0.45	0.44
1:F:356:THR:OG1	1:F:359:GLU:HG2	2.18	0.43
1:G:64:HIS:ND1	1:G:96:ALA:HB1	2.33	0.43
1:H:172:GLU:HG3	1:H:175:LYS:O	2.18	0.43
1:B:202:LYS:HE3	2:B:476:HOH:O	2.17	0.43
1:D:173:ASN:HD21	1:H:356:THR:HG21	1.83	0.43
1:A:388:LEU:CD2	1:B:385:THR:HG21	2.48	0.43
1:F:246:VAL:HG22	1:F:322:GLU:HG2	2.00	0.43
1:G:43:LEU:HA	1:G:46:LYS:HB2	1.98	0.43
1:F:244:VAL:HB	1:F:316:ARG:HG2	2.00	0.43
1:A:246:VAL:HG12	1:A:247:LEU:O	2.18	0.43
1:H:372:ARG:O	1:H:373:ASP:C	2.56	0.43
1:E:158:TRP:N	1:E:159:PRO:HD2	2.34	0.43
1:F:117:TYR:CE1	1:F:243:GLY:HA3	2.53	0.43
1:D:154:PRO:HA	1:D:157:THR:OG1	2.19	0.43
1:F:64:HIS:CE1	1:F:330:MET:O	2.72	0.43
1:E:455:LEU:CD1	1:H:456:ARG:HH12	2.30	0.43
1:D:434:LEU:HD23	1:D:434:LEU:HA	1.82	0.43
1:G:255:SER:O	1:G:257:PRO:HD3	2.19	0.43
1:C:382:ARG:HH11	1:C:382:ARG:CG	2.25	0.43
1:E:246:VAL:HG22	1:E:322:GLU:HG2	2.01	0.43
1:B:348:ILE:HD12	1:B:348:ILE:H	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:9:ILE:HG12	1:C:59:ILE:HG13	2.01	0.43
1:B:117:TYR:CE2	1:B:125:PRO:HD3	2.54	0.43
1:D:115:LEU:HD23	1:D:245:THR:CG2	2.48	0.43
1:H:390:GLN:HE21	1:H:390:GLN:HA	1.83	0.43
1:A:307:TYR:CE2	1:A:311:LEU:HD11	2.53	0.43
1:C:113:LEU:HD11	1:C:156:PHE:HA	2.01	0.43
1:D:151:LEU:HD12	1:D:205:ASN:O	2.19	0.43
1:C:209:ASP:C	1:C:209:ASP:OD1	2.56	0.43
1:F:60:ILE:HG23	1:F:60:ILE:O	2.19	0.43
1:F:388:LEU:HD12	1:H:384:VAL:CG1	2.49	0.43
1:G:370:ALA:C	1:G:372:ARG:N	2.72	0.43
1:H:272:ASN:HB3	1:H:275:LEU:HB2	2.00	0.43
1:A:450:ALA:CB	1:A:454:ARG:HH21	2.20	0.42
1:H:104:ILE:HD12	1:H:105:ALA:N	2.33	0.42
1:A:452:VAL:HG23	1:A:453:GLU:N	2.34	0.42
1:C:192:LEU:O	1:C:196:VAL:HG23	2.19	0.42
1:D:255:SER:O	1:D:257:PRO:HD3	2.19	0.42
1:G:68:GLY:HA3	1:G:332:ASN:O	2.19	0.42
1:B:246:VAL:HG21	1:B:322:GLU:OE1	2.20	0.42
1:C:43:LEU:HA	1:C:46:LYS:HB2	2.00	0.42
1:H:371:ALA:CB	1:H:376:ARG:CZ	2.97	0.42
1:G:59:ILE:HD11	1:G:61:PHE:CD1	2.54	0.42
1:A:199:ILE:HG21	1:A:206:ALA:HB2	2.02	0.42
1:H:424:LYS:O	1:H:428:GLN:HB3	2.19	0.42
1:E:455:LEU:CB	1:H:456:ARG:CZ	2.88	0.42
1:D:293:VAL:HG11	1:D:299:LEU:HD21	2.02	0.42
1:D:447:ASP:O	1:D:448:ALA:C	2.58	0.42
1:G:344:ARG:O	1:G:348:ILE:CD1	2.68	0.42
1:D:68:GLY:HA3	1:D:332:ASN:O	2.20	0.42
1:G:455:LEU:O	1:G:456:ARG:HG3	2.20	0.42
1:B:246:VAL:HG22	1:B:322:GLU:HG2	2.01	0.42
1:C:372:ARG:CG	1:C:372:ARG:HH11	2.33	0.42
1:H:293:VAL:HG12	1:H:299:LEU:HD21	2.01	0.42
1:H:117:TYR:CE1	1:H:125:PRO:HG3	2.55	0.42
1:C:110:VAL:O	1:C:301:ALA:HB3	2.19	0.42
1:F:246:VAL:HG21	1:F:322:GLU:OE1	2.20	0.42
1:D:158:TRP:HB3	1:D:159:PRO:HD3	2.02	0.42
1:F:402:VAL:CG1	1:G:402:VAL:CG1	2.93	0.42
1:A:341:TYR:HB3	1:C:405:GLN:NE2	2.28	0.42
1:E:440:THR:HG22	1:E:441:LEU:N	2.35	0.42
1:B:126:PRO:HD2	1:B:224:MET:SD	2.60	0.42
1:C:384:VAL:HG12	1:C:385:THR:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:158:TRP:O	1:H:159:PRO:C	2.58	0.41
1:C:158:TRP:HB3	1:C:159:PRO:HD3	2.00	0.41
1:F:195:LEU:HD12	1:F:195:LEU:C	2.40	0.41
1:H:455:LEU:C	1:H:456:ARG:CG	2.88	0.41
1:D:64:HIS:CE1	1:D:330:MET:O	2.71	0.41
1:C:454:ARG:O	1:C:455:LEU:C	2.54	0.41
1:F:450:ALA:CB	1:F:454:ARG:HH21	2.20	0.41
1:G:158:TRP:HB3	1:G:159:PRO:CD	2.50	0.41
1:H:183:VAL:O	1:H:183:VAL:HG12	2.21	0.41
1:A:158:TRP:O	1:A:161:ILE:N	2.53	0.41
1:B:450:ALA:CB	1:B:454:ARG:HH21	2.25	0.41
1:D:158:TRP:HB3	1:D:159:PRO:CD	2.50	0.41
1:C:10:TRP:CH2	1:C:50:VAL:HG21	2.55	0.41
1:C:192:LEU:HD12	1:C:192:LEU:O	2.19	0.41
1:D:8:VAL:HG13	1:D:57:PRO:HA	2.02	0.41
1:F:402:VAL:HG11	1:G:402:VAL:CG1	2.41	0.41
1:H:344:ARG:O	1:H:348:ILE:CD1	2.68	0.41
1:C:207:ASP:OD1	1:C:207:ASP:N	2.47	0.41
1:D:43:LEU:C	1:D:43:LEU:HD12	2.40	0.41
1:C:456:ARG:O	1:C:457:ARG:HB2	2.20	0.41
1:H:158:TRP:N	1:H:159:PRO:HD2	2.35	0.41
1:C:372:ARG:NH2	1:C:379:MSE:CE	2.84	0.41
1:E:341:TYR:CE2	1:G:406:ALA:HB2	2.54	0.41
1:F:158:TRP:N	1:F:159:PRO:HD2	2.35	0.41
1:G:47:PHE:HA	1:G:50:VAL:HG22	2.02	0.41
1:H:117:TYR:CZ	1:H:125:PRO:HG3	2.56	0.41
1:F:307:TYR:CE2	1:F:311:LEU:HD11	2.55	0.41
1:E:240:VAL:HG12	1:E:241:ASN:N	2.35	0.41
1:F:388:LEU:HD11	1:G:388:LEU:HD21	2.02	0.41
1:A:383:ASN:ND2	1:C:53:THR:CG2	2.84	0.41
1:C:43:LEU:HD12	1:C:44:GLU:N	2.36	0.41
1:B:64:HIS:CE1	1:B:330:MET:O	2.74	0.41
1:A:47:PHE:N	1:A:48:PRO:HD2	2.36	0.41
1:F:90:TYR:HA	1:F:91:PRO:HD2	1.78	0.41
1:E:388:LEU:HD23	1:F:385:THR:HG21	2.03	0.41
1:D:158:TRP:N	1:D:159:PRO:HD2	2.35	0.41
1:C:64:HIS:CD2	1:C:261:VAL:H	2.38	0.41
1:H:393:THR:HG22	1:H:397:LYS:HE2	2.03	0.41
1:B:114:SER:HA	1:B:323:ASN:ND2	2.35	0.41
1:D:93:THR:HG21	1:D:303:ALA:CB	2.51	0.41
1:H:375:LEU:O	1:H:378:VAL:HB	2.21	0.41
1:C:7:LEU:HB2	1:C:35:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:456:ARG:O	1:D:457:ARG:HG3	2.21	0.40
1:C:382:ARG:NH1	1:C:382:ARG:HG2	2.30	0.40
1:H:238:SER:OG	1:H:240:VAL:HG23	2.21	0.40
1:H:176:TYR:CZ	1:H:331:PRO:HA	2.56	0.40
1:F:455:LEU:HD12	1:G:456:ARG:NH1	2.34	0.40
1:H:158:TRP:HB3	1:H:159:PRO:HD3	2.03	0.40
1:H:93:THR:O	1:H:107:PRO:HG3	2.21	0.40
1:E:47:PHE:N	1:E:48:PRO:HD2	2.37	0.40
1:F:192:LEU:HD23	1:F:357:VAL:HG13	2.03	0.40
1:D:456:ARG:NH1	1:D:456:ARG:CA	2.82	0.40
1:H:455:LEU:O	1:H:456:ARG:HG3	2.21	0.40
1:C:152:GLN:NE2	1:C:207:ASP:HA	2.35	0.40
1:B:90:TYR:O	1:B:91:PRO:C	2.60	0.40
1:D:96:ALA:HB2	1:D:329:ILE:CG2	2.51	0.40
1:B:161:ILE:HA	1:B:191:GLY:HA3	2.03	0.40
1:C:106:TYR:CD2	1:C:280:LEU:HD13	2.56	0.40
1:G:455:LEU:C	1:G:456:ARG:HG3	2.41	0.40
1:G:455:LEU:O	1:G:456:ARG:CB	2.68	0.40
1:G:344:ARG:O	1:G:348:ILE:HD12	2.21	0.40
1:A:413:VAL:HG11	1:B:153:GLU:OE2	2.22	0.40
1:H:250:PHE:CE2	1:H:251:LYS:HD2	2.56	0.40
1:H:312:ALA:HB1	1:H:318:ALA:HB2	2.03	0.40
1:G:369:THR:HG23	1:G:369:THR:O	2.21	0.40
1:A:388:LEU:CD2	1:B:385:THR:CG2	3.00	0.40
1:F:382:ARG:NH1	1:F:382:ARG:CG	2.84	0.40
1:D:93:THR:HB	1:D:107:PRO:HB3	2.03	0.40
1:F:231:ALA:O	1:F:235:ILE:HG13	2.21	0.40
1:G:293:VAL:CG1	1:G:299:LEU:HD21	2.52	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	Distance(Å)	Clash(Å)
1:F:309:GLU:O	1:F:440:THR:OG1[1_454]	2.15	0.05

## 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	452/471 (96%)	419 (93%)	26 (6%)	7 (2%)	15	46
1	B	452/471 (96%)	425 (94%)	21 (5%)	6 (1%)	18	51
1	C	452/471 (96%)	414 (92%)	30 (7%)	8 (2%)	13	39
1	D	452/471 (96%)	417 (92%)	30 (7%)	5 (1%)	21	57
1	E	452/471 (96%)	424 (94%)	22 (5%)	6 (1%)	18	51
1	F	452/471 (96%)	422 (93%)	24 (5%)	6 (1%)	18	51
1	G	452/471 (96%)	427 (94%)	20 (4%)	5 (1%)	21	57
1	H	452/471 (96%)	413 (91%)	33 (7%)	6 (1%)	18	51
All	All	3616/3768 (96%)	3361 (93%)	206 (6%)	49 (1%)	16	49

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	ALA
1	A	424	LYS
1	B	424	LYS
1	C	367	ARG
1	C	370	ALA
1	C	456	ARG
1	D	371	ALA
1	D	456	ARG
1	E	424	LYS
1	F	424	LYS
1	G	370	ALA
1	G	456	ARG
1	H	371	ALA
1	H	456	ARG
1	C	454	ARG
1	C	455	LEU
1	D	455	LEU
1	F	371	ALA
1	G	455	LEU
1	H	178	ILE
1	H	455	LEU
1	A	42	LYS
1	A	165	GLY
1	B	165	GLY
1	C	178	ILE

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Mol	Chain	Res	Type
1	D	454	ARG
1	E	165	GLY
1	E	371	ALA
1	F	165	GLY
1	G	371	ALA
1	G	454	ARG
1	H	66	ARG
1	H	454	ARG
1	B	42	LYS
1	C	369	THR
1	C	373	ASP
1	B	334	PRO
1	D	168	ALA
1	E	42	LYS
1	E	334	PRO
1	F	42	LYS
1	F	334	PRO
1	A	334	PRO
1	B	74	GLY
1	A	81	PRO
1	E	81	PRO
1	A	74	GLY
1	B	81	PRO
1	F	81	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	A	362/376 (96%)	339 (94%)	23 (6%)	25	58
1	B	362/376 (96%)	339 (94%)	23 (6%)	25	58
1	C	362/376 (96%)	332 (92%)	30 (8%)	16	42
1	D	362/376 (96%)	330 (91%)	32 (9%)	14	38
1	E	362/376 (96%)	342 (94%)	20 (6%)	30	65
1	F	362/376 (96%)	342 (94%)	20 (6%)	30	65
1	G	362/376 (96%)	335 (92%)	27 (8%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	362/376 (96%)	335 (92%)	27 (8%)	19	47
All	All	2896/3008 (96%)	2694 (93%)	202 (7%)	21	52

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	34	LYS
1	A	42	LYS
1	A	43	LEU
1	A	55	ASP
1	A	59	ILE
1	A	102	LYS
1	A	142	LYS
1	A	172	GLU
1	A	218	ASN
1	A	341	TYR
1	A	368	ILE
1	A	372	ARG
1	A	376	ARG
1	A	382	ARG
1	A	388	LEU
1	A	390	GLN
1	A	426	GLN
1	A	435	GLU
1	A	439	THR
1	A	440	THR
1	A	449	SER
1	A	454	ARG
1	B	26	LYS
1	B	34	LYS
1	B	42	LYS
1	B	43	LEU
1	B	55	ASP
1	B	59	ILE
1	B	102	LYS
1	B	142	LYS
1	B	172	GLU
1	B	218	ASN
1	B	341	TYR
1	B	368	ILE
1	B	372	ARG

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Mol	Chain	Res	Type
1	B	376	ARG
1	B	382	ARG
1	B	388	LEU
1	B	390	GLN
1	B	426	GLN
1	B	435	GLU
1	B	439	THR
1	B	440	THR
1	B	449	SER
1	B	454	ARG
1	C	4	GLU
1	C	26	LYS
1	C	31	THR
1	C	34	LYS
1	C	42	LYS
1	C	59	ILE
1	C	65	ASP
1	C	87	ASP
1	C	172	GLU
1	C	175	LYS
1	C	184	ASP
1	C	218	ASN
1	C	237	THR
1	C	239	LYS
1	C	256	LYS
1	C	278	GLU
1	C	337	SER
1	C	345	THR
1	C	365	GLN
1	C	373	ASP
1	C	382	ARG
1	C	384	VAL
1	C	390	GLN
1	C	401	ASP
1	C	411	HIS
1	C	428	GLN
1	C	445	LEU
1	C	451	GLU
1	C	455	LEU
1	C	456	ARG
1	D	26	LYS
1	D	34	LYS

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Mol	Chain	Res	Type
1	D	42	LYS
1	D	59	ILE
1	D	65	ASP
1	D	133	PRO
1	D	145	SER
1	D	172	GLU
1	D	175	LYS
1	D	177	ASP
1	D	181	VAL
1	D	184	ASP
1	D	218	ASN
1	D	237	THR
1	D	238	SER
1	D	239	LYS
1	D	256	LYS
1	D	278	GLU
1	D	337	SER
1	D	365	GLN
1	D	382	ARG
1	D	384	VAL
1	D	389	GLN
1	D	390	GLN
1	D	411	HIS
1	D	417	MSE
1	D	428	GLN
1	D	445	LEU
1	D	446	GLN
1	D	451	GLU
1	D	455	LEU
1	D	456	ARG
1	E	26	LYS
1	E	34	LYS
1	E	42	LYS
1	E	43	LEU
1	E	55	ASP
1	E	59	ILE
1	E	102	LYS
1	E	142	LYS
1	E	172	GLU
1	E	218	ASN
1	E	341	TYR
1	E	376	ARG

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Mol	Chain	Res	Type
1	E	382	ARG
1	E	388	LEU
1	E	390	GLN
1	E	426	GLN
1	E	435	GLU
1	E	440	THR
1	E	449	SER
1	E	454	ARG
1	F	26	LYS
1	F	34	LYS
1	F	42	LYS
1	F	43	LEU
1	F	55	ASP
1	F	59	ILE
1	F	102	LYS
1	F	142	LYS
1	F	172	GLU
1	F	218	ASN
1	F	341	TYR
1	F	376	ARG
1	F	382	ARG
1	F	388	LEU
1	F	390	GLN
1	F	426	GLN
1	F	435	GLU
1	F	440	THR
1	F	449	SER
1	F	454	ARG
1	G	26	LYS
1	G	34	LYS
1	G	42	LYS
1	G	59	ILE
1	G	65	ASP
1	G	172	GLU
1	G	175	LYS
1	G	184	ASP
1	G	218	ASN
1	G	237	THR
1	G	239	LYS
1	G	256	LYS
1	G	278	GLU
1	G	337	SER

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Mol	Chain	Res	Type
1	G	365	GLN
1	G	369	THR
1	G	372	ARG
1	G	376	ARG
1	G	382	ARG
1	G	390	GLN
1	G	411	HIS
1	G	426	GLN
1	G	428	GLN
1	G	429	LYS
1	G	445	LEU
1	G	451	GLU
1	G	456	ARG
1	H	26	LYS
1	H	30	ASP
1	H	34	LYS
1	H	42	LYS
1	H	59	ILE
1	H	65	ASP
1	H	145	SER
1	H	172	GLU
1	H	175	LYS
1	H	184	ASP
1	H	237	THR
1	H	239	LYS
1	H	256	LYS
1	H	278	GLU
1	H	320	THR
1	H	337	SER
1	H	365	GLN
1	H	369	THR
1	H	376	ARG
1	H	382	ARG
1	H	390	GLN
1	H	411	HIS
1	H	428	GLN
1	H	445	LEU
1	H	451	GLU
1	H	455	LEU
1	H	456	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	86	GLN
1	A	218	ASN
1	A	383	ASN
1	A	390	GLN
1	A	411	HIS
1	B	49	GLN
1	B	64	HIS
1	B	86	GLN
1	B	173	ASN
1	B	218	ASN
1	B	389	GLN
1	B	390	GLN
1	C	64	HIS
1	C	72	GLN
1	C	86	GLN
1	C	124	ASN
1	C	152	GLN
1	C	218	ASN
1	C	234	ASN
1	C	390	GLN
1	C	405	GLN
1	D	64	HIS
1	D	72	GLN
1	D	152	GLN
1	D	173	ASN
1	D	218	ASN
1	D	234	ASN
1	D	389	GLN
1	D	390	GLN
1	D	405	GLN
1	D	446	GLN
1	E	49	GLN
1	E	64	HIS
1	E	86	GLN
1	E	218	ASN
1	E	390	GLN
1	F	49	GLN
1	F	64	HIS
1	F	86	GLN
1	F	218	ASN
1	F	386	HIS
1	F	389	GLN

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Mol	Chain	Res	Type
1	F	390	GLN
1	G	64	HIS
1	G	72	GLN
1	G	124	ASN
1	G	152	GLN
1	G	218	ASN
1	G	234	ASN
1	G	390	GLN
1	G	405	GLN
1	G	426	GLN
1	H	18	ASN
1	H	64	HIS
1	H	86	GLN
1	H	124	ASN
1	H	152	GLN
1	H	218	ASN
1	H	234	ASN
1	H	390	GLN
1	H	428	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	454/471 (96%)	0.47	14 (3%) 47 47	2, 25, 60, 86	0
1	B	454/471 (96%)	0.47	18 (3%) 36 37	2, 25, 60, 85	0
1	C	454/471 (96%)	0.57	37 (8%) 12 10	2, 38, 61, 80	0
1	D	454/471 (96%)	0.82	63 (13%) 4 3	2, 38, 62, 81	0
1	E	454/471 (96%)	0.53	29 (6%) 19 17	2, 25, 60, 85	0
1	F	454/471 (96%)	0.53	33 (7%) 15 13	2, 25, 60, 85	0
1	G	454/471 (96%)	1.85	173 (38%) 1 0	2, 37, 60, 79	0
1	H	454/471 (96%)	0.43	24 (5%) 25 26	2, 33, 59, 83	0
All	All	3632/3768 (96%)	0.71	391 (10%) 6 5	2, 31, 60, 86	0

All (391) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	52	ALA	15.2
1	G	53	THR	14.9
1	G	266	ILE	14.3
1	G	265	GLY	12.5
1	E	457	ARG	10.9
1	C	370	ALA	9.7
1	G	330	MET	9.6
1	E	5	GLY	8.7
1	A	53	THR	8.1
1	G	289	GLY	7.8
1	G	264	ALA	7.6
1	G	135	LEU	7.2
1	G	4	GLU	7.1
1	C	53	THR	6.9
1	G	6	LYS	6.7
1	G	299	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
1	G	33	ILE	6.5
1	D	352	SER	6.4
1	G	9	ILE	6.4
1	F	285	LEU	6.4
1	F	5	GLY	6.3
1	G	156	PHE	6.3
1	D	32	GLY	6.3
1	G	134	ALA	6.2
1	A	6	LYS	6.2
1	D	135	LEU	6.1
1	E	6	LYS	6.1
1	G	7	LEU	6.0
1	D	56	GLY	5.9
1	C	52	ALA	5.9
1	G	357	VAL	5.9
1	A	52	ALA	5.8
1	G	32	GLY	5.8
1	E	7	LEU	5.7
1	G	110	VAL	5.7
1	G	169	PHE	5.7
1	G	31	THR	5.6
1	F	274	GLU	5.6
1	G	343	VAL	5.6
1	G	339	PHE	5.6
1	G	198	LEU	5.5
1	E	4	GLU	5.5
1	G	201	ASN	5.5
1	G	106	TYR	5.3
1	G	248	PRO	5.3
1	D	357	VAL	5.2
1	G	190	ALA	5.2
1	G	20	LEU	5.2
1	F	54	GLY	5.1
1	E	283	TYR	5.1
1	F	52	ALA	5.0
1	G	157	THR	5.0
1	G	350	ALA	5.0
1	G	276	ALA	5.0
1	G	228	GLY	5.0
1	G	178	ILE	5.0
1	E	52	ALA	4.9
1	G	176	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	151	LEU	4.8
1	G	30	ASP	4.8
1	D	454	ARG	4.8
1	G	457	ARG	4.8
1	G	108	ILE	4.8
1	G	59	ILE	4.8
1	G	456	ARG	4.7
1	G	365	GLN	4.7
1	B	53	THR	4.7
1	G	347	VAL	4.7
1	G	262	LEU	4.7
1	C	59	ILE	4.7
1	H	4	GLU	4.6
1	G	293	VAL	4.6
1	G	237	THR	4.5
1	G	273	LYS	4.4
1	G	28	GLU	4.4
1	D	274	GLU	4.4
1	B	5	GLY	4.4
1	G	77	ALA	4.4
1	G	263	SER	4.4
1	B	457	ARG	4.4
1	G	260	GLY	4.3
1	D	195	LEU	4.2
1	G	5	GLY	4.2
1	F	53	THR	4.2
1	G	146	ALA	4.2
1	G	252	GLY	4.2
1	A	172	GLU	4.2
1	D	106	TYR	4.2
1	D	347	VAL	4.1
1	G	304	LEU	4.1
1	G	360	ALA	4.1
1	E	37	VAL	4.1
1	G	300	GLY	4.1
1	C	371	ALA	4.1
1	C	60	ILE	4.1
1	D	4	GLU	4.1
1	G	253	GLN	4.1
1	D	200	LYS	4.1
1	F	41	ASP	4.0
1	C	284	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	183	VAL	4.0
1	C	341	TYR	3.9
1	G	36	THR	3.9
1	D	5	GLY	3.9
1	C	21	ALA	3.9
1	E	8	VAL	3.9
1	G	197	ASP	3.9
1	G	274	GLU	3.9
1	G	92	PHE	3.9
1	G	34	LYS	3.9
1	G	320	THR	3.8
1	F	37	VAL	3.8
1	F	379	MSE	3.8
1	G	230	TRP	3.8
1	B	6	LYS	3.8
1	G	351	ALA	3.8
1	G	141	ALA	3.8
1	D	7	LEU	3.7
1	F	266	ILE	3.7
1	G	84	ALA	3.7
1	B	274	GLU	3.7
1	E	172	GLU	3.7
1	E	275	LEU	3.7
1	G	206	ALA	3.7
1	D	49	GLN	3.7
1	C	330	MET	3.7
1	G	227	ASN	3.7
1	D	351	ALA	3.6
1	D	55	ASP	3.6
1	G	168	ALA	3.6
1	G	58	ASP	3.6
1	D	354	ARG	3.6
1	G	219	LYS	3.6
1	D	26	LYS	3.6
1	H	330	MET	3.6
1	G	195	LEU	3.6
1	E	285	LEU	3.6
1	G	287	ASP	3.5
1	D	456	ARG	3.5
1	D	35	VAL	3.5
1	D	30	ASP	3.5
1	D	280	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	272	ASN	3.5
1	G	35	VAL	3.5
1	D	181	VAL	3.5
1	G	37	VAL	3.5
1	D	29	LYS	3.4
1	D	57	PRO	3.4
1	G	112	ALA	3.4
1	E	58	ASP	3.4
1	D	132	ILE	3.4
1	F	390	GLN	3.4
1	G	341	TYR	3.4
1	F	4	GLU	3.4
1	D	453	GLU	3.4
1	G	258	PHE	3.4
1	D	141	ALA	3.4
1	C	213	ALA	3.4
1	G	328	GLU	3.3
1	F	76	LEU	3.3
1	G	54	GLY	3.3
1	G	361	LEU	3.3
1	G	279	PHE	3.3
1	G	145	SER	3.3
1	G	167	TYR	3.3
1	B	330	MET	3.3
1	G	367	ARG	3.3
1	D	361	LEU	3.3
1	D	208	THR	3.3
1	D	378	VAL	3.2
1	D	178	ILE	3.2
1	G	78	GLU	3.2
1	D	279	PHE	3.2
1	G	294	ASN	3.2
1	F	10	TRP	3.2
1	G	132	ILE	3.2
1	G	83	LYS	3.2
1	G	337	SER	3.2
1	G	148	MET	3.1
1	G	127	LYS	3.1
1	E	35	VAL	3.1
1	H	456	ARG	3.1
1	G	27	PHE	3.1
1	G	47	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	352	SER	3.1
1	G	278	GLU	3.1
1	G	275	LEU	3.1
1	D	349	ASN	3.1
1	A	42	LYS	3.1
1	F	99	TYR	3.1
1	G	331	PRO	3.1
1	G	224	MET	3.1
1	G	340	TRP	3.0
1	F	6	LYS	3.0
1	D	194	PHE	3.0
1	E	47	PHE	3.0
1	G	368	ILE	3.0
1	H	172	GLU	3.0
1	D	196	VAL	3.0
1	G	82	ASP	3.0
1	C	266	ILE	3.0
1	G	129	TRP	3.0
1	D	169	PHE	3.0
1	E	378	VAL	3.0
1	B	52	ALA	3.0
1	G	160	LEU	2.9
1	G	223	ALA	2.9
1	H	85	PHE	2.9
1	F	172	GLU	2.9
1	G	205	ASN	2.9
1	G	122	LEU	2.9
1	G	203	HIS	2.9
1	B	106	TYR	2.9
1	C	367	ARG	2.9
1	D	273	LYS	2.9
1	F	456	ARG	2.9
1	G	292	ALA	2.9
1	G	307	TYR	2.9
1	G	164	ASP	2.9
1	G	186	ALA	2.8
1	G	104	ILE	2.8
1	G	121	LEU	2.8
1	C	220	GLY	2.8
1	E	284	LEU	2.8
1	G	295	LYS	2.8
1	D	77	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	31	THR	2.8
1	G	113	LEU	2.8
1	C	456	ARG	2.8
1	E	456	ARG	2.8
1	C	261	VAL	2.8
1	D	33	ILE	2.8
1	G	392	LEU	2.8
1	G	207	ASP	2.7
1	G	324	ALA	2.7
1	C	277	LYS	2.7
1	A	5	GLY	2.7
1	H	274	GLU	2.7
1	D	75	LEU	2.7
1	G	101	GLY	2.7
1	H	283	TYR	2.7
1	F	8	VAL	2.7
1	G	158	TRP	2.7
1	C	457	ARG	2.7
1	G	329	ILE	2.7
1	G	269	ALA	2.7
1	G	454	ARG	2.7
1	F	7	LEU	2.7
1	G	280	LEU	2.7
1	D	276	ALA	2.7
1	G	11	ILE	2.6
1	A	173	ASN	2.6
1	G	103	LEU	2.6
1	G	93	THR	2.6
1	C	161	ILE	2.6
1	F	38	GLU	2.6
1	H	352	SER	2.6
1	G	55	ASP	2.6
1	B	76	LEU	2.6
1	C	6	LYS	2.6
1	G	302	VAL	2.6
1	C	454	ARG	2.6
1	E	36	THR	2.6
1	D	330	MET	2.6
1	A	54	GLY	2.6
1	G	147	LEU	2.5
1	B	102	LYS	2.5
1	G	256	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	200	LYS	2.5
1	G	353	GLY	2.5
1	A	275	LEU	2.5
1	G	232	TRP	2.5
1	G	49	GLN	2.5
1	F	103	LEU	2.5
1	D	10	TRP	2.5
1	D	137	LYS	2.5
1	G	283	TYR	2.5
1	D	173	ASN	2.5
1	A	46	LYS	2.5
1	G	152	GLN	2.5
1	C	4	GLU	2.5
1	G	149	PHE	2.4
1	G	254	PRO	2.4
1	G	131	GLU	2.4
1	G	226	ILE	2.4
1	C	369	THR	2.4
1	B	456	ARG	2.4
1	G	171	TYR	2.4
1	D	28	GLU	2.4
1	G	159	PRO	2.4
1	B	455	LEU	2.4
1	E	103	LEU	2.4
1	G	75	LEU	2.4
1	G	259	VAL	2.4
1	F	47	PHE	2.4
1	D	363	ASP	2.4
1	H	173	ASN	2.4
1	G	137	LYS	2.4
1	E	66	ARG	2.4
1	C	167	TYR	2.3
1	B	403	GLU	2.3
1	C	26	LYS	2.3
1	B	33	ILE	2.3
1	C	235	ILE	2.3
1	D	80	THR	2.3
1	G	51	ALA	2.3
1	F	246	VAL	2.3
1	H	8	VAL	2.3
1	C	285	LEU	2.3
1	H	280	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	348	ILE	2.3
1	H	49	GLN	2.3
1	G	346	ALA	2.3
1	G	73	SER	2.3
1	F	231	ALA	2.3
1	D	9	ILE	2.3
1	A	456	ARG	2.3
1	D	161	ILE	2.2
1	D	275	LEU	2.2
1	G	107	PRO	2.2
1	G	61	PHE	2.2
1	G	140	LYS	2.2
1	G	282	ASN	2.2
1	A	378	VAL	2.2
1	F	35	VAL	2.2
1	D	167	TYR	2.2
1	B	388	LEU	2.2
1	D	6	LYS	2.2
1	G	229	PRO	2.2
1	H	91	PRO	2.2
1	A	284	LEU	2.2
1	E	20	LEU	2.2
1	H	30	ASP	2.2
1	E	11	ILE	2.2
1	G	220	GLY	2.2
1	B	273	LYS	2.2
1	C	25	LYS	2.2
1	E	279	PHE	2.2
1	A	330	MET	2.2
1	G	344	ARG	2.2
1	C	76	LEU	2.2
1	D	76	LEU	2.2
1	E	388	LEU	2.2
1	E	74	GLY	2.2
1	C	335	GLN	2.1
1	H	278	GLU	2.1
1	G	284	LEU	2.1
1	E	175	LYS	2.1
1	C	169	PHE	2.1
1	D	206	ALA	2.1
1	H	35	VAL	2.1
1	D	302	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	261	VAL	2.1
1	G	41	ASP	2.1
1	B	104	ILE	2.1
1	G	79	ILE	2.1
1	H	454	ARG	2.1
1	C	152	GLN	2.1
1	C	390	GLN	2.1
1	D	356	THR	2.1
1	G	115	LEU	2.1
1	F	17	TYR	2.1
1	H	432	GLU	2.1
1	E	75	LEU	2.1
1	C	78	GLU	2.1
1	H	106	TYR	2.1
1	G	231	ALA	2.1
1	D	152	GLN	2.1
1	H	282	ASN	2.1
1	D	133	PRO	2.1
1	F	59	ILE	2.1
1	D	151	LEU	2.1
1	C	31	THR	2.0
1	C	276	ALA	2.0
1	G	85	PHE	2.0
1	G	45	GLU	2.0
1	G	8	VAL	2.0
1	G	72	GLN	2.0
1	G	362	LYS	2.0
1	H	11	ILE	2.0
1	H	457	ARG	2.0
1	C	165	GLY	2.0
1	B	280	LEU	2.0
1	F	20	LEU	2.0
1	F	265	GLY	2.0
1	H	5	GLY	2.0
1	F	40	PRO	2.0
1	H	206	ALA	2.0
1	F	90	TYR	2.0
1	E	280	LEU	2.0
1	G	290	LEU	2.0



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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.