



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:04 PM GMT

PDB ID : 4GZA  
Title : Complex of mouse Plexin A2 - Semaphorin 3A - Neuropilin-1  
Authors : Janssen, B.J.C.; Malinauskas, T.; Siebold, C.; Jones, E.Y.  
Deposited on : 2012-09-06  
Resolution : 7.00 Å(reported)

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

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

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

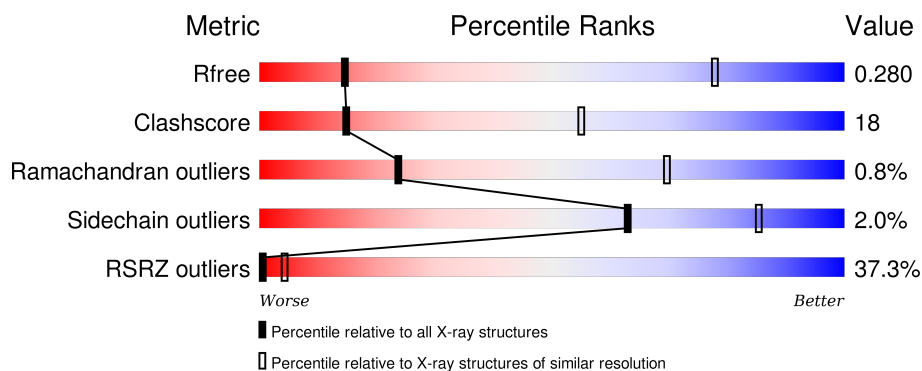
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 7.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	681	<div> <div>31%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	B	681	<div> <div>31%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	C	681	<div> <div>32%</div> <div>73%</div> <div>22%</div> <div>• •</div> </div>
1	D	681	<div> <div>35%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	E	681	<div> <div>46%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	681	<div><div><div>44%</div><div>73%</div><div>22%</div><div></div><div></div></div></div>
2	G	538	<div><div><div>33%</div><div>44%</div><div>41%</div><div>5%</div><div>10%</div></div></div>
3	H	577	<div><div><div>4%</div><div>17%</div><div></div><div>80%</div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35655 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 Plexin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	B	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	C	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	D	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	E	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	F	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	EXPRESSION TAG	UNP P70207
A	704	GLY	-	EXPRESSION TAG	UNP P70207
A	705	THR	-	EXPRESSION TAG	UNP P70207
A	706	LYS	-	EXPRESSION TAG	UNP P70207
A	707	HIS	-	EXPRESSION TAG	UNP P70207
A	708	HIS	-	EXPRESSION TAG	UNP P70207
A	709	HIS	-	EXPRESSION TAG	UNP P70207
A	710	HIS	-	EXPRESSION TAG	UNP P70207
A	711	HIS	-	EXPRESSION TAG	UNP P70207
A	712	HIS	-	EXPRESSION TAG	UNP P70207
B	32	GLU	-	EXPRESSION TAG	UNP P70207
B	704	GLY	-	EXPRESSION TAG	UNP P70207
B	705	THR	-	EXPRESSION TAG	UNP P70207
B	706	LYS	-	EXPRESSION TAG	UNP P70207
B	707	HIS	-	EXPRESSION TAG	UNP P70207
B	708	HIS	-	EXPRESSION TAG	UNP P70207
B	709	HIS	-	EXPRESSION TAG	UNP P70207

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Chain	Residue	Modelled	Actual	Comment	Reference
B	710	HIS	-	EXPRESSION TAG	UNP P70207
B	711	HIS	-	EXPRESSION TAG	UNP P70207
B	712	HIS	-	EXPRESSION TAG	UNP P70207
C	32	GLU	-	EXPRESSION TAG	UNP P70207
C	704	GLY	-	EXPRESSION TAG	UNP P70207
C	705	THR	-	EXPRESSION TAG	UNP P70207
C	706	LYS	-	EXPRESSION TAG	UNP P70207
C	707	HIS	-	EXPRESSION TAG	UNP P70207
C	708	HIS	-	EXPRESSION TAG	UNP P70207
C	709	HIS	-	EXPRESSION TAG	UNP P70207
C	710	HIS	-	EXPRESSION TAG	UNP P70207
C	711	HIS	-	EXPRESSION TAG	UNP P70207
C	712	HIS	-	EXPRESSION TAG	UNP P70207
D	32	GLU	-	EXPRESSION TAG	UNP P70207
D	704	GLY	-	EXPRESSION TAG	UNP P70207
D	705	THR	-	EXPRESSION TAG	UNP P70207
D	706	LYS	-	EXPRESSION TAG	UNP P70207
D	707	HIS	-	EXPRESSION TAG	UNP P70207
D	708	HIS	-	EXPRESSION TAG	UNP P70207
D	709	HIS	-	EXPRESSION TAG	UNP P70207
D	710	HIS	-	EXPRESSION TAG	UNP P70207
D	711	HIS	-	EXPRESSION TAG	UNP P70207
D	712	HIS	-	EXPRESSION TAG	UNP P70207
E	32	GLU	-	EXPRESSION TAG	UNP P70207
E	704	GLY	-	EXPRESSION TAG	UNP P70207
E	705	THR	-	EXPRESSION TAG	UNP P70207
E	706	LYS	-	EXPRESSION TAG	UNP P70207
E	707	HIS	-	EXPRESSION TAG	UNP P70207
E	708	HIS	-	EXPRESSION TAG	UNP P70207
E	709	HIS	-	EXPRESSION TAG	UNP P70207
E	710	HIS	-	EXPRESSION TAG	UNP P70207
E	711	HIS	-	EXPRESSION TAG	UNP P70207
E	712	HIS	-	EXPRESSION TAG	UNP P70207
F	32	GLU	-	EXPRESSION TAG	UNP P70207
F	704	GLY	-	EXPRESSION TAG	UNP P70207
F	705	THR	-	EXPRESSION TAG	UNP P70207
F	706	LYS	-	EXPRESSION TAG	UNP P70207
F	707	HIS	-	EXPRESSION TAG	UNP P70207
F	708	HIS	-	EXPRESSION TAG	UNP P70207
F	709	HIS	-	EXPRESSION TAG	UNP P70207
F	710	HIS	-	EXPRESSION TAG	UNP P70207
F	711	HIS	-	EXPRESSION TAG	UNP P70207

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Chain	Residue	Modelled	Actual	Comment	Reference
F	712	HIS	-	EXPRESSION TAG	UNP P70207

- Molecule 2 is a protein called Semaphorin-3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	484	Total	C	N	O	S	0	0	0
			3882	2474	669	720	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	18	GLU	-	EXPRESSION TAG	UNP O08665
G	19	THR	-	EXPRESSION TAG	UNP O08665
G	20	GLY	-	EXPRESSION TAG	UNP O08665
G	475	VAL	ILE	SEE REMARK 999	UNP O08665

- Molecule 3 is a protein called Neuropilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	117	Total	C	N	O	S	0	0	0
			944	611	152	176	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	19	GLU	-	EXPRESSION TAG	UNP P97333
H	20	THR	-	EXPRESSION TAG	UNP P97333
H	21	GLY	-	EXPRESSION TAG	UNP P97333
H	587	ARG	-	EXPRESSION TAG	UNP P97333
H	588	THR	-	EXPRESSION TAG	UNP P97333
H	589	LYS	-	EXPRESSION TAG	UNP P97333
H	590	HIS	-	EXPRESSION TAG	UNP P97333
H	591	HIS	-	EXPRESSION TAG	UNP P97333
H	592	HIS	-	EXPRESSION TAG	UNP P97333
H	593	HIS	-	EXPRESSION TAG	UNP P97333
H	594	HIS	-	EXPRESSION TAG	UNP P97333
H	595	HIS	-	EXPRESSION TAG	UNP P97333

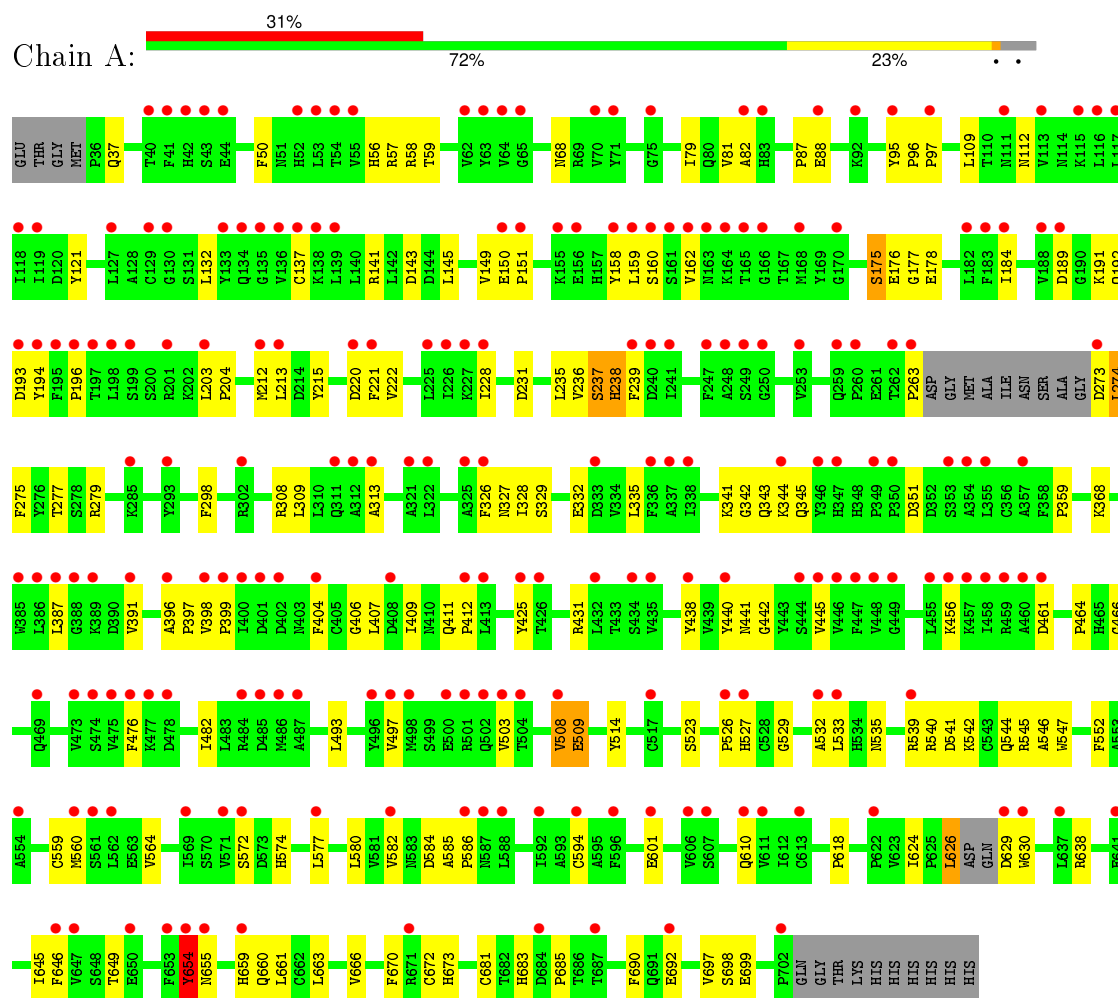
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Ca 1	0	0

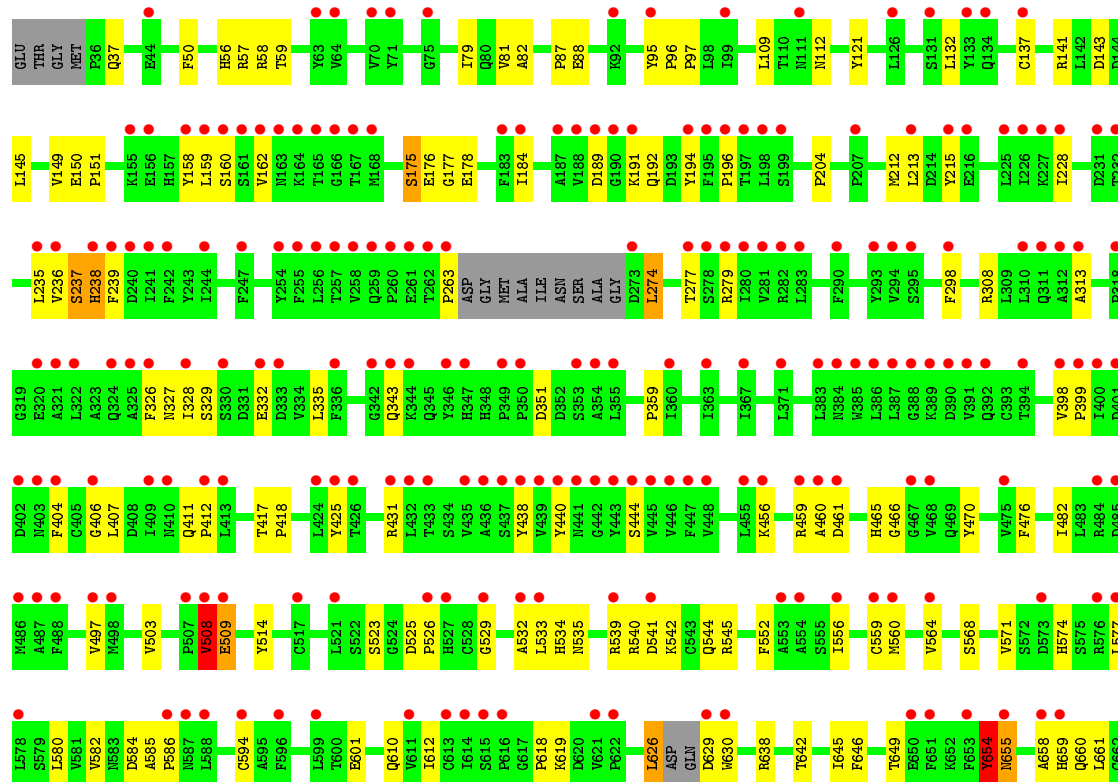
### 3 Residue-property plots

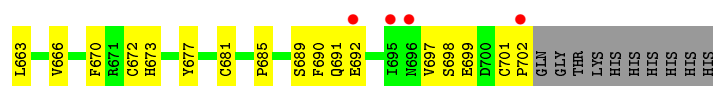
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Plexin-A2

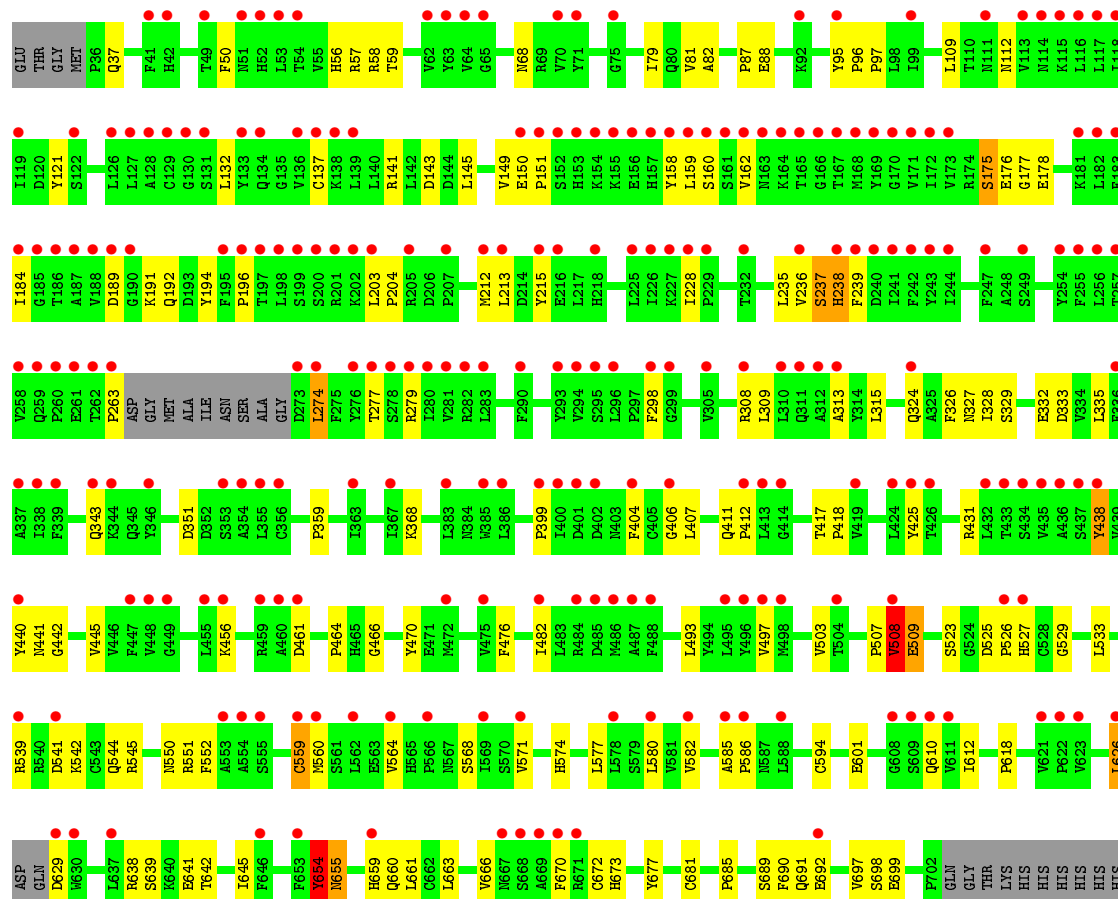
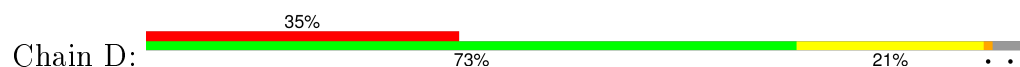




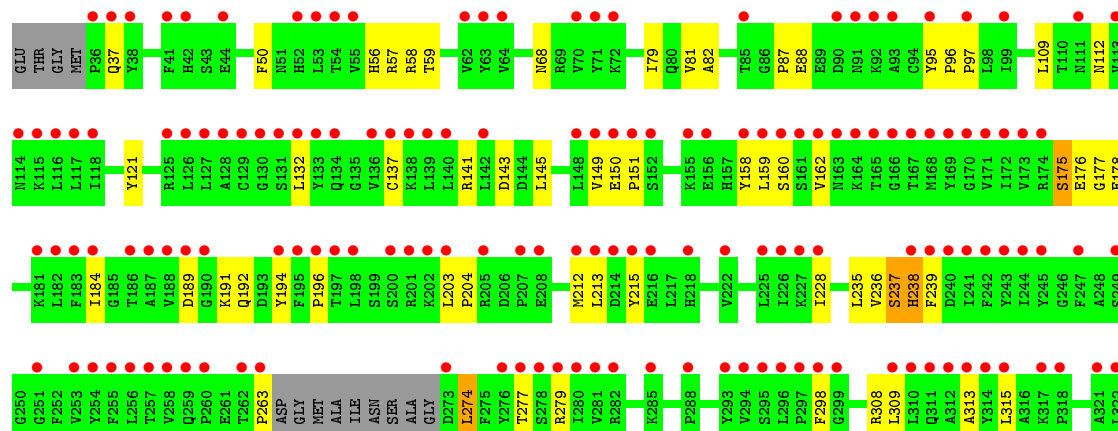


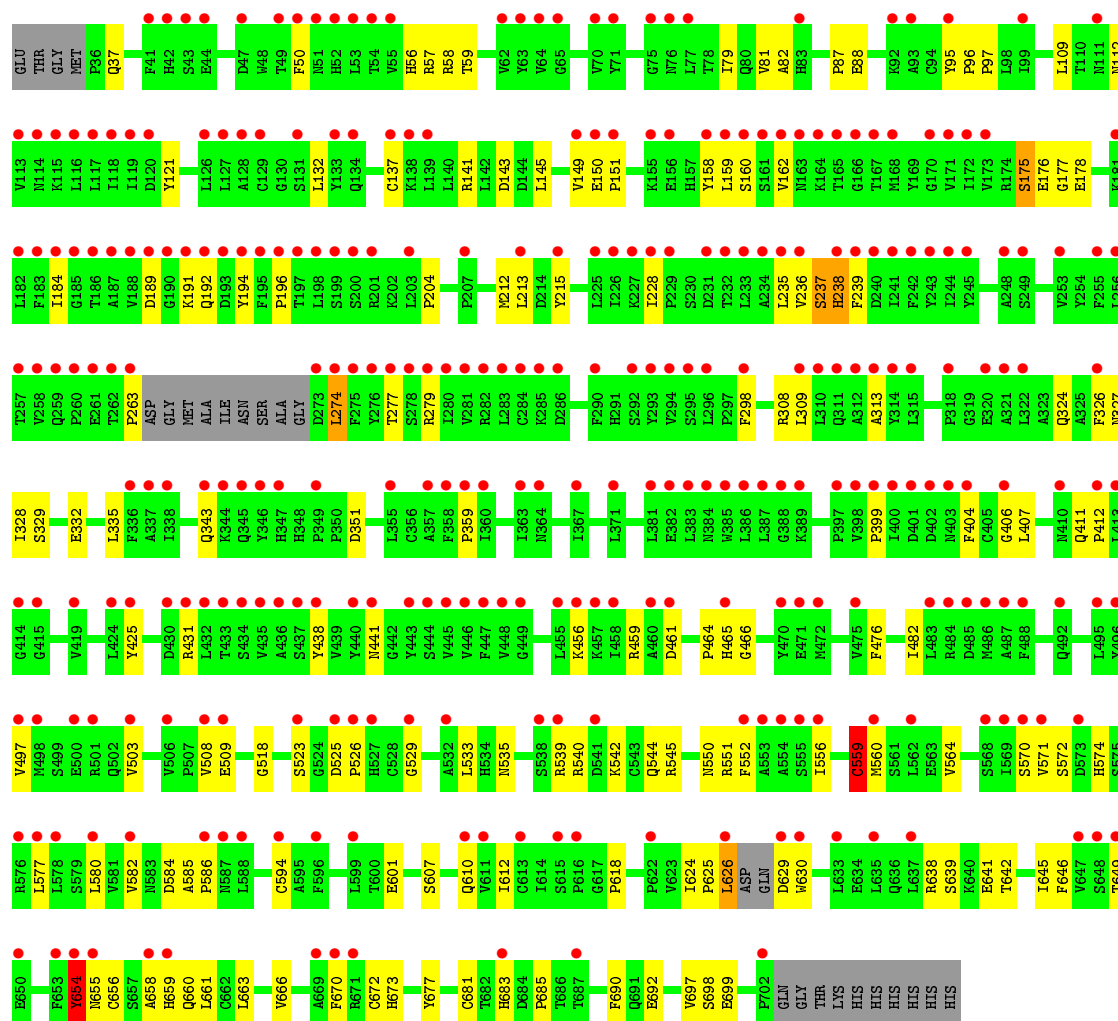


• Molecule 1: Plexin-A2

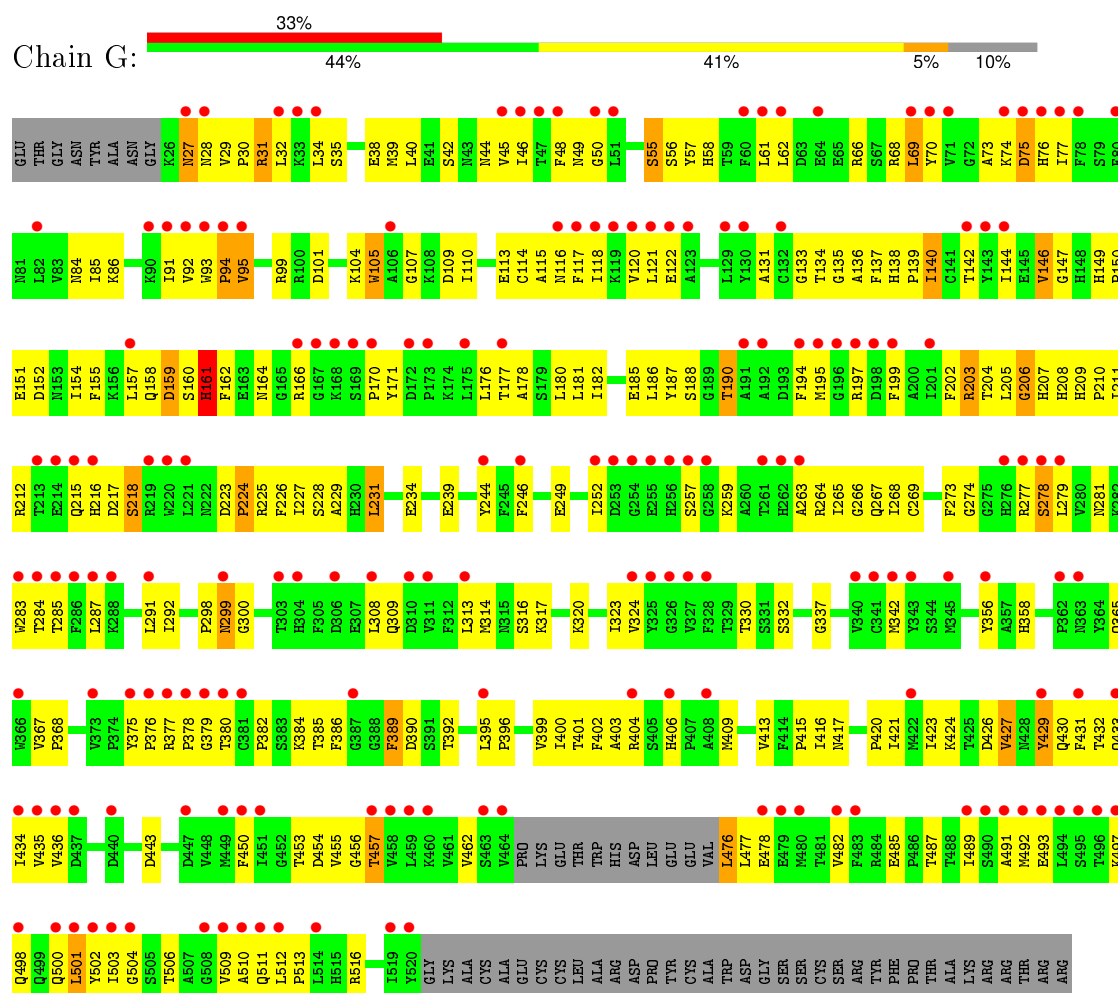


• Molecule 1: Plexin-A2

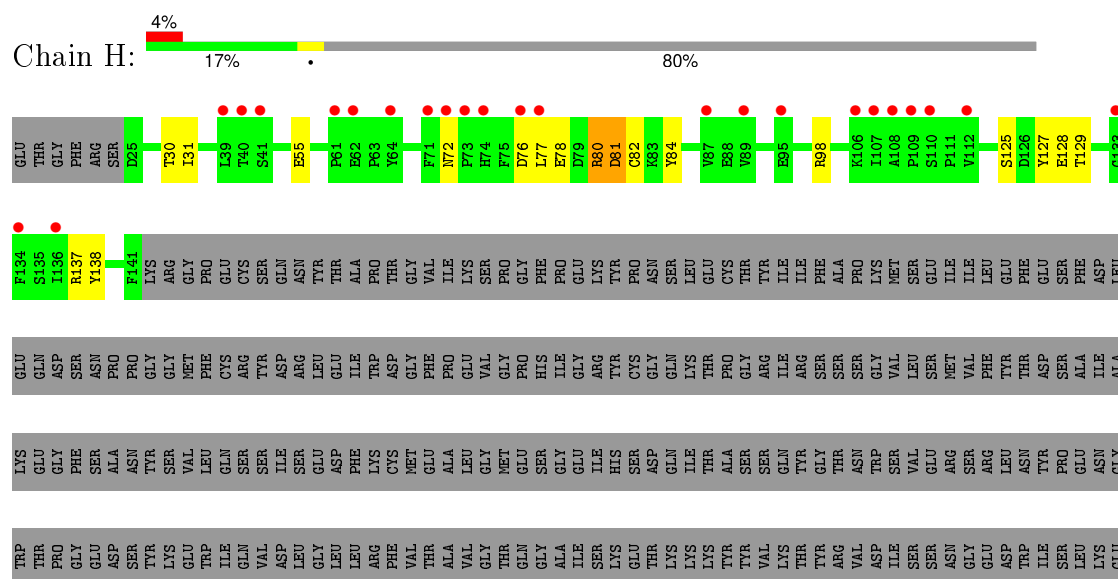




- Molecule 2: Semaphorin-3A



- Molecule 3: Neuropilin-1



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.63Å 293.60Å 252.18Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	125.51 – 7.00 125.51 – 7.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (125.51-7.00) 95.5 (125.51-7.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 6.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.285 , 0.285 0.286 , 0.280	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	293.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 423.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 20187 reflections	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	35655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	323.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.46	2/5260 (0.0%)	0.48	2/7138 (0.0%)
1	B	0.30	1/5260 (0.0%)	0.53	4/7138 (0.1%)
1	C	0.42	2/5260 (0.0%)	0.72	3/7138 (0.0%)
1	D	0.46	3/5261 (0.1%)	0.69	5/7141 (0.1%)
1	E	0.30	1/5261 (0.0%)	0.72	7/7141 (0.1%)
1	F	0.35	1/5261 (0.0%)	0.54	8/7141 (0.1%)
2	G	0.53	0/3988	0.72	0/5411
3	H	0.52	0/977	0.64	0/1325
All	All	0.41	10/36528 (0.0%)	0.63	29/49573 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	2
2	G	0	2
3	H	0	1
All	All	0	12

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	508	VAL	C-N	24.79	1.91	1.34
1	C	508	VAL	C-N	-21.01	0.85	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	559	CYS	C-N	19.66	1.79	1.34
1	F	508	VAL	C-N	12.94	1.63	1.34
1	D	654	TYR	C-N	-12.42	1.05	1.34
1	D	508	VAL	C-N	-10.42	1.10	1.34
1	A	654	TYR	C-N	8.14	1.52	1.34
1	E	559	CYS	C-N	-6.54	1.19	1.34
1	B	508	VAL	C-N	5.88	1.47	1.34
1	C	654	TYR	C-N	-5.74	1.20	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	654	TYR	O-C-N	-44.56	51.41	122.70
1	D	654	TYR	O-C-N	-40.97	57.14	122.70
1	E	654	TYR	O-C-N	-31.49	72.32	122.70
1	E	654	TYR	CA-C-N	21.86	165.30	117.20
1	E	654	TYR	C-N-CA	20.96	174.09	121.70
1	B	654	TYR	O-C-N	-12.84	102.16	122.70
1	C	508	VAL	O-C-N	-12.35	102.95	122.70
1	B	654	TYR	C-N-CA	12.17	152.12	121.70
1	B	508	VAL	O-C-N	-11.70	103.98	122.70
1	F	559	CYS	CA-C-N	-11.55	91.79	117.20
1	C	654	TYR	CA-C-N	11.43	142.34	117.20
1	F	654	TYR	CA-C-N	-11.23	92.50	117.20
1	E	559	CYS	O-C-N	10.82	140.01	122.70
1	A	654	TYR	O-C-N	-10.58	105.77	122.70
1	D	559	CYS	O-C-N	-10.16	106.45	122.70
1	F	559	CYS	C-N-CA	-9.56	97.81	121.70
1	F	508	VAL	O-C-N	-9.00	108.30	122.70
1	B	654	TYR	CA-C-N	8.76	136.47	117.20
1	E	559	CYS	CA-C-N	-8.66	98.15	117.20
1	D	508	VAL	CA-C-N	-8.39	98.75	117.20
1	F	654	TYR	C-N-CA	-8.34	100.86	121.70
1	D	508	VAL	C-N-CA	-8.31	100.92	121.70
1	E	559	CYS	C-N-CA	-8.24	101.09	121.70
1	F	559	CYS	O-C-N	-7.73	110.34	122.70
1	D	654	TYR	CA-C-N	7.47	133.63	117.20
1	F	508	VAL	C-N-CA	7.23	139.78	121.70
1	F	508	VAL	CA-C-N	5.97	130.34	117.20
1	A	508	VAL	O-C-N	-5.91	113.25	122.70
1	E	508	VAL	O-C-N	5.61	131.68	122.70



There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	654	TYR	Mainchain
1	B	508	VAL	Mainchain
1	C	508	VAL	Mainchain
1	C	654	TYR	Mainchain
1	D	508	VAL	Mainchain
1	D	654	TYR	Mainchain
1	E	654	TYR	Mainchain
1	F	559	CYS	Mainchain
1	F	654	TYR	Mainchain
2	G	429	TYR	Sidechain
2	G	57	TYR	Sidechain
3	H	80	ARG	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5138	0	4989	288	34
1	B	5138	0	4991	179	18
1	C	5138	0	4990	229	0
1	D	5138	0	4989	188	0
1	E	5138	0	4993	158	29
1	F	5138	0	4995	174	23
2	G	3882	0	3747	291	11
3	H	944	0	875	44	5
4	H	1	0	0	0	0
All	All	35655	0	34569	1242	63

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 18.

All (1242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LYS:CD	3:H:80:ARG:HH11	1.00	1.58
1:A:344:LYS:HD3	3:H:80:ARG:CD	1.23	1.57
1:A:222:VAL:CG2	2:G:166:ARG:HH12	1.17	1.54
1:D:577:LEU:HD11	1:F:607:SER:CB	1.44	1.47
1:E:324:GLN:NE2	1:F:518:GLY:HA3	1.23	1.47
1:A:221:PHE:HZ	2:G:202:PHE:CE2	1.32	1.45
1:A:368:LYS:NZ	1:B:630:TRP:HZ2	1.09	1.44
1:E:324:GLN:NE2	1:F:518:GLY:CA	1.80	1.43
1:E:324:GLN:HE22	1:F:518:GLY:CA	1.30	1.43
1:A:546:ALA:HB1	1:C:690:PHE:CE2	1.52	1.42
1:A:409:ILE:HG23	2:G:194:PHE:CE2	1.53	1.41
1:A:409:ILE:CG2	2:G:194:PHE:HE2	1.31	1.41
1:A:344:LYS:HD2	3:H:80:ARG:NH1	1.32	1.40
1:A:96:PRO:HD3	2:G:277:ARG:NE	1.10	1.40
1:C:568:SER:OG	1:C:670:PHE:HE1	1.06	1.37
1:A:221:PHE:CZ	2:G:202:PHE:CE2	2.14	1.34
1:A:344:LYS:CD	3:H:80:ARG:NH1	1.78	1.33
1:D:559:CYS:C	1:D:560:MET:N	1.79	1.33
1:A:442:GLY:N	1:C:691:GLN:HE22	1.22	1.33
1:A:440:TYR:CZ	1:C:692:GLU:OE2	1.80	1.32
1:E:518:GLY:HA3	1:F:324:GLN:NE2	1.44	1.32
1:C:465:HIS:HE1	1:D:523:SER:O	0.99	1.31
1:B:691:GLN:OE1	1:D:442:GLY:N	1.63	1.31
1:A:341:LYS:NZ	3:H:84:TYR:CE1	1.97	1.31
1:A:222:VAL:HG23	2:G:166:ARG:NH1	1.47	1.30
1:E:654:TYR:CD2	1:E:670:PHE:CD1	2.19	1.30
1:A:546:ALA:HB1	1:C:690:PHE:CZ	1.67	1.29
1:A:546:ALA:CB	1:C:690:PHE:HE2	1.46	1.29
1:C:626:LEU:CD1	1:D:399:PRO:HG3	1.62	1.28
1:E:465:HIS:HE1	1:F:523:SER:O	1.11	1.28
1:A:546:ALA:CB	1:C:690:PHE:CE2	2.15	1.27
1:A:409:ILE:CG2	2:G:194:PHE:CE2	2.10	1.27
1:E:465:HIS:CE1	1:F:523:SER:O	1.86	1.26
1:B:577:LEU:HD12	1:C:610:GLN:OE1	1.28	1.26
1:A:222:VAL:CG2	2:G:166:ARG:NH1	1.96	1.26
1:A:368:LYS:NZ	1:B:630:TRP:CZ2	2.02	1.26
1:A:96:PRO:CD	2:G:277:ARG:NE	1.98	1.26
1:A:221:PHE:CZ	2:G:202:PHE:CZ	2.23	1.25
1:E:654:TYR:HB3	1:E:670:PHE:CE2	1.72	1.25
1:A:508:VAL:C	1:A:509:GLU:N	1.91	1.24
1:D:577:LEU:CD1	1:F:607:SER:HB2	1.67	1.23
1:E:518:GLY:CA	1:F:324:GLN:NE2	2.02	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:HIS:CE1	1:D:523:SER:O	1.90	1.23
1:A:344:LYS:CD	3:H:80:ARG:CD	2.18	1.21
1:C:508:VAL:O	1:C:509:GLU:N	1.65	1.21
1:A:96:PRO:HD3	2:G:277:ARG:CZ	1.70	1.19
1:E:518:GLY:CA	1:F:324:GLN:HE22	1.55	1.19
1:C:508:VAL:C	1:C:509:GLU:CA	2.10	1.18
1:F:624:ILE:HG13	1:F:655:ASN:HB2	1.23	1.17
1:A:344:LYS:CD	3:H:80:ARG:HD3	1.75	1.16
1:A:626:LEU:CD1	1:B:399:PRO:HG3	1.74	1.16
1:D:612:ILE:CD1	1:F:612:ILE:HD12	1.76	1.15
1:E:523:SER:O	1:F:465:HIS:HE1	1.27	1.14
1:F:630:TRP:HB3	1:F:670:PHE:CE2	1.82	1.13
1:A:344:LYS:CG	3:H:80:ARG:NH1	2.09	1.13
1:E:654:TYR:CE2	1:E:670:PHE:CD1	2.36	1.12
1:F:629:ASP:OD1	1:F:659:HIS:NE2	1.82	1.12
1:B:610:GLN:OE1	1:C:577:LEU:HD12	1.48	1.12
1:F:533:LEU:HB3	1:F:642:THR:HG21	1.18	1.12
1:A:273:ASP:HB3	3:H:80:ARG:CZ	1.79	1.11
1:A:222:VAL:HG21	2:G:166:ARG:HH12	1.08	1.11
1:A:341:LYS:NZ	3:H:84:TYR:HE1	1.39	1.11
1:D:690:PHE:CG	1:E:540:ARG:HD2	1.74	1.11
1:A:442:GLY:N	1:C:691:GLN:NE2	1.99	1.10
1:A:96:PRO:HD3	2:G:277:ARG:CD	1.80	1.10
1:A:626:LEU:HD12	1:B:399:PRO:HG3	1.19	1.10
1:B:577:LEU:CD1	1:C:610:GLN:OE1	2.00	1.09
1:B:610:GLN:OE1	1:C:577:LEU:CG	2.00	1.09
1:A:552:PHE:CD2	1:C:690:PHE:CE1	2.41	1.08
1:C:508:VAL:CA	1:C:509:GLU:N	2.16	1.08
1:E:518:GLY:HA2	1:F:324:GLN:HE22	1.10	1.07
1:F:533:LEU:HB3	1:F:642:THR:CG2	1.85	1.06
1:C:630:TRP:HZ2	1:D:368:LYS:NZ	1.53	1.06
1:E:654:TYR:CD2	1:E:670:PHE:CE1	2.42	1.06
1:C:523:SER:HA	1:D:464:PRO:HD2	1.38	1.06
1:A:344:LYS:HD3	3:H:80:ARG:HD2	1.37	1.05
1:D:690:PHE:CG	1:E:540:ARG:CD	2.37	1.05
1:A:192:GLN:HE22	2:G:404:ARG:NH2	1.53	1.05
1:A:440:TYR:CE1	1:C:692:GLU:OE2	2.08	1.05
1:A:341:LYS:NZ	3:H:84:TYR:CD1	2.24	1.05
1:B:610:GLN:OE1	1:C:577:LEU:CD1	2.04	1.05
1:D:677:TYR:CZ	1:E:541:ASP:HB3	1.91	1.04
1:A:222:VAL:HG23	2:G:166:ARG:HH12	0.92	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:692:GLU:OE2	1:E:440:TYR:CD1	2.11	1.03
1:A:344:LYS:NZ	3:H:78:GLU:OE2	1.92	1.03
1:E:523:SER:O	1:F:465:HIS:CE1	2.11	1.03
1:C:654:TYR:CE2	1:C:670:PHE:CD1	2.47	1.03
1:E:654:TYR:CG	1:E:670:PHE:CG	2.46	1.02
1:C:626:LEU:HD11	1:D:399:PRO:HG3	1.41	1.01
1:A:630:TRP:HB3	1:A:670:PHE:CE2	1.94	1.01
1:B:610:GLN:OE1	1:C:577:LEU:HB2	1.60	1.01
1:B:691:GLN:OE1	1:D:441:ASN:C	1.96	1.01
1:E:654:TYR:CG	1:E:670:PHE:CD2	2.49	1.00
1:C:523:SER:HA	1:D:464:PRO:CD	1.91	1.00
1:E:654:TYR:CB	1:E:670:PHE:CE2	2.44	1.00
2:G:273:PHE:H	2:G:392:THR:HG21	1.24	1.00
1:E:324:GLN:HE22	1:F:518:GLY:HA2	0.86	1.00
2:G:287:LEU:HD22	2:G:409:MET:CE	1.91	1.00
1:A:464:PRO:HG3	1:B:514:TYR:HE1	1.23	0.99
1:F:624:ILE:HG13	1:F:655:ASN:CB	1.93	0.99
1:A:654:TYR:HB3	1:A:670:PHE:CD2	1.97	0.98
1:E:654:TYR:CD2	1:E:670:PHE:CG	2.52	0.97
1:B:610:GLN:OE1	1:C:577:LEU:CB	2.13	0.97
1:B:691:GLN:HB3	1:D:441:ASN:HA	1.43	0.97
1:A:344:LYS:HG2	3:H:80:ARG:NH1	1.80	0.96
1:E:654:TYR:CB	1:E:670:PHE:CD2	2.49	0.96
1:A:441:ASN:OD1	1:C:691:GLN:HB2	1.65	0.95
1:D:689:SER:HB3	1:E:540:ARG:HD3	1.47	0.95
1:A:344:LYS:HD3	3:H:80:ARG:HD3	0.98	0.95
1:A:546:ALA:HB3	1:C:690:PHE:HE2	1.31	0.95
1:B:610:GLN:CD	1:C:577:LEU:HD12	1.86	0.95
1:B:577:LEU:HD12	1:C:610:GLN:CD	1.86	0.95
1:A:654:TYR:CD2	1:A:670:PHE:CD1	2.56	0.94
1:F:630:TRP:CB	1:F:670:PHE:CE2	2.50	0.94
1:E:237:SER:HA	1:E:239:PHE:H	1.33	0.94
1:A:344:LYS:HD3	3:H:80:ARG:NE	1.82	0.94
1:A:237:SER:HA	1:A:239:PHE:H	1.33	0.94
1:E:324:GLN:OE1	1:F:556:ILE:HD11	1.67	0.93
1:A:221:PHE:CE1	2:G:202:PHE:HZ	1.87	0.93
1:A:344:LYS:CG	3:H:80:ARG:HH11	1.78	0.93
1:C:630:TRP:CZ2	1:D:368:LYS:NZ	2.38	0.92
1:A:654:TYR:CB	1:A:670:PHE:CD2	2.52	0.92
1:A:626:LEU:CD1	1:B:399:PRO:CG	2.48	0.92
1:F:630:TRP:HB3	1:F:670:PHE:HE2	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:TYR:CG	1:A:670:PHE:CB	2.53	0.92
1:A:442:GLY:H	1:C:691:GLN:HE22	1.15	0.92
1:A:654:TYR:CG	1:A:670:PHE:CG	2.57	0.92
1:A:221:PHE:CE1	2:G:202:PHE:CZ	2.58	0.91
1:B:610:GLN:CD	1:C:577:LEU:HB2	1.91	0.91
1:E:518:GLY:HA3	1:F:324:GLN:HE21	1.12	0.91
1:E:654:TYR:CE1	1:E:670:PHE:HB3	2.05	0.91
1:C:237:SER:HA	1:C:239:PHE:H	1.33	0.91
1:D:237:SER:HA	1:D:239:PHE:H	1.33	0.91
1:F:237:SER:HA	1:F:239:PHE:H	1.33	0.91
1:D:612:ILE:HD13	1:F:612:ILE:HD12	1.53	0.90
1:C:508:VAL:C	1:C:509:GLU:N	0.85	0.90
1:B:237:SER:HA	1:B:239:PHE:H	1.33	0.90
1:D:445:VAL:HG22	1:D:526:PRO:HG2	1.52	0.90
1:C:559:CYS:C	1:C:560:MET:N	2.24	0.90
1:D:577:LEU:HD11	1:F:607:SER:HB2	0.92	0.90
1:B:610:GLN:NE2	1:C:577:LEU:HB2	1.85	0.90
1:A:552:PHE:CG	1:C:690:PHE:CZ	2.60	0.90
1:A:221:PHE:CZ	2:G:202:PHE:HZ	1.87	0.89
1:B:654:TYR:CD2	1:B:670:PHE:CD1	2.60	0.89
1:A:409:ILE:HG22	2:G:194:PHE:HE2	1.33	0.89
1:D:612:ILE:CD1	1:F:612:ILE:CD1	2.49	0.89
1:A:345:GLN:OE1	3:H:127:TYR:OH	1.92	0.88
1:A:630:TRP:HB3	1:A:670:PHE:HE2	1.34	0.87
1:B:692:GLU:OE2	1:D:440:TYR:CD1	2.28	0.87
1:A:344:LYS:CD	3:H:80:ARG:CZ	2.52	0.87
1:A:654:TYR:CD2	1:A:670:PHE:HB3	2.09	0.87
1:A:464:PRO:CG	1:B:514:TYR:HE1	1.88	0.87
1:E:464:PRO:HD3	1:F:523:SER:HA	1.56	0.87
1:A:193:ASP:OD2	2:G:404:ARG:NH2	2.07	0.86
1:F:570:SER:HB2	1:F:683:HIS:CB	2.05	0.86
1:D:577:LEU:CD1	1:F:607:SER:CB	2.39	0.86
1:A:368:LYS:HZ2	1:B:630:TRP:HZ2	1.23	0.86
1:B:692:GLU:OE2	1:D:440:TYR:CG	2.29	0.86
1:A:221:PHE:CZ	2:G:202:PHE:HE2	1.69	0.86
1:A:464:PRO:HG3	1:B:514:TYR:CE1	2.10	0.85
1:C:440:TYR:HA	1:F:692:GLU:OE2	1.76	0.85
1:B:577:LEU:CG	1:C:610:GLN:OE1	2.23	0.85
1:A:514:TYR:HE1	1:B:464:PRO:HG3	1.41	0.85
1:A:654:TYR:CD2	1:A:670:PHE:CG	2.63	0.85
1:A:368:LYS:HZ3	1:B:630:TRP:HZ2	0.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:VAL:CG1	1:A:527:HIS:NE2	2.38	0.85
2:G:287:LEU:HD22	2:G:409:MET:HE1	1.57	0.85
1:D:568:SER:CB	1:D:670:PHE:CE1	2.60	0.85
1:A:445:VAL:HG22	1:A:526:PRO:HG2	1.57	0.84
1:B:691:GLN:OE1	1:D:442:GLY:CA	2.26	0.84
1:D:568:SER:CB	1:D:670:PHE:HE1	1.89	0.84
1:A:96:PRO:CD	2:G:277:ARG:CZ	2.48	0.84
1:C:630:TRP:HZ2	1:D:368:LYS:HZ1	1.24	0.84
1:A:559:CYS:O	1:A:584:ASP:OD2	1.96	0.84
2:G:94:PRO:O	2:G:95:VAL:HB	1.77	0.83
1:D:612:ILE:HD13	1:F:612:ILE:CD1	2.09	0.83
1:A:192:GLN:HE22	2:G:404:ARG:HH21	1.25	0.83
1:D:571:VAL:HG22	1:D:655:ASN:HB2	1.60	0.83
1:B:677:TYR:CZ	1:D:541:ASP:HB3	2.15	0.82
1:A:409:ILE:HG22	2:G:194:PHE:CE2	2.07	0.82
2:G:32:LEU:HD22	2:G:34:LEU:HD21	1.61	0.82
1:C:532:ALA:HB1	1:C:560:MET:CE	2.10	0.82
1:A:552:PHE:CD2	1:C:690:PHE:HE1	1.92	0.81
1:B:445:VAL:HG22	1:B:526:PRO:HG2	1.61	0.81
1:A:552:PHE:CB	1:C:690:PHE:HZ	1.94	0.81
1:A:532:ALA:HB1	1:A:560:MET:CE	2.11	0.81
1:B:610:GLN:HE22	1:C:577:LEU:HB2	1.45	0.81
1:C:571:VAL:HG22	1:C:655:ASN:HB2	1.63	0.81
2:G:44:ASN:OD1	2:G:516:ARG:HG3	1.81	0.81
1:D:533:LEU:HB3	1:D:642:THR:HG21	1.61	0.80
1:A:391:VAL:HG21	2:G:197:ARG:NH1	1.96	0.80
1:C:571:VAL:CG2	1:C:655:ASN:HB2	2.12	0.80
1:C:568:SER:CB	1:C:670:PHE:HE1	1.96	0.79
1:F:629:ASP:CG	1:F:659:HIS:CE1	2.55	0.79
1:A:192:GLN:NE2	2:G:404:ARG:NH2	2.29	0.79
1:A:654:TYR:CE2	1:A:670:PHE:HB3	2.17	0.79
1:A:552:PHE:CB	1:C:690:PHE:CZ	2.65	0.79
1:F:570:SER:CB	1:F:683:HIS:CG	2.65	0.79
1:A:540:ARG:CZ	1:C:690:PHE:HA	2.11	0.79
1:D:677:TYR:CE1	1:E:541:ASP:HB3	2.16	0.79
1:A:221:PHE:HZ	2:G:202:PHE:HE2	0.82	0.79
1:F:624:ILE:CG1	1:F:655:ASN:HB2	2.10	0.79
1:E:324:GLN:NE2	1:F:518:GLY:HA2	1.68	0.79
1:E:440:TYR:CE2	1:E:527:HIS:HA	2.19	0.78
2:G:273:PHE:N	2:G:392:THR:HG21	1.99	0.78
1:A:532:ALA:HB1	1:A:560:MET:HE2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ALA:HB3	1:C:690:PHE:CE2	2.10	0.78
1:D:577:LEU:HD12	1:F:610:GLN:OE1	1.82	0.78
2:G:489:ILE:HG23	2:G:503:ILE:HG23	1.64	0.78
2:G:269:CYS:SG	2:G:285:THR:HG21	2.23	0.78
2:G:453:THR:HG21	2:G:455:VAL:HG12	1.66	0.78
1:A:222:VAL:HG21	2:G:166:ARG:NH1	1.78	0.78
1:D:551:ARG:NH1	1:D:641:GLU:OE2	2.14	0.78
1:E:464:PRO:CD	1:F:523:SER:HA	2.14	0.78
1:C:508:VAL:O	1:C:509:GLU:CA	2.27	0.78
1:C:514:TYR:HE1	1:D:464:PRO:HG3	1.48	0.77
2:G:285:THR:HG22	2:G:285:THR:O	1.84	0.77
1:A:275:PHE:CE2	3:H:80:ARG:NE	2.45	0.77
1:C:654:TYR:CG	1:C:670:PHE:CD2	2.72	0.77
1:A:441:ASN:OD1	1:C:691:GLN:CB	2.32	0.77
1:A:391:VAL:HG21	2:G:197:ARG:CZ	2.14	0.77
1:B:690:PHE:HZ	1:D:552:PHE:CD2	2.03	0.77
1:C:654:TYR:CD2	1:C:670:PHE:CE2	2.73	0.77
2:G:152:ASP:HB2	2:G:154:ILE:HD11	1.65	0.77
1:C:568:SER:CB	1:C:670:PHE:CE1	2.68	0.77
1:C:654:TYR:CE2	1:C:670:PHE:CG	2.72	0.76
1:E:324:GLN:HE21	1:F:518:GLY:HA3	0.94	0.76
1:B:654:TYR:CD2	1:B:670:PHE:CG	2.73	0.76
1:B:654:TYR:HB3	1:B:670:PHE:CE2	2.19	0.76
2:G:215:GLN:HE21	2:G:216:HIS:CD2	2.03	0.76
1:E:654:TYR:HD2	1:E:670:PHE:CE1	2.00	0.76
1:A:342:GLY:HA3	3:H:84:TYR:OH	1.86	0.76
1:E:654:TYR:CE1	1:E:670:PHE:CB	2.69	0.76
1:E:654:TYR:CZ	1:E:670:PHE:HB3	2.20	0.76
1:A:440:TYR:OH	1:C:692:GLU:OE2	2.02	0.76
1:A:221:PHE:HE1	2:G:212:ARG:HD2	1.50	0.75
1:A:552:PHE:CG	1:C:690:PHE:CE1	2.74	0.75
1:D:677:TYR:CZ	1:E:541:ASP:CB	2.69	0.75
2:G:287:LEU:HB3	2:G:409:MET:HE3	1.67	0.75
1:A:654:TYR:CB	1:A:670:PHE:CG	2.70	0.75
1:B:577:LEU:HB2	1:C:610:GLN:OE1	1.86	0.75
1:B:551:ARG:NH1	1:B:641:GLU:OE2	2.14	0.75
2:G:402:PHE:O	2:G:403:ALA:HB3	1.86	0.75
1:C:626:LEU:HD13	1:D:399:PRO:HG3	1.65	0.75
1:A:387:LEU:HD22	2:G:197:ARG:HH12	1.52	0.74
1:C:540:ARG:HD2	1:F:690:PHE:CG	1.87	0.74
2:G:453:THR:CG2	2:G:455:VAL:HG12	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:PRO:HG3	1:D:626:LEU:HD12	1.69	0.74
1:D:577:LEU:CD1	1:F:610:GLN:OE1	2.34	0.74
1:A:654:TYR:CG	1:A:670:PHE:HB3	2.20	0.74
1:A:654:TYR:HB3	1:A:670:PHE:CE2	2.22	0.74
1:E:556:ILE:HD11	1:F:324:GLN:OE1	1.86	0.74
1:D:571:VAL:CG2	1:D:655:ASN:HB2	2.17	0.74
1:D:568:SER:HB2	1:D:670:PHE:CE1	2.22	0.74
1:B:610:GLN:OE1	1:C:577:LEU:HG	1.87	0.74
1:C:399:PRO:HG3	1:D:626:LEU:CD1	2.18	0.74
1:A:441:ASN:OD1	1:C:691:GLN:OE1	2.04	0.73
1:A:344:LYS:HD3	3:H:80:ARG:CZ	2.13	0.73
1:E:544:GLN:HG2	1:E:545:ARG:HG2	1.71	0.73
1:A:368:LYS:HZ1	1:B:630:TRP:HZ2	1.34	0.73
1:B:544:GLN:HG2	1:B:545:ARG:HG2	1.71	0.73
1:C:532:ALA:HB1	1:C:560:MET:HE2	1.71	0.73
1:F:544:GLN:HG2	1:F:545:ARG:HG2	1.71	0.73
1:C:654:TYR:CD2	1:C:670:PHE:CZ	2.77	0.72
1:D:544:GLN:HG2	1:D:545:ARG:HG2	1.71	0.72
1:B:677:TYR:CE1	1:D:541:ASP:HB3	2.24	0.72
1:A:95:TYR:C	2:G:277:ARG:NH2	2.43	0.72
1:A:544:GLN:HG2	1:A:545:ARG:HG2	1.71	0.72
1:A:96:PRO:CD	2:G:277:ARG:CD	2.58	0.72
1:A:96:PRO:CD	2:G:277:ARG:HE	1.98	0.72
1:D:577:LEU:HB2	1:F:610:GLN:OE1	1.90	0.72
1:A:399:PRO:HG3	1:B:626:LEU:CD1	2.20	0.72
1:A:192:GLN:NE2	2:G:404:ARG:HH21	1.88	0.72
1:A:464:PRO:CG	1:B:514:TYR:CE1	2.72	0.72
2:G:501:LEU:HD22	2:G:503:ILE:CD1	2.19	0.72
2:G:453:THR:HG22	2:G:455:VAL:H	1.54	0.71
1:A:654:TYR:HB3	1:A:670:PHE:CG	2.25	0.71
1:B:551:ARG:HH12	1:B:641:GLU:CD	1.92	0.71
1:C:544:GLN:HG2	1:C:545:ARG:HG2	1.71	0.71
2:G:498:GLN:O	2:G:500:GLN:HG2	1.90	0.71
1:D:612:ILE:HD12	1:F:612:ILE:HD12	1.69	0.71
2:G:186:LEU:HB2	2:G:205:LEU:HD22	1.71	0.71
2:G:170:PRO:HD3	2:G:190:THR:HG21	1.71	0.71
1:D:507:PRO:C	1:D:509:GLU:N	2.42	0.71
1:D:577:LEU:HD11	1:F:607:SER:OG	1.89	0.70
1:A:342:GLY:CA	3:H:84:TYR:OH	2.39	0.70
1:F:697:VAL:HG12	1:F:699:GLU:H	1.57	0.70
1:A:654:TYR:CD1	1:A:670:PHE:CB	2.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:VAL:HG12	1:A:699:GLU:H	1.56	0.70
1:C:697:VAL:HG12	1:C:699:GLU:H	1.56	0.70
1:A:344:LYS:HD2	3:H:80:ARG:HH11	0.54	0.70
1:B:692:GLU:OE2	1:D:441:ASN:N	2.24	0.70
1:D:677:TYR:CE1	1:E:541:ASP:CB	2.74	0.70
1:B:697:VAL:HG12	1:B:699:GLU:H	1.56	0.70
1:C:654:TYR:CD2	1:C:670:PHE:CD2	2.79	0.70
1:A:654:TYR:CD2	1:A:670:PHE:CB	2.71	0.70
1:D:697:VAL:HG12	1:D:699:GLU:H	1.56	0.70
1:A:344:LYS:CD	3:H:80:ARG:HD2	2.05	0.70
1:C:523:SER:HA	1:D:464:PRO:HD3	1.73	0.70
1:A:535:ASN:HB2	1:A:646:PHE:HA	1.73	0.70
1:E:654:TYR:CD1	1:E:670:PHE:CG	2.79	0.70
1:D:690:PHE:HE2	1:E:540:ARG:C	1.52	0.70
1:A:96:PRO:CG	2:G:277:ARG:HE	2.05	0.69
2:G:116:ASN:HA	2:G:134:THR:O	1.91	0.69
1:A:441:ASN:C	1:C:691:GLN:NE2	2.39	0.69
1:F:533:LEU:O	1:F:642:THR:OG1	2.04	0.69
1:A:95:TYR:O	2:G:277:ARG:NH1	2.25	0.69
1:F:629:ASP:OD1	1:F:659:HIS:CE1	2.45	0.69
2:G:273:PHE:H	2:G:392:THR:CG2	2.01	0.69
1:A:273:ASP:CB	3:H:80:ARG:CZ	2.67	0.69
1:F:533:LEU:CB	1:F:642:THR:HG21	2.10	0.69
2:G:433:GLN:HB2	2:G:492:MET:HE3	1.74	0.69
1:E:697:VAL:HG12	1:E:699:GLU:H	1.57	0.69
1:B:577:LEU:HB2	1:C:610:GLN:HE22	1.57	0.69
2:G:226:PHE:O	2:G:227:ILE:HD12	1.93	0.69
1:A:237:SER:HA	1:A:239:PHE:N	2.08	0.69
1:A:96:PRO:HG3	2:G:277:ARG:HE	1.57	0.69
1:B:237:SER:HA	1:B:239:PHE:N	2.08	0.68
1:E:654:TYR:CD1	1:E:670:PHE:CB	2.76	0.68
1:D:568:SER:OG	1:D:670:PHE:CE1	2.46	0.68
2:G:420:PRO:HG3	2:G:423:ILE:HD11	1.75	0.68
1:E:79:ILE:HD11	1:E:82:ALA:HB2	1.76	0.68
1:F:79:ILE:HD11	1:F:82:ALA:HB2	1.76	0.68
1:F:630:TRP:CG	1:F:670:PHE:HE2	2.12	0.68
1:C:237:SER:HA	1:C:239:PHE:N	2.07	0.68
1:C:626:LEU:HD12	1:D:399:PRO:HG3	1.69	0.68
2:G:330:THR:HG22	2:G:332:SER:H	1.57	0.68
1:A:273:ASP:HB3	3:H:80:ARG:NH1	2.09	0.68
1:E:564:VAL:HG22	1:E:580:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:SER:HB2	1:A:683:HIS:CE1	2.28	0.68
1:B:79:ILE:HD11	1:B:82:ALA:HB2	1.75	0.68
1:A:541:ASP:HB3	1:C:677:TYR:OH	1.94	0.68
1:C:534:HIS:CD2	1:C:642:THR:HB	2.28	0.67
1:A:96:PRO:CG	2:G:277:ARG:NE	2.57	0.67
1:F:237:SER:HA	1:F:239:PHE:N	2.08	0.67
1:B:577:LEU:HB2	1:C:610:GLN:NE2	2.09	0.67
1:D:237:SER:HA	1:D:239:PHE:N	2.08	0.67
1:B:564:VAL:HG22	1:B:580:LEU:HD13	1.76	0.67
1:E:654:TYR:HB3	1:E:670:PHE:CZ	2.29	0.67
1:D:79:ILE:HD11	1:D:82:ALA:HB2	1.75	0.67
1:A:95:TYR:C	2:G:277:ARG:CZ	2.63	0.67
1:D:666:VAL:HG11	1:D:698:SER:N	2.10	0.67
1:C:79:ILE:HD11	1:C:82:ALA:HB2	1.75	0.67
1:E:629:ASP:OD1	1:E:659:HIS:CE1	2.47	0.67
2:G:30:PRO:HG3	2:G:476:LEU:HD13	1.75	0.67
1:F:564:VAL:HG22	1:F:580:LEU:HD13	1.76	0.67
1:C:564:VAL:HG22	1:C:580:LEU:HD13	1.76	0.67
1:C:666:VAL:HG11	1:C:698:SER:N	2.10	0.67
1:A:79:ILE:HD11	1:A:82:ALA:HB2	1.76	0.67
2:G:502:TYR:C	2:G:503:ILE:HD12	2.16	0.67
1:B:666:VAL:HG11	1:B:698:SER:N	2.10	0.67
1:F:666:VAL:HG11	1:F:698:SER:N	2.10	0.67
1:A:523:SER:HA	1:B:464:PRO:HD2	1.78	0.66
2:G:274:GLY:O	2:G:392:THR:HG23	1.94	0.66
1:F:570:SER:CB	1:F:683:HIS:CB	2.72	0.66
2:G:516:ARG:HA	2:G:516:ARG:NE	2.10	0.66
1:F:533:LEU:HD13	1:F:642:THR:HG23	1.77	0.66
1:A:399:PRO:HG3	1:B:626:LEU:HD11	1.76	0.66
1:B:654:TYR:CG	1:B:670:PHE:CG	2.83	0.66
1:C:654:TYR:CE2	1:C:670:PHE:CE1	2.84	0.66
1:F:570:SER:HB2	1:F:683:HIS:HB2	1.76	0.66
1:D:533:LEU:HD22	1:D:639:SER:HB2	1.78	0.66
1:E:666:VAL:HG11	1:E:698:SER:N	2.10	0.66
1:E:523:SER:HA	1:F:464:PRO:HD3	1.75	0.66
1:D:564:VAL:HG22	1:D:580:LEU:HD13	1.76	0.66
1:A:552:PHE:HB2	1:C:690:PHE:HZ	1.59	0.66
1:C:626:LEU:HD11	1:D:399:PRO:CG	2.23	0.66
1:B:577:LEU:CB	1:C:610:GLN:OE1	2.43	0.66
2:G:180:LEU:HD11	2:G:182:ILE:HD13	1.78	0.66
1:A:666:VAL:HG11	1:A:698:SER:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:571:VAL:HG22	1:F:655:ASN:HA	1.78	0.66
1:E:237:SER:HA	1:E:239:PHE:N	2.07	0.66
1:A:564:VAL:HG22	1:A:580:LEU:HD13	1.76	0.66
1:D:533:LEU:HB3	1:D:642:THR:CG2	2.27	0.65
2:G:56:SER:HA	2:G:506:THR:HG22	1.77	0.65
1:B:654:TYR:HB3	1:B:670:PHE:CD2	2.31	0.65
1:D:568:SER:HG	1:D:670:PHE:HD1	1.39	0.65
2:G:404:ARG:HG2	2:G:404:ARG:HH11	1.62	0.65
1:F:630:TRP:CG	1:F:670:PHE:CE2	2.85	0.65
1:A:95:TYR:O	2:G:277:ARG:CZ	2.44	0.65
1:F:630:TRP:CB	1:F:670:PHE:HE2	1.97	0.65
2:G:95:VAL:HG23	2:G:116:ASN:HB2	1.78	0.65
1:A:523:SER:HA	1:B:464:PRO:CD	2.28	0.64
1:E:88:GLU:HB2	1:E:132:LEU:HD21	1.79	0.64
1:C:514:TYR:CE1	1:D:464:PRO:HG3	2.31	0.64
1:D:691:GLN:HB3	1:E:441:ASN:HA	1.78	0.64
1:E:532:ALA:HB1	1:E:560:MET:HE3	1.79	0.64
1:D:88:GLU:HB2	1:D:132:LEU:HD21	1.79	0.64
1:F:88:GLU:HB2	1:F:132:LEU:HD21	1.79	0.64
1:A:88:GLU:HB2	1:A:132:LEU:HD21	1.79	0.64
1:F:551:ARG:NH1	1:F:641:GLU:OE2	2.31	0.64
1:B:660:GLN:HB2	2:G:105:TRP:HE1	1.63	0.64
1:A:192:GLN:HE22	2:G:404:ARG:HH22	1.44	0.64
2:G:85:ILE:HG12	2:G:511:GLN:HE21	1.63	0.64
1:E:533:LEU:HB3	1:E:642:THR:HG21	1.79	0.64
1:B:654:TYR:CB	1:B:670:PHE:CD2	2.80	0.64
1:A:442:GLY:H	1:C:691:GLN:NE2	1.79	0.64
2:G:287:LEU:HD22	2:G:409:MET:HE2	1.77	0.63
1:A:654:TYR:CZ	1:A:670:PHE:HB3	2.33	0.63
1:C:88:GLU:HB2	1:C:132:LEU:HD21	1.79	0.63
1:E:568:SER:HB2	1:E:670:PHE:HE1	1.63	0.63
1:E:654:TYR:HB2	1:E:670:PHE:CD2	2.32	0.63
1:E:568:SER:CB	1:E:670:PHE:HE1	2.11	0.63
1:B:691:GLN:CD	1:D:442:GLY:N	2.51	0.63
1:A:508:VAL:HG13	1:A:527:HIS:NE2	2.14	0.63
1:B:677:TYR:OH	1:D:541:ASP:HB3	1.99	0.63
2:G:218:SER:HB2	2:G:252:ILE:HD11	1.80	0.63
2:G:48:PHE:CE2	2:G:50:GLY:HA2	2.33	0.63
2:G:209:HIS:HD2	2:G:210:PRO:O	1.82	0.63
2:G:317:LYS:HE2	2:G:317:LYS:HA	1.79	0.63
1:A:344:LYS:HZ2	3:H:80:ARG:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:TYR:CD2	1:C:670:PHE:CE1	2.87	0.63
2:G:85:ILE:H	2:G:511:GLN:HE22	1.46	0.63
1:B:534:HIS:NE2	1:B:642:THR:HB	2.14	0.63
2:G:203:ARG:NH2	2:G:273:PHE:CE2	2.65	0.62
1:A:344:LYS:HG2	3:H:80:ARG:CZ	2.29	0.62
1:D:274:LEU:HD12	1:D:274:LEU:H	1.64	0.62
1:A:654:TYR:CD1	1:A:670:PHE:HB2	2.34	0.62
1:B:88:GLU:HB2	1:B:132:LEU:HD21	1.79	0.62
1:C:629:ASP:OD1	1:C:659:HIS:CE1	2.53	0.62
2:G:396:PRO:HG2	2:G:399:VAL:HG12	1.81	0.62
1:D:568:SER:OG	1:D:670:PHE:CD1	2.51	0.62
1:D:654:TYR:CD2	1:D:670:PHE:CG	2.88	0.62
1:C:654:TYR:CZ	1:C:670:PHE:CG	2.88	0.62
1:A:630:TRP:CB	1:A:670:PHE:CE2	2.77	0.62
1:B:690:PHE:CZ	1:D:552:PHE:CD2	2.87	0.62
1:F:274:LEU:H	1:F:274:LEU:HD12	1.64	0.62
1:A:552:PHE:HD2	1:C:690:PHE:HE1	1.43	0.62
2:G:249:GLU:OE2	2:G:264:ARG:CD	2.47	0.62
1:A:654:TYR:CD1	1:A:670:PHE:HB3	2.34	0.61
2:G:154:ILE:HD12	2:G:154:ILE:H	1.65	0.61
1:B:508:VAL:CG1	1:B:527:HIS:NE2	2.63	0.61
1:F:572:SER:HB2	1:F:683:HIS:CE1	2.35	0.61
2:G:118:ILE:N	2:G:118:ILE:HD12	2.16	0.61
1:C:534:HIS:CE1	1:C:642:THR:HG22	2.35	0.61
1:F:570:SER:HG	1:F:683:HIS:CG	2.19	0.61
2:G:164:ASN:HD22	2:G:166:ARG:H	1.47	0.61
1:A:442:GLY:CA	1:C:691:GLN:HE22	2.10	0.61
1:A:222:VAL:HG21	2:G:166:ARG:CZ	2.30	0.61
1:A:546:ALA:HB1	1:C:690:PHE:HZ	1.53	0.61
2:G:285:THR:HG23	2:G:379:GLY:HA2	1.82	0.61
1:B:274:LEU:H	1:B:274:LEU:HD12	1.64	0.61
2:G:427:VAL:HG21	2:G:429:TYR:OH	2.00	0.61
1:C:274:LEU:H	1:C:274:LEU:HD12	1.64	0.61
1:D:654:TYR:HB3	1:D:670:PHE:CE2	2.35	0.61
1:A:396:ALA:CB	2:G:107:GLY:HA3	2.31	0.61
1:E:274:LEU:HD12	1:E:274:LEU:H	1.64	0.61
1:D:191:LYS:HB3	1:D:194:TYR:HB2	1.83	0.61
1:A:274:LEU:H	1:A:274:LEU:HD12	1.64	0.61
2:G:85:ILE:H	2:G:511:GLN:NE2	1.99	0.61
1:A:547:TRP:HA	1:C:689:SER:CB	2.31	0.60
1:E:191:LYS:HB3	1:E:194:TYR:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ARG:HG3	1:C:526:PRO:HG3	1.82	0.60
1:D:692:GLU:OE2	1:E:440:TYR:CG	2.55	0.60
2:G:164:ASN:ND2	2:G:166:ARG:H	1.98	0.60
1:C:654:TYR:CD2	1:C:670:PHE:CG	2.89	0.60
2:G:453:THR:HG22	2:G:455:VAL:N	2.15	0.60
2:G:268:ILE:HD13	2:G:283:TRP:CD2	2.35	0.60
1:A:464:PRO:HD2	1:B:523:SER:HA	1.82	0.60
1:F:191:LYS:HB3	1:F:194:TYR:HB2	1.83	0.60
1:F:654:TYR:HB3	1:F:670:PHE:CD2	2.37	0.60
1:A:398:VAL:HG22	2:G:105:TRP:O	2.00	0.60
1:A:397:PRO:HD2	2:G:107:GLY:HA2	1.83	0.60
1:D:508:VAL:CG1	1:D:527:HIS:NE2	2.65	0.60
1:B:191:LYS:HB3	1:B:194:TYR:HB2	1.83	0.60
1:A:273:ASP:HB3	3:H:80:ARG:NE	2.14	0.60
1:B:577:LEU:HB2	1:C:610:GLN:CD	2.22	0.60
1:A:191:LYS:HB3	1:A:194:TYR:HB2	1.83	0.60
2:G:66:ARG:HA	2:G:150:PRO:CB	2.32	0.60
1:F:654:TYR:CD2	1:F:670:PHE:HB3	2.36	0.60
2:G:154:ILE:N	2:G:154:ILE:HD12	2.17	0.60
1:E:629:ASP:CG	1:E:659:HIS:CE1	2.75	0.60
2:G:501:LEU:HD22	2:G:503:ILE:HD11	1.84	0.60
1:F:626:LEU:HD21	1:F:658:ALA:O	2.01	0.60
2:G:105:TRP:CE3	2:G:105:TRP:HA	2.36	0.59
2:G:66:ARG:HA	2:G:150:PRO:HB3	1.84	0.59
1:C:626:LEU:CD1	1:D:399:PRO:CG	2.58	0.59
1:D:692:GLU:OE2	1:E:440:TYR:HA	2.02	0.59
1:B:663:LEU:HD23	1:B:698:SER:HB2	1.84	0.59
2:G:209:HIS:CD2	2:G:210:PRO:O	2.56	0.59
2:G:313:LEU:HD22	2:G:324:VAL:HG22	1.83	0.59
1:C:191:LYS:HB3	1:C:194:TYR:HB2	1.83	0.59
1:E:654:TYR:CD2	1:E:670:PHE:CZ	2.90	0.59
2:G:226:PHE:C	2:G:227:ILE:HD12	2.22	0.59
1:C:663:LEU:HD23	1:C:698:SER:HB2	1.84	0.59
1:F:663:LEU:HD23	1:F:698:SER:HB2	1.84	0.59
1:E:663:LEU:HD23	1:E:698:SER:HB2	1.84	0.59
1:A:663:LEU:HD23	1:A:698:SER:HB2	1.84	0.59
1:B:533:LEU:HD22	1:B:639:SER:HB2	1.84	0.59
2:G:367:VAL:HG13	2:G:368:PRO:HD2	1.85	0.59
1:B:559:CYS:C	1:B:560:MET:N	2.56	0.59
2:G:176:LEU:O	2:G:190:THR:HG23	2.03	0.59
2:G:48:PHE:CZ	2:G:50:GLY:HA2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:NZ	3:H:84:TYR:HD1	1.93	0.59
1:D:97:PRO:HG2	1:D:158:TYR:CE1	2.38	0.59
1:D:663:LEU:HD23	1:D:698:SER:HB2	1.84	0.59
2:G:249:GLU:OE2	2:G:264:ARG:HD2	2.03	0.59
1:D:438:TYR:HH	1:D:527:HIS:CD2	2.21	0.59
1:C:654:TYR:CZ	1:C:670:PHE:HB3	2.38	0.58
1:E:629:ASP:OD1	1:E:659:HIS:NE2	2.36	0.58
2:G:46:ILE:O	2:G:85:ILE:HD11	2.03	0.58
1:F:97:PRO:HG2	1:F:158:TYR:CE1	2.38	0.58
2:G:404:ARG:NH1	2:G:404:ARG:HG2	2.18	0.58
1:A:654:TYR:HB2	1:A:670:PHE:CD2	2.35	0.58
1:E:532:ALA:HB1	1:E:560:MET:CE	2.33	0.58
1:A:97:PRO:HG2	1:A:158:TYR:CE1	2.38	0.58
1:E:97:PRO:HG2	1:E:158:TYR:CE1	2.38	0.58
1:E:523:SER:HA	1:F:464:PRO:CD	2.32	0.58
2:G:186:LEU:O	2:G:203:ARG:HA	2.04	0.58
1:C:571:VAL:HG22	1:C:655:ASN:CB	2.32	0.58
2:G:493:GLU:O	2:G:501:LEU:HD23	2.04	0.58
1:B:690:PHE:CZ	1:D:552:PHE:CE2	2.92	0.58
2:G:178:ALA:O	2:G:188:SER:HA	2.03	0.58
1:C:97:PRO:HG2	1:C:158:TYR:CE1	2.38	0.58
1:C:541:ASP:HB3	1:F:677:TYR:CZ	2.39	0.58
1:A:547:TRP:HA	1:C:689:SER:HB3	1.85	0.58
1:A:341:LYS:HZ2	3:H:84:TYR:HE1	0.67	0.58
1:C:654:TYR:CG	1:C:670:PHE:CE2	2.91	0.58
1:F:629:ASP:CG	1:F:659:HIS:NE2	2.54	0.58
2:G:501:LEU:HD22	2:G:503:ILE:HD12	1.86	0.58
1:F:626:LEU:HD22	1:F:658:ALA:HB1	1.85	0.58
2:G:70:TYR:OH	2:G:146:VAL:HG21	2.04	0.58
2:G:140:ILE:H	2:G:140:ILE:HD13	1.68	0.58
1:F:533:LEU:HD22	1:F:639:SER:OG	2.03	0.58
2:G:227:ILE:O	2:G:228:SER:HB3	2.04	0.57
1:D:175:SER:OG	1:D:178:GLU:HG2	2.04	0.57
1:B:97:PRO:HG2	1:B:158:TYR:CE1	2.38	0.57
1:C:654:TYR:CD2	1:C:670:PHE:CD1	2.93	0.57
1:A:175:SER:OG	1:A:178:GLU:HG2	2.05	0.57
1:A:552:PHE:HB3	1:C:690:PHE:CE1	2.40	0.57
1:C:629:ASP:HA	1:C:658:ALA:HB1	1.86	0.57
2:G:435:VAL:HG23	2:G:450:PHE:HB2	1.87	0.57
1:B:175:SER:OG	1:B:178:GLU:HG2	2.04	0.57
1:E:407:LEU:O	1:E:411:GLN:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:187:TYR:CE2	2:G:203:ARG:HD3	2.40	0.57
1:D:533:LEU:HD22	1:D:639:SER:CB	2.35	0.57
1:F:175:SER:OG	1:F:178:GLU:HG2	2.04	0.57
2:G:309:GLN:OE1	2:G:309:GLN:HA	2.05	0.57
1:A:274:LEU:O	3:H:80:ARG:NH2	2.13	0.57
1:B:407:LEU:O	1:B:411:GLN:HG2	2.05	0.57
1:C:425:TYR:OH	1:C:456:LYS:HE2	2.05	0.57
2:G:120:VAL:O	2:G:131:ALA:HA	2.04	0.57
1:D:577:LEU:CB	1:F:610:GLN:OE1	2.52	0.57
1:C:465:HIS:NE2	1:D:470:TYR:HA	2.20	0.57
2:G:170:PRO:HD3	2:G:177:THR:OG1	2.05	0.57
2:G:265:ILE:HB	2:G:291:LEU:HD11	1.87	0.57
1:D:407:LEU:O	1:D:411:GLN:HG2	2.05	0.57
1:B:612:ILE:HG13	1:C:577:LEU:HD13	1.86	0.56
1:C:175:SER:OG	1:C:178:GLU:HG2	2.05	0.56
2:G:135:GLY:H	2:G:139:PRO:HA	1.68	0.56
1:E:175:SER:OG	1:E:178:GLU:HG2	2.05	0.56
1:F:529:GLY:HA3	1:F:552:PHE:CZ	2.40	0.56
1:A:407:LEU:O	1:A:411:GLN:HG2	2.05	0.56
1:A:222:VAL:HG21	2:G:166:ARG:HH22	1.70	0.56
1:A:654:TYR:HD2	1:A:670:PHE:CD1	2.16	0.56
1:D:529:GLY:HA3	1:D:552:PHE:CZ	2.40	0.56
1:F:407:LEU:O	1:F:411:GLN:HG2	2.05	0.56
1:C:407:LEU:O	1:C:411:GLN:HG2	2.05	0.56
1:C:529:GLY:HA3	1:C:552:PHE:CZ	2.40	0.56
1:F:425:TYR:OH	1:F:456:LYS:HE2	2.05	0.56
1:E:571:VAL:HG21	1:E:655:ASN:HB2	1.88	0.56
1:A:629:ASP:OD1	1:A:659:HIS:NE2	2.38	0.56
1:A:514:TYR:CE1	1:B:464:PRO:HG3	2.30	0.56
2:G:457:THR:H	2:G:489:ILE:HD11	1.70	0.56
1:E:529:GLY:HA3	1:E:552:PHE:CZ	2.41	0.56
1:F:570:SER:OG	1:F:683:HIS:CG	2.59	0.56
1:E:425:TYR:OH	1:E:456:LYS:HE2	2.05	0.56
1:A:425:TYR:OH	1:A:456:LYS:HE2	2.05	0.56
1:F:535:ASN:OD1	1:F:646:PHE:HA	2.05	0.56
1:B:529:GLY:HA3	1:B:552:PHE:CZ	2.40	0.56
1:E:626:LEU:HD21	1:E:658:ALA:O	2.05	0.56
1:F:570:SER:HB2	1:F:683:HIS:HB3	1.86	0.56
1:E:568:SER:HB2	1:E:670:PHE:CE1	2.40	0.56
2:G:285:THR:CG2	2:G:285:THR:O	2.52	0.56
1:B:425:TYR:OH	1:B:456:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:LEU:HG	1:D:236:VAL:HG23	1.88	0.56
1:A:344:LYS:CE	3:H:80:ARG:HD3	2.35	0.55
1:C:568:SER:OG	1:C:670:PHE:CE1	1.98	0.55
1:A:398:VAL:CG2	2:G:105:TRP:O	2.53	0.55
2:G:402:PHE:O	2:G:403:ALA:CB	2.52	0.55
2:G:45:VAL:HG11	2:G:482:VAL:HG13	1.88	0.55
1:C:235:LEU:HG	1:C:236:VAL:HG23	1.88	0.55
1:A:654:TYR:CE1	1:A:670:PHE:HB3	2.42	0.55
2:G:104:LYS:HD2	2:G:110:ILE:HD11	1.87	0.55
1:A:222:VAL:HG21	2:G:166:ARG:NH2	2.22	0.55
1:A:529:GLY:HA3	1:A:552:PHE:CZ	2.41	0.55
2:G:420:PRO:CG	2:G:423:ILE:HD11	2.37	0.55
1:E:235:LEU:HG	1:E:236:VAL:HG23	1.88	0.55
2:G:426:ASP:N	2:G:426:ASP:OD1	2.40	0.55
1:A:221:PHE:CE1	2:G:212:ARG:HD2	2.36	0.55
1:F:533:LEU:HD22	1:F:639:SER:CB	2.37	0.55
1:C:571:VAL:HG21	1:C:655:ASN:HB2	1.88	0.55
1:D:425:TYR:OH	1:D:456:LYS:HE2	2.05	0.55
2:G:389:PHE:H	2:G:389:PHE:HD1	1.53	0.55
1:C:535:ASN:CG	1:C:646:PHE:HA	2.27	0.55
2:G:249:GLU:OE2	2:G:264:ARG:HD3	2.07	0.55
1:A:235:LEU:HG	1:A:236:VAL:HG23	1.88	0.55
1:C:574:HIS:ND1	1:C:618:PRO:HD3	2.22	0.55
1:A:552:PHE:CG	1:C:690:PHE:HZ	2.13	0.54
1:D:689:SER:HB3	1:E:540:ARG:CD	2.31	0.54
1:E:574:HIS:ND1	1:E:618:PRO:HD3	2.22	0.54
1:F:574:HIS:ND1	1:F:618:PRO:HD3	2.23	0.54
1:A:221:PHE:HE1	2:G:212:ARG:CD	2.20	0.54
1:A:220:ASP:OD2	2:G:209:HIS:NE2	2.40	0.54
1:B:235:LEU:HG	1:B:236:VAL:HG23	1.88	0.54
1:B:574:HIS:ND1	1:B:618:PRO:HD3	2.22	0.54
1:F:235:LEU:HG	1:F:236:VAL:HG23	1.89	0.54
2:G:378:PRO:HG3	2:G:399:VAL:HG23	1.87	0.54
2:G:30:PRO:HG3	2:G:476:LEU:CD1	2.37	0.54
2:G:32:LEU:HB2	2:G:478:GLU:HB3	1.89	0.54
1:D:574:HIS:ND1	1:D:618:PRO:HD3	2.22	0.54
2:G:161:HIS:O	2:G:162:PHE:HB2	2.08	0.54
2:G:401:THR:O	2:G:404:ARG:HB3	2.07	0.54
1:D:571:VAL:HG22	1:D:655:ASN:CB	2.34	0.54
1:E:399:PRO:HG3	1:F:626:LEU:HD11	1.90	0.54
1:A:87:PRO:HB2	1:A:109:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:ILE:HD11	1:F:612:ILE:CD1	2.38	0.54
2:G:384:LYS:HB3	2:G:384:LYS:NZ	2.23	0.54
1:D:87:PRO:HB2	1:D:109:LEU:HD11	1.90	0.53
2:G:39:MET:HE3	2:G:44:ASN:HB3	1.89	0.53
1:C:534:HIS:CE1	1:C:642:THR:CG2	2.92	0.53
1:B:87:PRO:HB2	1:B:109:LEU:HD11	1.90	0.53
2:G:31:ARG:HD2	2:G:31:ARG:N	2.23	0.53
2:G:199:PHE:CZ	2:G:225:ARG:NH1	2.76	0.53
2:G:279:LEU:HD12	2:G:400:ILE:HG23	1.90	0.53
1:A:344:LYS:NZ	3:H:80:ARG:HD2	2.23	0.53
1:C:508:VAL:C	1:C:509:GLU:CB	2.77	0.53
2:G:134:THR:HG23	2:G:171:TYR:O	2.08	0.53
1:B:535:ASN:HB2	1:B:646:PHE:HA	1.90	0.53
2:G:218:SER:HB2	2:G:252:ILE:CD1	2.39	0.53
1:A:574:HIS:ND1	1:A:618:PRO:HD3	2.22	0.53
2:G:93:TRP:CH2	2:G:142:THR:HG22	2.43	0.53
1:B:534:HIS:CD2	1:B:642:THR:HB	2.44	0.53
1:E:87:PRO:HB2	1:E:109:LEU:HD11	1.90	0.53
1:C:508:VAL:CG1	1:C:539:ARG:NH2	2.72	0.53
2:G:56:SER:CA	2:G:506:THR:HG22	2.38	0.53
2:G:267:GLN:O	2:G:268:ILE:HG13	2.09	0.53
2:G:204:THR:O	2:G:205:LEU:HB2	2.09	0.53
1:F:87:PRO:HB2	1:F:109:LEU:HD11	1.90	0.53
1:A:552:PHE:CB	1:C:690:PHE:CE1	2.92	0.52
1:A:231:ASP:CG	2:G:217:ASP:HA	2.30	0.52
1:C:459:ARG:CG	1:C:526:PRO:HG3	2.39	0.52
1:C:87:PRO:HB2	1:C:109:LEU:HD11	1.90	0.52
1:F:533:LEU:HD11	1:F:641:GLU:OE1	2.09	0.52
1:D:507:PRO:O	1:D:509:GLU:N	2.42	0.52
1:C:535:ASN:HB2	1:C:646:PHE:HA	1.92	0.52
1:A:540:ARG:NH1	1:C:689:SER:O	2.42	0.52
1:C:568:SER:HB2	1:C:670:PHE:CE1	2.44	0.52
2:G:503:ILE:N	2:G:503:ILE:HD12	2.25	0.52
2:G:427:VAL:HG13	2:G:429:TYR:CD2	2.44	0.52
1:C:459:ARG:CD	1:C:526:PRO:HG3	2.39	0.52
2:G:453:THR:H	2:G:489:ILE:HD12	1.75	0.52
2:G:35:SER:OG	2:G:38:GLU:HG3	2.09	0.52
1:A:559:CYS:O	1:A:584:ASP:CG	2.48	0.52
2:G:149:HIS:C	2:G:151:GLU:H	2.13	0.52
1:A:552:PHE:HD2	1:C:690:PHE:CE1	2.17	0.52
1:D:235:LEU:HD21	1:D:263:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ARG:HB2	1:C:343:GLN:HG2	1.92	0.52
1:A:96:PRO:N	2:G:277:ARG:CZ	2.72	0.52
1:C:654:TYR:CZ	1:C:670:PHE:CB	2.93	0.52
1:F:235:LEU:HD21	1:F:263:PRO:HG2	1.92	0.52
1:A:308:ARG:HB2	1:A:343:GLN:HG2	1.92	0.52
1:A:274:LEU:N	1:A:274:LEU:HD12	2.25	0.51
1:B:610:GLN:CG	1:C:577:LEU:HD12	2.40	0.51
1:D:274:LEU:N	1:D:274:LEU:HD12	2.25	0.51
1:C:470:TYR:CE1	1:C:525:ASP:CG	2.84	0.51
1:A:547:TRP:HA	1:C:689:SER:OG	2.09	0.51
1:C:559:CYS:O	1:C:584:ASP:OD2	2.27	0.51
1:F:274:LEU:N	1:F:274:LEU:HD12	2.25	0.51
1:E:235:LEU:HD21	1:E:263:PRO:HG2	1.93	0.51
1:B:176:GLU:HG3	1:B:177:GLY:N	2.26	0.51
1:A:344:LYS:CE	3:H:80:ARG:CD	2.88	0.51
1:D:677:TYR:CE1	1:E:541:ASP:HB2	2.45	0.51
2:G:46:ILE:HB	2:G:511:GLN:HB3	1.91	0.51
2:G:46:ILE:HD12	2:G:511:GLN:NE2	2.26	0.51
1:C:274:LEU:HD12	1:C:274:LEU:N	2.26	0.51
2:G:66:ARG:O	2:G:68:ARG:HG3	2.11	0.51
1:D:176:GLU:HG3	1:D:177:GLY:N	2.26	0.51
1:E:308:ARG:HB2	1:E:343:GLN:HG2	1.92	0.51
1:A:235:LEU:HD21	1:A:263:PRO:HG2	1.93	0.51
1:A:176:GLU:HG3	1:A:177:GLY:N	2.26	0.51
1:C:176:GLU:HG3	1:C:177:GLY:N	2.26	0.51
2:G:274:GLY:HA2	2:G:284:THR:HG23	1.93	0.51
1:E:461:ASP:O	1:E:466:GLY:O	2.29	0.51
1:B:308:ARG:HB2	1:B:343:GLN:HG2	1.92	0.51
1:D:308:ARG:HB2	1:D:343:GLN:HG2	1.92	0.51
1:E:274:LEU:N	1:E:274:LEU:HD12	2.25	0.51
1:A:624:ILE:HG13	1:A:655:ASN:HB2	1.93	0.51
1:E:176:GLU:HG3	1:E:177:GLY:N	2.26	0.51
1:A:461:ASP:O	1:A:466:GLY:O	2.29	0.51
1:F:308:ARG:HB2	1:F:343:GLN:HG2	1.92	0.51
1:B:612:ILE:CD1	1:C:577:LEU:HD13	2.40	0.51
2:G:455:VAL:O	2:G:455:VAL:HG13	2.10	0.51
1:C:235:LEU:HD21	1:C:263:PRO:HG2	1.93	0.51
1:D:574:HIS:CE1	1:D:618:PRO:HD3	2.46	0.51
1:E:654:TYR:CE2	1:E:670:PHE:HD1	2.17	0.50
1:B:690:PHE:HZ	1:D:552:PHE:CE2	2.28	0.50
1:B:574:HIS:CE1	1:B:618:PRO:HD3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:LEU:HD11	1:B:399:PRO:CG	2.38	0.50
2:G:462:VAL:CG2	2:G:477:LEU:HD11	2.41	0.50
2:G:234:GLU:O	2:G:320:LYS:HD3	2.12	0.50
1:A:221:PHE:CE1	2:G:202:PHE:CE2	2.88	0.50
1:B:274:LEU:N	1:B:274:LEU:HD12	2.25	0.50
2:G:109:ASP:HB3	2:G:113:GLU:HG3	1.93	0.50
1:A:275:PHE:CD2	3:H:80:ARG:NE	2.78	0.50
1:D:508:VAL:HG13	1:D:527:HIS:CE1	2.46	0.50
1:F:574:HIS:CE1	1:F:618:PRO:HD3	2.46	0.50
1:B:235:LEU:HD21	1:B:263:PRO:HG2	1.93	0.50
1:F:176:GLU:HG3	1:F:177:GLY:N	2.26	0.50
1:A:552:PHE:HB3	1:C:690:PHE:CZ	2.44	0.50
1:A:514:TYR:HE1	1:B:464:PRO:CG	2.20	0.50
1:E:629:ASP:CG	1:E:659:HIS:HE1	2.14	0.50
1:E:574:HIS:CE1	1:E:618:PRO:HD3	2.46	0.50
1:F:539:ARG:HD2	1:F:542:LYS:NZ	2.27	0.50
1:A:539:ARG:HD2	1:A:542:LYS:NZ	2.27	0.50
1:B:461:ASP:O	1:B:466:GLY:O	2.29	0.50
1:B:654:TYR:CZ	1:B:670:PHE:HB3	2.46	0.50
1:E:518:GLY:HA2	1:F:324:GLN:NE2	1.87	0.50
1:F:630:TRP:CB	1:F:670:PHE:CZ	2.93	0.50
1:D:654:TYR:CG	1:D:670:PHE:CD2	3.00	0.50
2:G:140:ILE:HD13	2:G:140:ILE:N	2.27	0.50
1:C:574:HIS:CE1	1:C:618:PRO:HD3	2.46	0.50
1:A:574:HIS:CE1	1:A:618:PRO:HD3	2.46	0.50
2:G:491:ALA:HB3	2:G:504:GLY:HA3	1.94	0.49
1:D:461:ASP:O	1:D:466:GLY:O	2.29	0.49
1:B:551:ARG:NH1	1:B:641:GLU:CD	2.62	0.49
1:A:399:PRO:HG3	1:B:626:LEU:HD13	1.94	0.49
2:G:313:LEU:CD2	2:G:324:VAL:HG22	2.42	0.49
1:A:508:VAL:HG13	1:A:527:HIS:CE1	2.48	0.49
1:C:539:ARG:HD2	1:C:542:LYS:NZ	2.27	0.49
2:G:157:LEU:HD13	2:G:157:LEU:O	2.13	0.49
1:D:673:HIS:CD2	1:D:685:PRO:HG3	2.48	0.49
1:F:461:ASP:O	1:F:466:GLY:O	2.29	0.49
1:E:95:TYR:HA	1:E:96:PRO:C	2.33	0.49
2:G:202:PHE:CZ	2:G:212:ARG:HD2	2.48	0.49
2:G:178:ALA:HB1	2:G:228:SER:HA	1.94	0.49
1:E:137:CYS:SG	1:E:159:LEU:HD11	2.53	0.49
2:G:69:LEU:O	2:G:69:LEU:HD13	2.12	0.49
1:A:508:VAL:CG1	1:A:527:HIS:CD2	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:VAL:O	1:C:509:GLU:HA	2.11	0.49
1:B:237:SER:OG	1:B:238:HIS:HA	2.13	0.49
2:G:453:THR:HG22	2:G:455:VAL:HG12	1.93	0.49
1:E:539:ARG:HD2	1:E:542:LYS:NZ	2.27	0.49
1:A:560:MET:CE	1:A:586:PRO:HD3	2.43	0.49
2:G:118:ILE:CD1	2:G:118:ILE:N	2.76	0.49
1:C:461:ASP:O	1:C:466:GLY:O	2.29	0.49
1:B:95:TYR:HA	1:B:96:PRO:C	2.33	0.49
1:C:137:CYS:SG	1:C:159:LEU:HD11	2.53	0.49
1:A:673:HIS:CD2	1:A:685:PRO:HG3	2.48	0.49
1:D:445:VAL:CG2	1:D:526:PRO:HG2	2.33	0.49
2:G:399:VAL:HG13	2:G:400:ILE:H	1.77	0.49
1:C:560:MET:CE	1:C:586:PRO:HD3	2.43	0.49
1:E:673:HIS:CD2	1:E:685:PRO:HG3	2.48	0.49
1:A:464:PRO:CD	1:B:523:SER:HA	2.42	0.49
2:G:206:GLY:O	2:G:208:HIS:N	2.41	0.49
1:F:137:CYS:SG	1:F:159:LEU:HD11	2.53	0.49
1:D:560:MET:CE	1:D:586:PRO:HD3	2.43	0.49
1:E:568:SER:HG	1:E:670:PHE:HE1	1.59	0.49
1:B:560:MET:CE	1:B:586:PRO:HD3	2.43	0.49
1:D:137:CYS:SG	1:D:159:LEU:HD11	2.53	0.49
1:B:137:CYS:SG	1:B:159:LEU:HD11	2.53	0.49
1:A:660:GLN:C	1:A:661:LEU:HD12	2.34	0.49
1:C:673:HIS:CD2	1:C:685:PRO:HG3	2.48	0.48
1:C:95:TYR:HA	1:C:96:PRO:C	2.33	0.48
1:F:50:PHE:CE2	1:F:503:VAL:HG23	2.48	0.48
1:D:95:TYR:HA	1:D:96:PRO:C	2.33	0.48
1:C:514:TYR:HE1	1:D:464:PRO:CG	2.22	0.48
1:E:237:SER:OG	1:E:238:HIS:HA	2.13	0.48
2:G:429:TYR:O	2:G:430:GLN:HG3	2.14	0.48
1:D:539:ARG:HD2	1:D:542:LYS:NZ	2.27	0.48
1:D:660:GLN:C	1:D:661:LEU:HD12	2.34	0.48
1:F:560:MET:CE	1:F:586:PRO:HD3	2.43	0.48
1:D:690:PHE:HE2	1:E:541:ASP:N	2.06	0.48
1:F:237:SER:OG	1:F:238:HIS:HA	2.13	0.48
1:B:539:ARG:HD2	1:B:542:LYS:NZ	2.27	0.48
1:A:50:PHE:CE2	1:A:503:VAL:HG23	2.48	0.48
2:G:170:PRO:CD	2:G:190:THR:HG21	2.42	0.48
1:E:560:MET:CE	1:E:586:PRO:HD3	2.43	0.48
1:D:50:PHE:CE2	1:D:503:VAL:HG23	2.48	0.48
1:F:673:HIS:CD2	1:F:685:PRO:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:HIS:CD2	1:B:685:PRO:HG3	2.48	0.48
1:C:237:SER:OG	1:C:238:HIS:HA	2.13	0.48
1:E:660:GLN:C	1:E:661:LEU:HD12	2.34	0.48
1:E:351:ASP:HA	1:E:431:ARG:HB2	1.96	0.48
1:D:237:SER:OG	1:D:238:HIS:HA	2.13	0.48
1:A:137:CYS:SG	1:A:159:LEU:HD11	2.53	0.48
1:A:237:SER:OG	1:A:238:HIS:HA	2.13	0.48
1:B:508:VAL:HB	1:B:539:ARG:NH2	2.28	0.48
1:F:559:CYS:HB3	1:F:560:MET:H	1.31	0.48
1:D:417:THR:HA	1:D:418:PRO:HD3	1.74	0.48
1:C:654:TYR:CE1	1:C:670:PHE:CB	2.96	0.48
2:G:427:VAL:HG11	2:G:429:TYR:CE1	2.48	0.48
1:E:50:PHE:CE2	1:E:503:VAL:HG23	2.48	0.48
1:C:660:GLN:C	1:C:661:LEU:HD12	2.34	0.48
1:B:691:GLN:CB	1:D:441:ASN:HA	2.31	0.48
1:A:445:VAL:CG2	1:A:526:PRO:HG2	2.36	0.48
1:A:326:PHE:CG	1:A:359:PRO:HG3	2.49	0.48
1:B:50:PHE:CE2	1:B:503:VAL:HG23	2.48	0.48
1:C:50:PHE:CE2	1:C:503:VAL:HG23	2.48	0.48
1:F:660:GLN:C	1:F:661:LEU:HD12	2.34	0.48
1:C:326:PHE:CG	1:C:359:PRO:HG3	2.49	0.48
1:A:327:ASN:O	1:A:327:ASN:CG	2.52	0.48
1:B:141:ARG:HD2	1:B:143:ASP:OD1	2.14	0.47
1:F:594:CYS:O	1:F:601:GLU:HA	2.14	0.47
1:E:141:ARG:HD2	1:E:143:ASP:OD1	2.14	0.47
1:E:327:ASN:CG	1:E:327:ASN:O	2.52	0.47
1:E:326:PHE:CG	1:E:359:PRO:HG3	2.49	0.47
2:G:285:THR:HG23	2:G:379:GLY:CA	2.44	0.47
2:G:211:ILE:CD1	2:G:281:ASN:HA	2.44	0.47
1:F:95:TYR:HA	1:F:96:PRO:C	2.33	0.47
1:F:351:ASP:HA	1:F:431:ARG:HB2	1.96	0.47
2:G:263:ALA:O	2:G:264:ARG:HG2	2.15	0.47
1:A:594:CYS:O	1:A:601:GLU:HA	2.14	0.47
2:G:453:THR:CG2	2:G:454:ASP:N	2.78	0.47
1:A:141:ARG:HD2	1:A:143:ASP:OD1	2.15	0.47
1:F:141:ARG:HD2	1:F:143:ASP:OD1	2.15	0.47
1:A:95:TYR:HA	1:A:96:PRO:C	2.33	0.47
1:D:654:TYR:CD2	1:D:670:PHE:CD1	3.02	0.47
1:B:660:GLN:C	1:B:661:LEU:HD12	2.34	0.47
2:G:427:VAL:CG1	2:G:429:TYR:H	2.27	0.47
2:G:246:PHE:CZ	2:G:265:ILE:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ASP:HA	1:D:431:ARG:HB2	1.96	0.47
1:E:654:TYR:CD1	1:E:670:PHE:HB2	2.49	0.47
2:G:287:LEU:HD11	2:G:379:GLY:HA3	1.96	0.47
1:C:594:CYS:O	1:C:601:GLU:HA	2.14	0.47
1:B:327:ASN:CG	1:B:327:ASN:O	2.52	0.47
2:G:377:ARG:O	2:G:380:THR:HB	2.14	0.47
1:C:327:ASN:CG	1:C:327:ASN:O	2.52	0.47
1:A:508:VAL:CG1	1:A:527:HIS:CE1	2.97	0.47
1:F:326:PHE:CG	1:F:359:PRO:HG3	2.49	0.47
1:F:629:ASP:CG	1:F:659:HIS:HE1	2.16	0.47
2:G:482:VAL:HG12	2:G:510:ALA:HB1	1.97	0.47
2:G:509:VAL:HG12	2:G:510:ALA:N	2.30	0.47
1:B:508:VAL:HG13	1:B:527:HIS:NE2	2.29	0.47
1:D:594:CYS:O	1:D:601:GLU:HA	2.14	0.47
1:D:141:ARG:HD2	1:D:143:ASP:OD1	2.14	0.47
1:B:638:ARG:HB2	1:B:645:ILE:HD13	1.97	0.47
1:A:409:ILE:CG2	2:G:194:PHE:CD2	2.89	0.47
2:G:160:SER:HB3	2:G:161:HIS:CE1	2.49	0.47
1:F:327:ASN:CG	1:F:327:ASN:O	2.52	0.47
1:F:459:ARG:HD3	1:F:526:PRO:HG3	1.97	0.47
1:B:594:CYS:O	1:B:601:GLU:HA	2.14	0.47
1:F:533:LEU:HD13	1:F:641:GLU:HB3	1.96	0.46
1:F:570:SER:HB3	1:F:683:HIS:CG	2.49	0.46
2:G:92:VAL:HG12	2:G:94:PRO:HD3	1.97	0.46
1:C:417:THR:HA	1:C:418:PRO:HD3	1.74	0.46
1:A:476:PHE:CE2	1:A:482:ILE:HD13	2.51	0.46
1:E:594:CYS:O	1:E:601:GLU:HA	2.14	0.46
1:A:508:VAL:HG11	1:A:527:HIS:NE2	2.27	0.46
1:B:326:PHE:CG	1:B:359:PRO:HG3	2.49	0.46
1:C:351:ASP:HA	1:C:431:ARG:HB2	1.96	0.46
1:C:539:ARG:HB2	1:C:542:LYS:HD3	1.97	0.46
1:F:654:TYR:CG	1:F:670:PHE:CB	2.98	0.46
1:F:533:LEU:HB3	1:F:642:THR:HG23	1.86	0.46
1:A:630:TRP:CB	1:A:670:PHE:CZ	2.98	0.46
1:B:159:LEU:HD13	1:B:184:ILE:HD13	1.98	0.46
1:C:141:ARG:HD2	1:C:143:ASP:OD1	2.14	0.46
1:D:326:PHE:CG	1:D:359:PRO:HG3	2.49	0.46
2:G:164:ASN:ND2	2:G:166:ARG:HG3	2.31	0.46
1:D:577:LEU:HD11	1:F:607:SER:HB3	1.75	0.46
1:B:654:TYR:CE2	1:B:670:PHE:HB3	2.50	0.46
1:A:96:PRO:N	2:G:277:ARG:NH2	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:LEU:HD13	1:F:184:ILE:HD13	1.98	0.46
1:B:328:ILE:HB	1:B:332:GLU:OE1	2.16	0.46
2:G:358:HIS:CD2	2:G:406:HIS:HE1	2.33	0.46
1:C:328:ILE:HB	1:C:332:GLU:OE1	2.16	0.46
1:D:327:ASN:CG	1:D:327:ASN:O	2.52	0.46
1:E:476:PHE:CE2	1:E:482:ILE:HD13	2.51	0.46
1:A:638:ARG:HB2	1:A:645:ILE:HD13	1.97	0.46
1:D:638:ARG:HB2	1:D:645:ILE:HD13	1.97	0.46
1:F:81:VAL:HG11	1:F:145:LEU:HB2	1.98	0.46
1:F:533:LEU:CD1	1:F:641:GLU:OE1	2.64	0.46
1:A:464:PRO:HG2	1:B:514:TYR:CE1	2.51	0.46
1:B:539:ARG:HB2	1:B:542:LYS:HD3	1.97	0.46
1:E:539:ARG:HB2	1:E:542:LYS:HD3	1.97	0.46
1:B:81:VAL:HG11	1:B:145:LEU:HB2	1.98	0.46
1:E:277:THR:HG22	1:E:279:ARG:HG3	1.98	0.46
1:D:476:PHE:CE2	1:D:482:ILE:HD13	2.51	0.46
1:F:476:PHE:CE2	1:F:482:ILE:HD13	2.51	0.46
1:B:351:ASP:HA	1:B:431:ARG:HB2	1.96	0.46
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.83	0.46
1:F:539:ARG:HB2	1:F:542:LYS:HD3	1.97	0.46
1:A:539:ARG:HB2	1:A:542:LYS:HD3	1.97	0.46
1:A:159:LEU:HD13	1:A:184:ILE:HD13	1.98	0.46
1:F:672:CYS:HB3	1:F:681:CYS:SG	2.56	0.46
1:D:328:ILE:HB	1:D:332:GLU:OE1	2.16	0.46
2:G:115:ALA:HB3	2:G:117:PHE:CE1	2.50	0.46
2:G:134:THR:O	2:G:136:ALA:N	2.43	0.46
1:D:691:GLN:CB	1:E:441:ASN:HA	2.43	0.46
1:D:539:ARG:HB2	1:D:542:LYS:HD3	1.97	0.46
1:B:476:PHE:CE2	1:B:482:ILE:HD13	2.51	0.46
1:D:550:ASN:HB2	1:D:586:PRO:HA	1.97	0.46
2:G:180:LEU:HD11	2:G:182:ILE:CD1	2.46	0.46
1:F:638:ARG:HB2	1:F:645:ILE:HD13	1.97	0.46
1:A:351:ASP:HA	1:A:431:ARG:HB2	1.96	0.46
1:E:329:SER:HB3	1:E:332:GLU:HG3	1.98	0.46
1:E:654:TYR:CG	1:E:670:PHE:CE2	2.92	0.46
1:A:112:ASN:HB2	1:A:132:LEU:HD22	1.98	0.46
1:B:329:SER:HB3	1:B:332:GLU:HG3	1.98	0.46
1:D:329:SER:HB3	1:D:332:GLU:HG3	1.98	0.46
2:G:342:MET:HG3	2:G:421:ILE:CG1	2.46	0.46
1:C:81:VAL:HG11	1:C:145:LEU:HB2	1.98	0.46
1:D:81:VAL:HG11	1:D:145:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:323:ILE:HD12	2:G:323:ILE:N	2.31	0.46
2:G:432:THR:CG2	2:G:454:ASP:HB3	2.46	0.45
1:B:112:ASN:HB2	1:B:132:LEU:HD22	1.98	0.45
1:F:559:CYS:O	1:F:584:ASP:HB2	2.16	0.45
1:F:277:THR:HG22	1:F:279:ARG:HG3	1.98	0.45
1:C:277:THR:HG22	1:C:279:ARG:HG3	1.98	0.45
1:C:638:ARG:HB2	1:C:645:ILE:HD13	1.97	0.45
1:A:274:LEU:O	3:H:80:ARG:CZ	2.63	0.45
1:C:654:TYR:HB3	1:C:670:PHE:CE2	2.50	0.45
1:C:112:ASN:HB2	1:C:132:LEU:HD22	1.98	0.45
1:C:329:SER:HB3	1:C:332:GLU:HG3	1.98	0.45
1:C:672:CYS:HB3	1:C:681:CYS:SG	2.56	0.45
1:A:342:GLY:HA2	3:H:84:TYR:OH	2.16	0.45
1:C:514:TYR:CE1	1:D:464:PRO:CG	2.98	0.45
1:B:660:GLN:HB2	2:G:105:TRP:NE1	2.31	0.45
1:A:231:ASP:OD2	2:G:218:SER:N	2.45	0.45
1:E:328:ILE:HB	1:E:332:GLU:OE1	2.16	0.45
1:C:476:PHE:CE2	1:C:482:ILE:HD13	2.51	0.45
2:G:399:VAL:HG13	2:G:400:ILE:N	2.32	0.45
1:B:533:LEU:HA	1:B:533:LEU:HD23	1.84	0.45
1:D:508:VAL:HB	1:D:539:ARG:NH2	2.32	0.45
2:G:110:ILE:HA	2:G:114:CYS:HB2	1.98	0.45
1:E:638:ARG:HB2	1:E:645:ILE:HD13	1.97	0.45
1:B:672:CYS:HB3	1:B:681:CYS:SG	2.56	0.45
1:D:112:ASN:HB2	1:D:132:LEU:HD22	1.98	0.45
1:D:508:VAL:CG1	1:D:527:HIS:CD2	3.00	0.45
1:A:328:ILE:HB	1:A:332:GLU:OE1	2.16	0.45
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.84	0.45
1:B:568:SER:HB2	1:B:670:PHE:CE1	2.51	0.45
1:B:577:LEU:HD13	1:C:612:ILE:CD1	2.45	0.45
1:B:612:ILE:HD13	1:C:612:ILE:HD13	1.97	0.45
1:D:159:LEU:HD13	1:D:184:ILE:HD13	1.98	0.45
2:G:512:LEU:HD23	2:G:513:PRO:O	2.17	0.45
1:A:277:THR:HG22	1:A:279:ARG:HG3	1.98	0.45
1:B:630:TRP:HB3	1:B:670:PHE:HE2	1.81	0.45
1:B:661:LEU:HD11	2:G:105:TRP:CD1	2.52	0.45
1:E:159:LEU:HD13	1:E:184:ILE:HD13	1.98	0.45
1:F:328:ILE:HB	1:F:332:GLU:OE1	2.16	0.45
1:A:672:CYS:HB3	1:A:681:CYS:SG	2.56	0.45
1:B:612:ILE:HD12	1:C:612:ILE:HG21	1.99	0.45
1:D:677:TYR:CE2	1:E:541:ASP:HB3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:239:GLU:OE1	2:G:384:LYS:HG3	2.17	0.45
2:G:152:ASP:HB2	2:G:154:ILE:CD1	2.40	0.45
2:G:427:VAL:HG13	2:G:429:TYR:CE2	2.52	0.45
1:E:411:GLN:HA	1:E:412:PRO:C	2.38	0.45
2:G:27:ASN:ND2	2:G:28:ASN:H	2.14	0.45
1:D:277:THR:HG22	1:D:279:ARG:HG3	1.98	0.45
2:G:77:ILE:CD1	2:G:144:ILE:HD11	2.47	0.45
1:C:571:VAL:CG2	1:C:655:ASN:CB	2.89	0.45
1:B:661:LEU:HD11	2:G:105:TRP:HD1	1.82	0.45
2:G:105:TRP:HE3	2:G:105:TRP:HA	1.80	0.45
1:C:159:LEU:HD13	1:C:184:ILE:HD13	1.98	0.45
1:A:329:SER:HB3	1:A:332:GLU:HG3	1.98	0.45
1:A:162:VAL:CG2	1:A:189:ASP:HB2	2.47	0.45
1:E:81:VAL:HG11	1:E:145:LEU:HB2	1.98	0.45
1:A:547:TRP:HB3	1:C:677:TYR:HB3	2.00	0.44
1:F:570:SER:CB	1:F:683:HIS:HB3	2.45	0.44
2:G:95:VAL:HG13	2:G:99:ARG:HB3	1.99	0.44
2:G:502:TYR:CD1	2:G:502:TYR:N	2.85	0.44
2:G:91:ILE:HD13	2:G:157:LEU:HB2	1.98	0.44
1:D:551:ARG:HH12	1:D:641:GLU:CD	2.13	0.44
1:E:112:ASN:HB2	1:E:132:LEU:HD22	1.98	0.44
1:C:535:ASN:CB	1:C:646:PHE:HA	2.47	0.44
2:G:512:LEU:HD23	2:G:512:LEU:C	2.38	0.44
1:B:162:VAL:CG2	1:B:189:ASP:HB2	2.47	0.44
1:E:672:CYS:HB3	1:E:681:CYS:SG	2.56	0.44
2:G:277:ARG:O	2:G:278:SER:O	2.35	0.44
1:B:612:ILE:CG1	1:C:577:LEU:HD13	2.47	0.44
1:E:533:LEU:HD13	1:E:642:THR:HG23	2.00	0.44
1:E:533:LEU:HD23	1:E:533:LEU:HA	1.84	0.44
1:F:411:GLN:HA	1:F:412:PRO:C	2.38	0.44
1:C:411:GLN:HA	1:C:412:PRO:C	2.38	0.44
1:A:81:VAL:HG11	1:A:145:LEU:HB2	1.98	0.44
1:D:672:CYS:HB3	1:D:681:CYS:SG	2.56	0.44
1:B:277:THR:HG22	1:B:279:ARG:HG3	1.98	0.44
1:E:417:THR:HA	1:E:418:PRO:HD3	1.74	0.44
1:F:329:SER:HB3	1:F:332:GLU:HG3	1.98	0.44
3:H:80:ARG:O	3:H:82:CYS:N	2.51	0.44
1:F:654:TYR:HB3	1:F:670:PHE:CG	2.52	0.44
1:C:560:MET:HE2	1:C:586:PRO:HD3	2.00	0.44
1:F:112:ASN:HB2	1:F:132:LEU:HD22	1.98	0.44
1:D:411:GLN:HA	1:D:412:PRO:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:VAL:CG2	1:F:189:ASP:HB2	2.47	0.44
1:C:162:VAL:CG2	1:C:189:ASP:HB2	2.48	0.44
1:F:482:ILE:HG23	1:F:497:VAL:HG13	2.00	0.44
1:A:409:ILE:HG21	2:G:194:PHE:HE2	1.57	0.44
1:C:629:ASP:CG	1:C:659:HIS:CE1	2.91	0.44
1:E:162:VAL:CG2	1:E:189:ASP:HB2	2.48	0.44
1:F:149:VAL:HG22	1:F:150:GLU:N	2.33	0.44
1:B:630:TRP:HB3	1:B:670:PHE:CE2	2.53	0.44
1:D:525:ASP:HA	1:D:526:PRO:HD3	1.86	0.44
2:G:149:HIS:HB2	2:G:152:ASP:OD2	2.17	0.44
1:A:231:ASP:OD1	2:G:217:ASP:HA	2.18	0.44
2:G:66:ARG:HA	2:G:150:PRO:HB2	1.98	0.44
1:C:191:LYS:N	1:C:191:LYS:HD2	2.33	0.44
1:C:482:ILE:HG23	1:C:497:VAL:HG13	2.00	0.44
1:C:149:VAL:HG22	1:C:150:GLU:N	2.33	0.44
1:D:690:PHE:CE2	1:E:541:ASP:N	2.85	0.44
2:G:287:LEU:HD11	2:G:378:PRO:O	2.17	0.44
1:A:523:SER:HA	1:B:464:PRO:HD3	1.99	0.44
1:C:459:ARG:HG3	1:C:526:PRO:CG	2.47	0.44
1:B:191:LYS:HD2	1:B:191:LYS:N	2.33	0.44
1:A:411:GLN:HA	1:A:412:PRO:C	2.38	0.44
2:G:382:PRO:HA	2:G:389:PHE:CZ	2.53	0.44
1:D:149:VAL:HG22	1:D:150:GLU:N	2.33	0.44
1:A:547:TRP:CA	1:C:689:SER:OG	2.66	0.43
1:F:654:TYR:CD1	1:F:656:CYS:SG	3.11	0.43
1:A:396:ALA:HB2	2:G:107:GLY:HA3	1.98	0.43
1:E:191:LYS:HD2	1:E:191:LYS:N	2.33	0.43
1:D:508:VAL:HG13	1:D:527:HIS:NE2	2.33	0.43
1:C:313:ALA:HB1	1:C:335:LEU:HD11	2.00	0.43
1:E:149:VAL:HG22	1:E:150:GLU:N	2.33	0.43
1:B:313:ALA:HB1	1:B:335:LEU:HD11	2.00	0.43
1:E:57:ARG:HG2	1:E:121:TYR:CE1	2.53	0.43
2:G:181:LEU:HA	2:G:185:GLU:O	2.17	0.43
1:B:525:ASP:HA	1:B:526:PRO:HD3	1.85	0.43
2:G:492:MET:HG3	2:G:501:LEU:HD21	2.01	0.43
1:F:191:LYS:HD2	1:F:191:LYS:N	2.33	0.43
1:A:191:LYS:HD2	1:A:191:LYS:N	2.33	0.43
1:D:629:ASP:OD1	1:D:659:HIS:CE1	2.71	0.43
1:B:411:GLN:HA	1:B:412:PRO:C	2.38	0.43
1:D:482:ILE:HG23	1:D:497:VAL:HG13	2.00	0.43
1:B:482:ILE:HG23	1:B:497:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ASP:CB	3:H:80:ARG:NE	2.79	0.43
1:F:535:ASN:CG	1:F:645:ILE:O	2.57	0.43
1:D:313:ALA:HB1	1:D:335:LEU:HD11	2.00	0.43
1:D:56:HIS:HB3	1:D:59:THR:OG1	2.19	0.43
1:A:149:VAL:HG22	1:A:150:GLU:N	2.33	0.43
1:B:149:VAL:HG22	1:B:150:GLU:N	2.33	0.43
1:F:56:HIS:HB3	1:F:59:THR:OG1	2.19	0.43
1:F:57:ARG:HG2	1:F:121:TYR:CE1	2.54	0.43
2:G:292:ILE:O	2:G:415:PRO:HD3	2.18	0.43
3:H:76:ASP:O	3:H:77:LEU:HD23	2.19	0.43
2:G:75:ASP:HB3	2:G:94:PRO:HB3	2.01	0.43
2:G:118:ILE:HA	2:G:133:GLY:CA	2.49	0.43
2:G:356:TYR:OH	2:G:377:ARG:NH1	2.51	0.43
1:A:313:ALA:HB1	1:A:335:LEU:HD11	2.00	0.43
1:D:162:VAL:CG2	1:D:189:ASP:HB2	2.47	0.43
1:A:96:PRO:HD3	2:G:277:ARG:HD3	1.88	0.43
1:D:191:LYS:HD2	1:D:191:LYS:N	2.33	0.43
2:G:375:TYR:CD1	2:G:376:PRO:HA	2.54	0.43
1:D:470:TYR:CE1	1:D:525:ASP:CG	2.92	0.43
1:F:533:LEU:CD1	1:F:641:GLU:CD	2.87	0.43
2:G:287:LEU:CD2	2:G:409:MET:CE	2.82	0.43
1:D:57:ARG:HG2	1:D:121:TYR:CE1	2.54	0.43
1:E:56:HIS:HB3	1:E:59:THR:OG1	2.19	0.43
2:G:503:ILE:CD1	2:G:503:ILE:N	2.82	0.43
1:B:560:MET:HE2	1:B:586:PRO:HD3	2.01	0.43
1:A:482:ILE:HG23	1:A:497:VAL:HG13	2.00	0.43
1:B:417:THR:HA	1:B:418:PRO:HD3	1.74	0.43
1:E:196:PRO:HG3	1:E:215:TYR:OH	2.19	0.43
1:C:57:ARG:HG2	1:C:121:TYR:CE1	2.53	0.43
1:C:654:TYR:HD2	1:C:670:PHE:CZ	2.34	0.42
2:G:137:PHE:CD2	2:G:171:TYR:HB3	2.53	0.42
1:B:533:LEU:HB3	1:B:642:THR:HG21	2.01	0.42
2:G:84:ASN:C	2:G:86:LYS:H	2.22	0.42
1:A:57:ARG:HG2	1:A:121:TYR:CE1	2.54	0.42
1:D:654:TYR:CD2	1:D:670:PHE:CD2	3.07	0.42
2:G:182:ILE:CD1	2:G:231:LEU:HG	2.48	0.42
1:A:151:PRO:HG2	1:A:213:LEU:HD12	2.02	0.42
2:G:229:ALA:HA	2:G:244:TYR:O	2.19	0.42
1:D:196:PRO:HG3	1:D:215:TYR:OH	2.19	0.42
2:G:39:MET:HE3	2:G:45:VAL:HG13	2.01	0.42
1:E:192:GLN:HG3	1:E:228:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:CYS:HA	1:C:702:PRO:HD3	1.89	0.42
2:G:431:PHE:CD1	2:G:431:PHE:N	2.83	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.84	0.42
2:G:203:ARG:NH2	2:G:273:PHE:CZ	2.87	0.42
2:G:208:HIS:ND1	2:G:209:HIS:N	2.68	0.42
1:D:192:GLN:HG3	1:D:228:ILE:O	2.19	0.42
1:D:610:GLN:HE22	1:F:577:LEU:HB3	1.84	0.42
1:A:56:HIS:HB3	1:A:59:THR:OG1	2.19	0.42
1:B:57:ARG:HG2	1:B:121:TYR:CE1	2.54	0.42
2:G:121:LEU:C	2:G:122:GLU:HG2	2.40	0.42
1:F:204:PRO:HD2	1:F:212:MET:SD	2.60	0.42
1:B:192:GLN:HG3	1:B:228:ILE:O	2.19	0.42
1:B:619:LYS:HD3	1:B:619:LYS:HA	1.91	0.42
1:E:654:TYR:CE2	1:E:670:PHE:CG	2.91	0.42
1:D:571:VAL:HG21	1:D:655:ASN:HB2	2.00	0.42
1:C:482:ILE:HD12	1:C:497:VAL:HG11	2.02	0.42
1:F:313:ALA:HB1	1:F:335:LEU:HD11	2.00	0.42
1:F:476:PHE:HE2	1:F:482:ILE:HD13	1.85	0.42
1:F:482:ILE:HD12	1:F:497:VAL:HG11	2.02	0.42
1:D:151:PRO:HG2	1:D:213:LEU:HD12	2.01	0.42
1:F:57:ARG:HG3	1:F:58:ARG:HG3	2.02	0.42
1:A:196:PRO:HG3	1:A:215:TYR:OH	2.19	0.42
1:B:56:HIS:HB3	1:B:59:THR:OG1	2.19	0.42
1:C:619:LYS:HD3	1:C:619:LYS:HA	1.91	0.42
1:F:309:LEU:HA	1:F:309:LEU:HD23	1.89	0.42
1:C:56:HIS:HB3	1:C:59:THR:OG1	2.19	0.42
1:F:624:ILE:HG13	1:F:655:ASN:HB3	1.91	0.42
1:E:482:ILE:HD12	1:E:497:VAL:HG11	2.02	0.42
1:E:482:ILE:HG23	1:E:497:VAL:HG13	2.00	0.42
1:C:204:PRO:HD2	1:C:212:MET:SD	2.60	0.42
1:C:192:GLN:HG3	1:C:228:ILE:O	2.20	0.42
1:A:204:PRO:HD2	1:A:212:MET:SD	2.60	0.42
2:G:55:SER:O	2:G:73:ALA:HB1	2.19	0.42
1:E:37:GLN:HA	1:E:37:GLN:OE1	2.20	0.42
1:B:691:GLN:HE22	1:D:442:GLY:HA2	1.85	0.42
1:B:577:LEU:HD13	1:C:612:ILE:HD11	2.02	0.42
1:C:508:VAL:HG11	1:C:539:ARG:NH2	2.34	0.42
2:G:402:PHE:O	2:G:404:ARG:N	2.50	0.42
2:G:453:THR:HG22	2:G:454:ASP:N	2.34	0.42
1:F:550:ASN:HB2	1:F:586:PRO:HA	2.02	0.42
1:A:57:ARG:HG3	1:A:58:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLN:HA	1:C:37:GLN:OE1	2.20	0.42
1:C:398:VAL:HA	1:C:399:PRO:HD3	1.93	0.42
1:E:626:LEU:HG	1:F:399:PRO:HG3	1.79	0.42
1:A:476:PHE:HE2	1:A:482:ILE:HD13	1.85	0.42
1:F:654:TYR:HD1	1:F:656:CYS:SG	2.42	0.41
1:A:192:GLN:HG3	1:A:228:ILE:O	2.20	0.41
1:B:459:ARG:HG3	1:B:526:PRO:HG3	2.00	0.41
2:G:427:VAL:HG12	2:G:429:TYR:H	1.85	0.41
1:E:87:PRO:HB2	1:E:109:LEU:CD1	2.51	0.41
1:D:482:ILE:HD12	1:D:497:VAL:HG11	2.02	0.41
1:C:476:PHE:HE2	1:C:482:ILE:HD13	1.85	0.41
1:E:313:ALA:HB1	1:E:335:LEU:HD11	2.01	0.41
2:G:74:LYS:O	2:G:76:HIS:N	2.54	0.41
1:B:476:PHE:HE2	1:B:482:ILE:HD13	1.85	0.41
1:E:149:VAL:HG22	1:E:151:PRO:HD3	2.02	0.41
1:C:57:ARG:HG3	1:C:58:ARG:HG3	2.02	0.41
1:B:196:PRO:HG3	1:B:215:TYR:OH	2.19	0.41
2:G:56:SER:HB3	2:G:58:HIS:CD2	2.54	0.41
1:C:525:ASP:HA	1:C:526:PRO:HD3	1.86	0.41
1:C:541:ASP:HB3	1:F:677:TYR:CE1	2.55	0.41
2:G:244:TYR:HA	2:G:266:GLY:O	2.21	0.41
1:E:204:PRO:HD2	1:E:212:MET:SD	2.60	0.41
1:F:192:GLN:HG3	1:F:228:ILE:O	2.20	0.41
1:B:204:PRO:HD2	1:B:212:MET:SD	2.60	0.41
1:E:203:LEU:HD23	1:E:203:LEU:HA	1.84	0.41
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.20	0.41
2:G:416:ILE:O	2:G:417:ASN:HB2	2.20	0.41
1:D:663:LEU:CD2	1:D:698:SER:HB2	2.51	0.41
2:G:427:VAL:CG2	2:G:429:TYR:OH	2.69	0.41
1:A:87:PRO:HB2	1:A:109:LEU:CD1	2.51	0.41
1:E:476:PHE:HE2	1:E:482:ILE:HD13	1.85	0.41
1:F:196:PRO:HG3	1:F:215:TYR:OH	2.20	0.41
1:D:37:GLN:OE1	1:D:37:GLN:HA	2.20	0.41
2:G:223:ASP:N	2:G:224:PRO:CD	2.83	0.41
1:A:37:GLN:HA	1:A:37:GLN:OE1	2.20	0.41
1:F:571:VAL:CG2	1:F:655:ASN:HA	2.48	0.41
2:G:401:THR:C	2:G:402:PHE:O	2.58	0.41
1:A:482:ILE:HD12	1:A:497:VAL:HG11	2.02	0.41
1:B:149:VAL:HG22	1:B:151:PRO:HD3	2.02	0.41
1:D:204:PRO:HD2	1:D:212:MET:SD	2.60	0.41
1:C:196:PRO:HG3	1:C:215:TYR:OH	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:PHE:CD2	1:C:690:PHE:CZ	2.92	0.41
2:G:274:GLY:HA2	2:G:284:THR:CG2	2.51	0.41
1:A:345:GLN:HG2	3:H:128:GLU:OE2	2.21	0.41
1:D:533:LEU:HD23	1:D:533:LEU:HA	1.84	0.41
1:A:663:LEU:CD2	1:A:698:SER:HB2	2.50	0.41
1:D:493:LEU:HA	1:D:539:ARG:NH2	2.35	0.41
1:B:482:ILE:HD12	1:B:497:VAL:HG11	2.02	0.41
2:G:316:SER:HB2	2:G:323:ILE:CD1	2.51	0.41
2:G:77:ILE:HD13	2:G:144:ILE:HD11	2.02	0.41
1:B:151:PRO:HG2	1:B:213:LEU:HD12	2.01	0.41
1:A:547:TRP:HB2	1:C:689:SER:OG	2.20	0.41
1:D:560:MET:HE2	1:D:586:PRO:HD3	2.03	0.41
2:G:287:LEU:CD1	2:G:379:GLY:HA3	2.49	0.41
2:G:287:LEU:CD2	2:G:409:MET:HE1	2.40	0.41
2:G:434:ILE:CG1	2:G:435:VAL:N	2.83	0.41
1:D:87:PRO:HB2	1:D:109:LEU:CD1	2.51	0.41
1:C:87:PRO:HB2	1:C:109:LEU:CD1	2.51	0.41
2:G:342:MET:HG3	2:G:421:ILE:HG12	2.02	0.41
1:E:151:PRO:HG2	1:E:213:LEU:HD12	2.02	0.41
1:D:315:LEU:HD11	1:D:333:ASP:HB3	2.03	0.41
1:E:582:VAL:CG1	1:E:585:ALA:HB2	2.51	0.41
1:E:398:VAL:HA	1:E:399:PRO:HD3	1.93	0.41
1:D:68:ASN:ND2	1:D:87:PRO:HG3	2.36	0.41
1:C:151:PRO:HG2	1:C:213:LEU:HD12	2.02	0.41
1:D:57:ARG:HG3	1:D:58:ARG:HG3	2.02	0.41
1:B:57:ARG:HG3	1:B:58:ARG:HG3	2.02	0.41
1:B:404:PHE:CE2	1:B:406:GLY:HA2	2.56	0.41
1:E:309:LEU:HD23	1:E:309:LEU:HA	1.89	0.41
1:B:654:TYR:CG	1:B:670:PHE:CD2	3.09	0.41
2:G:392:THR:O	2:G:395:LEU:HD12	2.21	0.41
1:B:470:TYR:CE1	1:B:525:ASP:CG	2.94	0.41
1:A:391:VAL:HG11	2:G:195:MET:HE1	2.03	0.41
1:C:663:LEU:CD2	1:C:698:SER:HB2	2.50	0.41
2:G:180:LEU:HD13	2:G:180:LEU:C	2.41	0.41
2:G:427:VAL:HG21	2:G:429:TYR:CZ	2.55	0.41
1:B:68:ASN:ND2	1:B:87:PRO:HG3	2.36	0.41
1:F:151:PRO:HG2	1:F:213:LEU:HD12	2.01	0.41
1:C:149:VAL:HG22	1:C:151:PRO:HD3	2.02	0.41
1:E:57:ARG:HG3	1:E:58:ARG:HG3	2.02	0.41
1:D:582:VAL:CG1	1:D:585:ALA:HB2	2.51	0.41
1:C:556:ILE:HD11	1:D:324:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:PHE:CE2	1:D:406:GLY:HA2	2.56	0.41
1:A:404:PHE:CE2	1:A:406:GLY:HA2	2.56	0.41
1:A:564:VAL:HG23	1:A:649:THR:HG21	2.03	0.41
2:G:263:ALA:C	2:G:264:ARG:HG2	2.42	0.41
1:E:626:LEU:C	1:F:399:PRO:HA	2.40	0.41
1:A:68:ASN:ND2	1:A:87:PRO:HG3	2.36	0.41
1:E:68:ASN:ND2	1:E:87:PRO:HG3	2.36	0.41
1:A:493:LEU:HD22	1:A:539:ARG:CZ	2.51	0.41
1:F:149:VAL:HG22	1:F:151:PRO:HD3	2.03	0.41
1:E:404:PHE:CE2	1:E:406:GLY:HA2	2.56	0.41
1:A:582:VAL:CG1	1:A:585:ALA:HB2	2.51	0.41
1:B:582:VAL:CG1	1:B:585:ALA:HB2	2.51	0.41
1:C:508:VAL:N	1:C:509:GLU:N	2.67	0.40
2:G:427:VAL:CG2	2:G:429:TYR:CZ	3.04	0.40
1:D:149:VAL:HG22	1:D:151:PRO:HD3	2.02	0.40
3:H:31:ILE:HG21	3:H:138:TYR:CZ	2.56	0.40
1:C:582:VAL:CG1	1:C:585:ALA:HB2	2.51	0.40
1:B:315:LEU:HD11	1:B:333:ASP:HB3	2.03	0.40
2:G:62:LEU:C	2:G:62:LEU:HD13	2.41	0.40
1:A:409:ILE:HG22	2:G:194:PHE:CD2	2.53	0.40
1:F:564:VAL:HG23	1:F:649:THR:HG21	2.03	0.40
1:B:508:VAL:CG1	1:B:527:HIS:CD2	3.03	0.40
2:G:337:GLY:HA2	2:G:424:LYS:O	2.22	0.40
1:C:404:PHE:CE2	1:C:406:GLY:HA2	2.56	0.40
1:E:315:LEU:HD11	1:E:333:ASP:HB3	2.03	0.40
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.83	0.40
2:G:164:ASN:HD22	2:G:166:ARG:HG3	1.86	0.40
2:G:268:ILE:HD13	2:G:283:TRP:CE2	2.56	0.40
2:G:135:GLY:HA3	2:G:138:HIS:O	2.21	0.40
2:G:400:ILE:O	2:G:402:PHE:O	2.38	0.40
1:E:564:VAL:HG23	1:E:649:THR:HG21	2.03	0.40
2:G:29:VAL:HA	2:G:30:PRO:HD3	1.86	0.40
1:D:508:VAL:CG1	1:D:527:HIS:CE1	3.04	0.40
1:B:87:PRO:HB2	1:B:109:LEU:CD1	2.51	0.40
1:F:459:ARG:CD	1:F:526:PRO:HG3	2.52	0.40
1:F:525:ASP:HA	1:F:526:PRO:HD3	1.86	0.40
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.89	0.40
1:F:37:GLN:HA	1:F:37:GLN:OE1	2.20	0.40
1:D:309:LEU:HA	1:D:309:LEU:HD23	1.88	0.40
1:E:349:PRO:HA	1:E:350:PRO:HD3	1.96	0.40
1:B:612:ILE:HD11	1:C:577:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:624:ILE:HA	1:F:625:PRO:HD2	1.94	0.40
1:D:654:TYR:CE2	1:D:670:PHE:CD1	3.09	0.40
2:G:482:VAL:O	2:G:482:VAL:HG12	2.21	0.40
1:C:564:VAL:HG23	1:C:649:THR:HG21	2.03	0.40
1:E:626:LEU:O	1:F:399:PRO:HA	2.21	0.40
2:G:160:SER:O	2:G:161:HIS:C	2.60	0.40
1:F:582:VAL:CG1	1:F:585:ALA:HB2	2.51	0.40
1:F:404:PHE:CE2	1:F:406:GLY:HA2	2.56	0.40
1:B:565:HIS:HA	1:B:566:PRO:HA	1.96	0.40
1:C:533:LEU:HD23	1:C:533:LEU:HA	1.84	0.40
1:C:444:SER:HB3	1:C:460:ALA:HB3	2.04	0.40

All (63) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:PHE:CE1	1:F:540:ARG:NE[3_455]	0.68	1.52
1:A:690:PHE:CE2	1:F:540:ARG:CG[3_455]	0.78	1.42
1:B:541:ASP:N	1:E:690:PHE:CE2[3_455]	0.79	1.41
1:A:577:LEU:CD1	1:E:610:GLN:OE1[3_455]	0.87	1.33
1:B:540:ARG:C	1:E:690:PHE:CZ[3_455]	0.87	1.33
1:B:540:ARG:CB	1:E:690:PHE:CE1[3_455]	0.88	1.32
2:G:386:PHE:CZ	3:H:72:ASN:ND2[2_554]	0.89	1.31
1:A:690:PHE:CE1	1:F:540:ARG:CZ[3_455]	0.94	1.26
1:A:577:LEU:CG	1:E:610:GLN:OE1[3_455]	1.00	1.20
1:A:690:PHE:CE2	1:F:540:ARG:CD[3_455]	1.06	1.14
1:B:541:ASP:N	1:E:690:PHE:CZ[3_455]	1.06	1.14
2:G:365:GLN:NE2	2:G:365:GLN:NE2[2_554]	1.13	1.07
1:A:690:PHE:CD1	1:F:540:ARG:NE[3_455]	1.20	1.00
2:G:386:PHE:CE1	3:H:72:ASN:ND2[2_554]	1.21	0.99
1:A:690:PHE:CD2	1:F:540:ARG:CD[3_455]	1.21	0.99
1:A:690:PHE:CZ	1:F:540:ARG:NE[3_455]	1.22	0.98
1:A:610:GLN:OE1	1:E:577:LEU:CD1[3_455]	1.30	0.90
1:A:692:GLU:OE2	1:F:441:ASN:N[3_455]	1.30	0.90
1:A:577:LEU:CD1	1:E:610:GLN:CD[3_455]	1.31	0.89
1:B:541:ASP:CA	1:E:690:PHE:CE2[3_455]	1.35	0.85
1:A:610:GLN:OE1	1:E:577:LEU:CG[3_455]	1.39	0.81
2:G:385:THR:CG2	3:H:137:ARG:NH1[2_554]	1.43	0.77
1:B:540:ARG:CA	1:E:690:PHE:CE1[3_455]	1.45	0.75
1:A:690:PHE:CE2	1:F:540:ARG:CB[3_455]	1.47	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:386:PHE:CZ	3:H:72:ASN:CG[2_554]	1.49	0.71
1:B:441:ASN:N	1:E:691:GLN:OE1[3_455]	1.50	0.70
1:B:540:ARG:CA	1:E:690:PHE:CZ[3_455]	1.51	0.69
2:G:259:LYS:CE	2:G:299:ASN:O[2_554]	1.58	0.62
1:A:690:PHE:CZ	1:F:540:ARG:CD[3_455]	1.62	0.58
1:A:690:PHE:CE1	1:F:540:ARG:NH2[3_455]	1.66	0.54
2:G:365:GLN:CA	2:G:365:GLN:OE1[2_554]	1.70	0.50
1:B:540:ARG:CD	1:E:689:SER:O[3_455]	1.71	0.49
1:A:690:PHE:CZ	1:F:540:ARG:CG[3_455]	1.72	0.48
1:B:540:ARG:CB	1:E:690:PHE:CD1[3_455]	1.81	0.39
1:A:690:PHE:CZ	1:F:540:ARG:CZ[3_455]	1.81	0.39
1:A:690:PHE:CG	1:F:540:ARG:CD[3_455]	1.82	0.38
1:B:540:ARG:C	1:E:690:PHE:CE2[3_455]	1.85	0.35
1:A:690:PHE:CE2	1:F:540:ARG:NE[3_455]	1.87	0.33
1:A:610:GLN:OE1	1:E:577:LEU:CB[3_455]	1.87	0.33
1:A:690:PHE:CG	1:F:540:ARG:NE[3_455]	1.87	0.33
1:A:692:GLU:OE2	1:F:441:ASN:CA[3_455]	1.90	0.30
2:G:365:GLN:CD	2:G:365:GLN:NE2[2_554]	1.92	0.28
2:G:259:LYS:CD	2:G:300:GLY:CA[2_554]	1.93	0.27
1:A:690:PHE:CD1	1:F:540:ARG:CZ[3_455]	1.94	0.26
1:A:690:PHE:CD2	1:F:540:ARG:CG[3_455]	1.98	0.22
1:A:577:LEU:CB	1:E:610:GLN:NE2[3_455]	2.00	0.20
1:A:577:LEU:CG	1:E:610:GLN:CD[3_455]	2.01	0.19
1:B:540:ARG:O	1:E:690:PHE:CZ[3_455]	2.02	0.18
2:G:259:LYS:CD	2:G:300:GLY:C[2_554]	2.03	0.17
1:A:610:GLN:CD	1:E:577:LEU:CD1[3_455]	2.04	0.16
1:B:540:ARG:CB	1:E:690:PHE:CZ[3_455]	2.05	0.15
1:B:540:ARG:C	1:E:690:PHE:CE1[3_455]	2.05	0.15
1:B:541:ASP:CB	1:E:690:PHE:CE2[3_455]	2.06	0.14
1:B:541:ASP:CB	1:E:690:PHE:CD2[3_455]	2.07	0.13
1:B:540:ARG:CG	1:E:690:PHE:CE1[3_455]	2.08	0.12
1:A:577:LEU:CB	1:E:610:GLN:OE1[3_455]	2.08	0.12
1:B:541:ASP:N	1:E:690:PHE:CD2[3_455]	2.09	0.11
1:A:690:PHE:CE1	1:F:540:ARG:CD[3_455]	2.10	0.10
1:A:690:PHE:CD2	1:F:540:ARG:NE[3_455]	2.11	0.09
1:A:690:PHE:CE1	1:F:540:ARG:NH1[3_455]	2.17	0.03
1:A:690:PHE:CD1	1:F:540:ARG:CD[3_455]	2.18	0.02
1:A:577:LEU:CD1	1:E:610:GLN:CG[3_455]	2.19	0.01
2:G:386:PHE:CZ	3:H:72:ASN:CB[2_554]	2.19	0.01

## 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	648/681 (95%)	628 (97%)	18 (3%)	2 (0%)	46	83
1	B	648/681 (95%)	629 (97%)	16 (2%)	3 (0%)	34	77
1	C	648/681 (95%)	627 (97%)	17 (3%)	4 (1%)	30	74
1	D	650/681 (95%)	630 (97%)	16 (2%)	4 (1%)	30	74
1	E	650/681 (95%)	632 (97%)	15 (2%)	3 (0%)	34	77
1	F	650/681 (95%)	631 (97%)	17 (3%)	2 (0%)	46	83
2	G	480/538 (89%)	408 (85%)	55 (12%)	17 (4%)	4	39
3	H	115/577 (20%)	106 (92%)	7 (6%)	2 (2%)	11	55
All	All	4489/5201 (86%)	4291 (96%)	161 (4%)	37 (1%)	24	69

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	655	ASN
2	G	161	HIS
2	G	207	HIS
2	G	257	SER
3	H	81	ASP
3	H	129	THR
1	B	508	VAL
1	C	655	ASN
1	E	655	ASN
2	G	42	SER
2	G	75	ASP
2	G	95	VAL
2	G	147	GLY
2	G	158	GLN
2	G	159	ASP
2	G	206	GLY
2	G	278	SER

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Mol	Chain	Res	Type
2	G	456	GLY
1	A	160	SER
1	A	175	SER
1	B	160	SER
1	B	175	SER
1	C	160	SER
1	C	175	SER
1	C	508	VAL
1	D	160	SER
1	D	175	SER
1	E	160	SER
1	E	175	SER
1	F	160	SER
1	F	175	SER
2	G	55	SER
2	G	49	ASN
2	G	299	ASN
2	G	298	PRO
1	D	508	VAL
2	G	146	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	578/597 (97%)	571 (99%)	7 (1%)	78	90
1	B	578/597 (97%)	571 (99%)	7 (1%)	78	90
1	C	578/597 (97%)	571 (99%)	7 (1%)	78	90
1	D	578/597 (97%)	571 (99%)	7 (1%)	78	90
1	E	578/597 (97%)	571 (99%)	7 (1%)	78	90
1	F	578/597 (97%)	571 (99%)	7 (1%)	78	90
2	G	428/472 (91%)	397 (93%)	31 (7%)	18	55
3	H	102/506 (20%)	97 (95%)	5 (5%)	31	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3998/4560 (88%)	3920 (98%)	78 (2%)	63 85

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	A	238	HIS
1	A	274	LEU
1	A	298	PHE
1	A	438	TYR
1	A	509	GLU
1	A	626	LEU
1	B	237	SER
1	B	238	HIS
1	B	274	LEU
1	B	298	PHE
1	B	438	TYR
1	B	509	GLU
1	B	626	LEU
1	C	237	SER
1	C	238	HIS
1	C	274	LEU
1	C	298	PHE
1	C	438	TYR
1	C	509	GLU
1	C	626	LEU
1	D	237	SER
1	D	238	HIS
1	D	274	LEU
1	D	298	PHE
1	D	438	TYR
1	D	509	GLU
1	D	626	LEU
1	E	237	SER
1	E	238	HIS
1	E	274	LEU
1	E	298	PHE
1	E	438	TYR
1	E	509	GLU
1	E	626	LEU
1	F	237	SER
1	F	238	HIS

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Mol	Chain	Res	Type
1	F	274	LEU
1	F	298	PHE
1	F	438	TYR
1	F	509	GLU
1	F	626	LEU
2	G	27	ASN
2	G	31	ARG
2	G	40	LEU
2	G	61	LEU
2	G	69	LEU
2	G	94	PRO
2	G	101	ASP
2	G	105	TRP
2	G	140	ILE
2	G	155	PHE
2	G	159	ASP
2	G	161	HIS
2	G	190	THR
2	G	203	ARG
2	G	218	SER
2	G	224	PRO
2	G	231	LEU
2	G	308	LEU
2	G	314	MET
2	G	389	PHE
2	G	390	ASP
2	G	413	VAL
2	G	427	VAL
2	G	436	VAL
2	G	443	ASP
2	G	457	THR
2	G	476	LEU
2	G	485	GLU
2	G	487	THR
2	G	497	LYS
2	G	501	LEU
3	H	30	THR
3	H	55	GLU
3	H	81	ASP
3	H	98	ARG
3	H	125	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	465	HIS
1	A	683	HIS
1	B	465	HIS
1	B	534	HIS
1	B	660	GLN
1	C	465	HIS
1	C	565	HIS
1	C	659	HIS
1	D	659	HIS
1	E	324	GLN
1	E	465	HIS
1	E	659	HIS
1	F	324	GLN
1	F	465	HIS
2	G	27	ASN
2	G	76	HIS
2	G	164	ASN
2	G	209	HIS
2	G	215	GLN
2	G	216	HIS
2	G	370	GLN
2	G	406	HIS
2	G	411	ASN
2	G	417	ASN
2	G	433	GLN
2	G	511	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

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	656/681 (96%)	1.57	212 (32%) <b>1</b> <b>5</b>	287, 291, 313, 313	0
1	B	656/681 (96%)	1.64	209 (31%) <b>1</b> <b>5</b>	290, 308, 308, 308	0
1	C	656/681 (96%)	1.66	218 (33%) <b>0</b> <b>5</b>	278, 322, 327, 327	0
1	D	656/681 (96%)	1.75	237 (36%) <b>0</b> <b>4</b>	294, 342, 342, 342	0
1	E	656/681 (96%)	2.22	312 (47%) <b>0</b> <b>4</b>	304, 341, 351, 351	0
1	F	656/681 (96%)	2.35	303 (46%) <b>0</b> <b>4</b>	305, 348, 370, 370	0
2	G	484/538 (89%)	1.75	177 (36%) <b>0</b> <b>4</b>	340, 340, 340, 340	0
3	H	117/577 (20%)	1.05	24 (20%) <b>1</b> <b>7</b>	370, 370, 370, 370	0
All	All	4537/5201 (87%)	1.83	1692 (37%) <b>0</b> <b>4</b>	278, 322, 348, 370	0

All (1692) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	189	ASP	14.7
1	B	629	ASP	13.4
1	F	262	THR	12.2
1	F	190	GLY	11.7
1	E	436	ALA	11.7
1	F	273	ASP	11.2
1	F	165	THR	11.1
1	F	294	VAL	11.1
1	F	412	PRO	10.4
1	F	263	PRO	10.3
1	E	400	ILE	9.8
1	F	163	ASN	9.8
1	C	262	THR	9.5
1	D	622	PRO	9.4
1	F	413	LEU	9.4
1	F	485	ASP	9.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	326	GLY	9.3
1	E	312	ALA	9.2
1	F	385	TRP	9.2
1	F	239	PHE	9.1
1	C	629	ASP	9.0
1	E	240	ASP	9.0
1	F	188	VAL	8.9
1	E	311	GLN	8.7
1	C	622	PRO	8.7
1	D	156	GLU	8.6
1	B	162	VAL	8.5
1	F	486	MET	8.4
1	C	385	TRP	8.4
1	F	118	ILE	8.4
1	F	401	ASP	8.4
1	E	435	VAL	8.3
1	C	263	PRO	8.3
1	F	162	VAL	8.3
1	E	399	PRO	8.2
1	F	161	SER	8.1
1	F	54	THR	8.1
1	F	183	PHE	8.0
1	F	484	ARG	7.9
1	E	338	ILE	7.8
1	E	434	SER	7.8
1	F	293	TYR	7.8
1	E	244	ILE	7.8
1	D	262	THR	7.7
2	G	494	LEU	7.7
1	E	239	PHE	7.7
1	F	166	GLY	7.6
1	F	311	GLN	7.5
1	B	343	GLN	7.5
1	F	312	ALA	7.4
1	E	437	SER	7.4
1	C	189	ASP	7.4
1	F	402	ASP	7.4
1	D	401	ASP	7.3
1	F	184	ILE	7.2
1	F	295	SER	7.2
1	E	402	ASP	7.2
1	D	228	ILE	7.2

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Mol	Chain	Res	Type	RSRZ
1	F	172	ILE	7.2
1	F	53	LEU	7.1
1	D	137	CYS	7.1
1	E	263	PRO	7.1
1	E	447	PHE	7.1
1	B	189	ASP	7.0
1	F	403	ASN	7.0
1	B	161	SER	7.0
1	F	240	ASP	7.0
1	E	228	ILE	7.0
1	E	629	ASP	7.0
1	D	239	PHE	7.0
1	E	262	THR	7.0
1	E	165	THR	6.9
1	C	240	ASP	6.9
1	E	692	GLU	6.9
2	G	167	GLY	6.9
1	B	311	GLN	6.9
1	B	170	GLY	6.8
1	C	402	ASP	6.8
1	B	163	ASN	6.8
1	E	432	LEU	6.8
1	F	282	ARG	6.7
2	G	493	GLU	6.7
1	C	228	ILE	6.7
1	A	475	VAL	6.7
1	F	197	THR	6.7
2	G	120	VAL	6.7
1	E	163	ASN	6.6
1	F	436	ALA	6.6
1	F	119	ILE	6.6
1	E	385	TRP	6.6
1	E	438	TYR	6.6
1	E	484	ARG	6.6
1	E	401	ASP	6.5
1	B	402	ASP	6.4
1	D	629	ASP	6.4
1	D	294	VAL	6.4
1	A	53	LEU	6.4
2	G	503	ILE	6.4
1	E	486	MET	6.4
1	B	401	ASP	6.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	400	ILE	6.3
2	G	510	ALA	6.3
1	F	196	PRO	6.3
1	D	257	THR	6.3
1	A	448	VAL	6.3
1	D	161	SER	6.3
1	B	404	PHE	6.3
1	D	256	LEU	6.3
1	A	486	MET	6.2
1	D	240	ASP	6.2
1	F	434	SER	6.2
1	E	346	TYR	6.2
1	F	435	VAL	6.2
1	B	436	ALA	6.2
1	C	161	SER	6.2
1	B	554	ALA	6.2
1	F	553	ALA	6.2
1	F	346	TYR	6.2
2	G	197	ARG	6.2
2	G	284	THR	6.2
1	E	310	LEU	6.1
2	G	378	PRO	6.1
1	F	438	TYR	6.1
1	F	117	LEU	6.1
1	E	133	TYR	6.1
1	C	553	ALA	6.1
1	F	199	SER	6.0
1	D	295	SER	6.0
1	D	159	LEU	6.0
1	F	383	LEU	6.0
1	B	54	THR	6.0
1	F	186	THR	6.0
1	E	168	MET	6.0
1	E	508	VAL	6.0
1	F	437	SER	6.0
1	E	95	TYR	5.9
1	E	188	VAL	5.9
1	D	263	PRO	5.9
1	D	346	TYR	5.9
1	B	553	ALA	5.9
1	F	310	LEU	5.9
1	A	354	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	F	226	ILE	5.9
1	D	162	VAL	5.9
1	D	311	GLN	5.9
1	F	257	THR	5.9
1	C	239	PHE	5.8
1	C	259	GLN	5.8
1	F	228	ILE	5.8
1	F	164	LYS	5.8
1	A	399	PRO	5.8
1	D	293	TYR	5.8
1	C	404	PHE	5.8
1	F	554	ALA	5.8
1	F	399	PRO	5.8
1	D	171	VAL	5.8
1	D	255	PHE	5.8
1	D	258	VAL	5.8
1	B	312	ALA	5.8
1	F	256	LEU	5.8
1	A	400	ILE	5.8
2	G	509	VAL	5.7
1	F	344	LYS	5.7
1	D	189	ASP	5.7
1	F	343	GLN	5.7
1	F	261	GLU	5.6
1	E	187	ALA	5.6
1	F	64	VAL	5.6
1	F	92	LYS	5.6
1	D	282	ARG	5.6
1	C	273	ASP	5.6
1	C	257	THR	5.6
1	E	354	ALA	5.6
1	A	497	VAL	5.6
1	A	64	VAL	5.5
1	E	337	ALA	5.5
1	A	262	THR	5.5
1	C	156	GLU	5.5
1	D	244	ILE	5.5
1	E	137	CYS	5.5
1	B	165	THR	5.5
1	A	163	ASN	5.5
2	G	93	TRP	5.5
1	A	221	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	115	LYS	5.5
1	D	432	LEU	5.5
1	F	170	GLY	5.4
1	F	447	PHE	5.4
1	F	386	LEU	5.4
2	G	458	VAL	5.4
1	D	385	TRP	5.4
1	E	448	VAL	5.4
1	D	183	PHE	5.4
1	C	349	PRO	5.4
1	E	456	LYS	5.4
2	G	325	TYR	5.3
1	A	71	TYR	5.3
1	E	298	PHE	5.3
1	B	497	VAL	5.3
1	F	52	HIS	5.3
1	D	310	LEU	5.3
1	E	446	VAL	5.3
1	F	198	LEU	5.3
1	D	259	GLN	5.3
1	D	281	VAL	5.3
1	E	54	THR	5.3
1	B	171	VAL	5.2
1	A	159	LEU	5.2
1	F	560	MET	5.2
1	A	487	ALA	5.2
1	D	312	ALA	5.2
1	A	42	HIS	5.2
1	A	133	TYR	5.2
1	E	560	MET	5.2
1	F	448	VAL	5.2
1	F	445	VAL	5.2
1	F	338	ILE	5.2
1	D	170	GLY	5.2
1	F	647	VAL	5.2
1	C	398	VAL	5.2
1	F	404	PHE	5.2
1	B	403	ASN	5.1
1	F	63	TYR	5.1
1	B	199	SER	5.1
1	F	255	PHE	5.1
1	E	53	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
2	G	463	SER	5.1
1	C	190	GLY	5.1
1	C	260	PRO	5.1
2	G	62	LEU	5.1
1	D	215	TYR	5.1
1	A	161	SER	5.1
1	C	432	LEU	5.1
1	F	227	LYS	5.1
1	E	398	VAL	5.1
1	D	241	ILE	5.1
1	E	158	TYR	5.1
1	E	256	LEU	5.1
1	E	313	ALA	5.1
2	G	380	THR	5.1
1	A	485	ASP	5.1
1	E	485	ASP	5.1
1	D	277	THR	5.1
1	F	187	ALA	5.0
1	C	241	ILE	5.0
1	F	182	LEU	5.0
1	E	277	THR	5.0
1	E	445	VAL	5.0
1	D	160	SER	5.0
1	C	293	TYR	5.0
1	E	655	ASN	5.0
1	D	172	ILE	5.0
1	E	134	GLN	5.0
1	E	257	THR	5.0
1	E	554	ALA	5.0
1	D	184	ILE	5.0
1	D	338	ILE	5.0
1	F	241	ILE	5.0
1	F	337	ALA	5.0
1	F	387	LEU	5.0
1	F	414	GLY	4.9
1	E	433	THR	4.9
1	F	496	TYR	4.9
1	B	53	LEU	4.9
1	D	163	ASN	4.9
2	G	192	ALA	4.9
1	F	171	VAL	4.9
1	E	201	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	354	ALA	4.9
1	F	159	LEU	4.9
1	F	588	LEU	4.9
1	B	190	GLY	4.9
1	F	280	ILE	4.9
1	E	553	ALA	4.9
1	B	255	PHE	4.9
1	A	240	ASP	4.9
1	A	401	ASP	4.9
1	D	138	LYS	4.9
1	E	166	GLY	4.8
1	D	343	GLN	4.8
1	F	181	LYS	4.8
2	G	327	VAL	4.8
3	H	41	SER	4.8
2	G	379	GLY	4.8
3	H	108	ALA	4.8
1	E	63	TYR	4.8
1	C	311	GLN	4.8
1	F	115	LYS	4.8
2	G	387	GLY	4.8
1	B	655	ASN	4.8
2	G	216	HIS	4.8
1	E	349	PRO	4.8
1	A	425	TYR	4.8
1	E	343	GLN	4.8
1	F	168	MET	4.8
1	F	432	LEU	4.7
2	G	220	TRP	4.7
1	D	197	THR	4.7
1	D	199	SER	4.7
1	D	64	VAL	4.7
1	C	282	ARG	4.7
1	C	467	GLY	4.7
2	G	214	GLU	4.7
1	D	400	ILE	4.7
1	C	425	TYR	4.7
1	E	156	GLU	4.7
1	E	412	PRO	4.7
1	C	159	LEU	4.7
1	F	281	VAL	4.7
1	B	438	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	412	PRO	4.7
1	A	622	PRO	4.7
1	F	444	SER	4.7
1	B	262	THR	4.7
1	B	228	ILE	4.7
1	C	438	TYR	4.6
1	F	527	HIS	4.6
1	B	115	LYS	4.6
1	C	256	LEU	4.6
1	E	255	PHE	4.6
2	G	459	LEU	4.6
1	D	165	THR	4.6
1	B	160	SER	4.6
1	E	294	VAL	4.6
1	C	318	PRO	4.6
2	G	92	VAL	4.6
2	G	478	GLU	4.6
2	G	502	TYR	4.6
1	A	560	MET	4.6
1	E	159	LEU	4.6
1	A	41	PHE	4.6
1	E	278	SER	4.6
1	E	599	LEU	4.6
1	C	401	ASP	4.6
1	C	346	TYR	4.5
1	F	456	LYS	4.5
1	F	487	ALA	4.5
1	D	118	ILE	4.5
1	E	207	PRO	4.5
1	A	629	ASP	4.5
1	E	509	GLU	4.5
1	F	236	VAL	4.5
1	E	150	GLU	4.5
1	D	280	ILE	4.5
1	A	588	LEU	4.5
1	E	131	SER	4.5
1	F	244	ILE	4.5
1	B	63	TYR	4.5
1	C	403	ASN	4.5
1	E	293	TYR	4.5
1	E	507	PRO	4.5
1	F	51	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	276	TYR	4.4
1	E	245	TYR	4.4
1	E	517	CYS	4.4
1	A	387	LEU	4.4
1	B	239	PHE	4.4
1	F	235	LEU	4.4
2	G	498	GLN	4.4
1	A	447	PHE	4.4
3	H	109	PRO	4.4
1	A	426	THR	4.4
1	E	371	LEU	4.4
1	B	164	LYS	4.4
1	F	629	ASP	4.4
2	G	48	PHE	4.4
1	B	226	ILE	4.4
1	F	446	VAL	4.4
3	H	134	PHE	4.4
1	F	167	THR	4.4
1	B	622	PRO	4.4
1	F	126	LEU	4.4
1	F	191	LYS	4.4
2	G	480	MET	4.4
1	E	404	PHE	4.4
1	A	54	THR	4.3
1	A	228	ILE	4.3
1	E	186	THR	4.3
1	A	220	ASP	4.3
1	E	425	TYR	4.3
1	C	388	GLY	4.3
1	F	127	LEU	4.3
1	B	447	PHE	4.3
1	D	158	TYR	4.3
1	E	170	GLY	4.3
1	D	402	ASP	4.3
1	B	432	LEU	4.3
1	D	413	LEU	4.3
1	A	165	THR	4.3
3	H	61	PRO	4.3
1	D	448	VAL	4.3
1	B	282	ARG	4.3
1	F	274	LEU	4.3
1	D	71	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	404	PHE	4.3
1	B	281	VAL	4.3
1	D	242	PHE	4.3
1	C	461	ASP	4.3
1	D	497	VAL	4.3
1	F	397	PRO	4.3
2	G	491	ALA	4.3
1	B	71	TYR	4.3
1	D	150	GLU	4.3
1	C	258	VAL	4.3
1	C	44	GLU	4.2
1	C	196	PRO	4.2
1	D	70	VAL	4.2
1	B	184	ILE	4.2
1	A	249	SER	4.2
1	E	139	LEU	4.2
1	B	188	VAL	4.2
1	B	337	ALA	4.2
1	F	137	CYS	4.2
1	E	273	ASP	4.2
1	E	136	VAL	4.2
1	E	92	LYS	4.2
1	C	695	ILE	4.2
2	G	482	VAL	4.2
1	F	488	PHE	4.2
2	G	169	SER	4.2
1	B	313	ALA	4.2
1	D	337	ALA	4.2
2	G	520	TYR	4.2
1	C	294	VAL	4.2
1	F	55	VAL	4.2
1	C	333	ASP	4.2
1	E	282	ARG	4.2
1	F	626	LEU	4.2
1	D	196	PRO	4.2
1	F	243	TYR	4.2
1	D	117	LEU	4.2
1	E	413	LEU	4.2
1	F	313	ALA	4.2
2	G	495	SER	4.2
1	E	99	ILE	4.1
1	E	296	LEU	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	377	ARG	4.1
1	C	386	LEU	4.1
1	E	616	PRO	4.1
2	G	362	PRO	4.1
1	F	398	VAL	4.1
1	D	129	CYS	4.1
1	E	431	ARG	4.1
1	C	133	TYR	4.1
1	C	298	PHE	4.1
1	B	435	VAL	4.1
2	G	106	ALA	4.1
1	B	293	TYR	4.1
2	G	215	GLN	4.1
1	E	116	LEU	4.1
1	E	161	SER	4.1
1	A	83	HIS	4.1
2	G	119	LYS	4.1
1	F	50	PHE	4.1
1	E	213	LEU	4.1
1	D	53	LEU	4.1
1	B	385	TRP	4.1
1	A	554	ALA	4.1
1	E	258	VAL	4.1
1	A	239	PHE	4.1
1	E	164	LYS	4.0
1	F	285	LYS	4.0
2	G	254	GLY	4.0
1	C	261	GLU	4.0
2	G	219	ARG	4.0
1	A	402	ASP	4.0
1	C	696	ASN	4.0
1	B	294	VAL	4.0
1	D	486	MET	4.0
1	F	283	LEU	4.0
1	C	162	VAL	4.0
1	A	496	TYR	4.0
1	B	355	LEU	4.0
1	E	455	LEU	4.0
1	D	355	LEU	4.0
1	C	447	PHE	4.0
1	D	131	SER	4.0
1	E	152	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	433	THR	4.0
1	B	240	ASP	4.0
1	C	188	VAL	4.0
1	A	116	LEU	4.0
1	C	191	LYS	4.0
1	F	441	ASN	4.0
1	C	313	ALA	4.0
1	C	406	GLY	4.0
1	F	249	SER	4.0
1	E	138	LYS	4.0
1	E	280	ILE	4.0
1	B	259	GLN	4.0
1	F	160	SER	4.0
1	B	64	VAL	4.0
1	D	198	LEU	4.0
1	E	355	LEU	4.0
1	B	456	LYS	4.0
1	C	468	VAL	4.0
1	A	195	PHE	4.0
1	D	560	MET	4.0
1	B	448	VAL	4.0
1	E	527	HIS	4.0
1	F	259	GLN	3.9
1	B	276	TYR	3.9
2	G	77	ILE	3.9
1	F	156	GLU	3.9
1	C	328	ILE	3.9
1	E	647	VAL	3.9
1	D	92	LYS	3.9
1	C	508	VAL	3.9
1	D	554	ALA	3.9
1	A	435	VAL	3.9
1	D	313	ALA	3.9
1	F	248	ALA	3.9
1	E	196	PRO	3.9
1	B	261	GLU	3.9
1	F	195	PHE	3.9
3	H	39	LEU	3.9
1	C	134	GLN	3.9
1	F	347	HIS	3.9
1	E	586	PRO	3.9
1	E	295	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	400	ILE	3.9
1	E	203	LEU	3.9
1	C	460	ALA	3.9
1	D	278	SER	3.9
1	A	63	TYR	3.9
1	C	412	PRO	3.9
1	C	390	ASP	3.9
1	A	596	PHE	3.9
1	C	280	ILE	3.9
1	A	137	CYS	3.9
1	A	162	VAL	3.9
1	D	260	PRO	3.9
1	E	189	ASP	3.8
1	E	259	GLN	3.8
1	E	281	VAL	3.8
1	F	139	LEU	3.8
2	G	492	MET	3.8
1	B	183	PHE	3.8
1	F	455	LEU	3.8
1	C	616	PRO	3.8
2	G	173	PRO	3.8
1	D	200	SER	3.8
1	D	588	LEU	3.8
1	E	443	TYR	3.8
1	A	160	SER	3.8
1	A	456	LYS	3.8
1	E	169	TYR	3.8
1	C	194	TYR	3.8
2	G	157	LEU	3.8
1	E	190	GLY	3.8
2	G	376	PRO	3.8
1	D	456	LYS	3.8
1	E	475	VAL	3.8
1	C	509	GLU	3.8
1	E	128	ALA	3.8
1	E	626	LEU	3.8
1	C	325	ALA	3.8
1	D	128	ALA	3.8
1	B	168	MET	3.8
1	A	118	ILE	3.8
1	B	338	ILE	3.8
1	E	162	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	G	70	TYR	3.8
1	E	127	LEU	3.8
1	B	310	LEU	3.8
1	D	298	PHE	3.8
2	G	519	ILE	3.8
1	E	344	LYS	3.8
1	D	488	PHE	3.8
1	E	183	PHE	3.8
1	F	433	THR	3.8
1	D	227	LYS	3.8
1	D	201	ARG	3.8
1	B	616	PRO	3.8
2	G	460	LYS	3.8
1	A	166	GLY	3.8
1	A	117	LEU	3.8
1	B	630	TRP	3.8
1	B	62	VAL	3.7
1	C	283	LEU	3.7
1	C	392	GLN	3.7
1	F	242	PHE	3.7
1	C	355	LEU	3.7
1	B	92	LYS	3.7
1	B	412	PRO	3.7
2	G	464	VAL	3.7
1	F	371	LEU	3.7
1	E	314	TYR	3.7
1	E	615	SER	3.7
1	C	226	ILE	3.7
2	G	450	PHE	3.7
1	B	172	ILE	3.7
1	D	247	PHE	3.7
1	C	444	SER	3.7
1	F	616	PRO	3.7
1	A	55	VAL	3.7
1	C	459	ARG	3.7
1	E	117	LEU	3.7
1	A	385	TRP	3.7
1	E	241	ILE	3.7
1	D	273	ASP	3.7
1	E	414	GLY	3.7
2	G	170	PRO	3.7
1	A	398	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	460	ALA	3.7
1	E	367	ILE	3.7
1	E	200	SER	3.7
1	C	281	VAL	3.7
1	F	471	GLU	3.7
1	B	484	ARG	3.7
1	F	497	VAL	3.7
1	E	356	CYS	3.7
1	B	263	PRO	3.7
1	F	116	LEU	3.7
1	E	194	TYR	3.7
1	F	134	GLN	3.7
1	B	198	LEU	3.7
1	F	345	GLN	3.7
1	C	529	GLY	3.7
1	F	192	GLN	3.7
1	C	651	PHE	3.7
1	D	54	THR	3.6
1	B	131	SER	3.6
1	C	160	SER	3.6
1	C	526	PRO	3.6
1	E	279	ARG	3.6
1	D	243	TYR	3.6
1	F	461	ASP	3.6
1	C	615	SER	3.6
1	E	70	VAL	3.6
1	E	38	TYR	3.6
1	E	336	PHE	3.6
1	E	646	PHE	3.6
1	D	564	VAL	3.6
1	D	585	ALA	3.6
1	D	216	GLU	3.6
1	F	460	ALA	3.6
1	D	63	TYR	3.6
1	D	226	ILE	3.6
1	F	359	PRO	3.6
1	A	503	VAL	3.6
1	E	113	VAL	3.6
1	E	149	VAL	3.6
1	F	201	ARG	3.6
1	E	160	SER	3.6
1	E	689	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	G	47	THR	3.6
1	A	92	LYS	3.6
1	A	134	GLN	3.6
1	D	447	PHE	3.6
1	A	136	VAL	3.6
1	B	166	GLY	3.6
2	G	457	THR	3.6
2	G	285	THR	3.6
1	C	527	HIS	3.6
2	G	172	ASP	3.6
1	A	389	LYS	3.6
1	D	95	TYR	3.6
1	E	172	ILE	3.6
1	D	582	VAL	3.6
3	H	73	PRO	3.6
1	D	610	GLN	3.6
1	E	215	TYR	3.6
1	F	194	TYR	3.6
1	B	119	ILE	3.6
1	C	399	PRO	3.6
1	E	496	TYR	3.6
1	F	260	PRO	3.5
1	C	448	VAL	3.5
1	E	243	TYR	3.5
1	C	195	PHE	3.5
1	A	346	TYR	3.5
1	D	111	ASN	3.5
2	G	258	GLY	3.5
1	E	167	THR	3.5
1	A	527	HIS	3.5
2	G	168	LYS	3.5
1	B	486	MET	3.5
1	C	350	PRO	3.5
1	E	630	TRP	3.5
1	A	164	LYS	3.5
2	G	33	LYS	3.5
2	G	257	SER	3.5
1	F	384	ASN	3.5
1	E	114	ASN	3.5
2	G	32	LEU	3.5
1	A	355	LEU	3.5
1	C	137	CYS	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	213	THR	3.5
1	B	440	TYR	3.5
1	F	71	TYR	3.5
1	F	594	CYS	3.5
1	F	238	HIS	3.5
2	G	34	LEU	3.5
1	A	455	LEU	3.5
2	G	252	ILE	3.5
1	D	236	VAL	3.5
1	F	284	CYS	3.5
2	G	511	GLN	3.5
2	G	436	VAL	3.5
1	C	92	LYS	3.5
1	A	70	VAL	3.5
1	D	436	ALA	3.5
1	F	658	ALA	3.5
1	A	196	PRO	3.5
1	C	443	TYR	3.5
1	D	249	SER	3.5
1	E	444	SER	3.5
1	D	213	LEU	3.5
2	G	94	PRO	3.5
1	A	502	GLN	3.5
1	A	517	CYS	3.5
1	F	498	MET	3.5
1	E	315	LEU	3.5
1	D	336	PHE	3.5
1	F	622	PRO	3.4
1	B	503	VAL	3.4
1	E	171	VAL	3.4
1	F	232	THR	3.4
2	G	253	ASP	3.4
1	D	279	ARG	3.4
2	G	299	ASN	3.4
1	D	461	ASP	3.4
1	D	621	VAL	3.4
1	C	235	LEU	3.4
1	B	133	TYR	3.4
1	E	64	VAL	3.4
1	E	129	CYS	3.4
1	B	527	HIS	3.4
1	D	173	VAL	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	95	TYR	3.4
1	B	541	ASP	3.4
1	C	440	TYR	3.4
1	E	226	ILE	3.4
1	B	150	GLU	3.4
1	C	389	LYS	3.4
1	C	278	SER	3.4
1	C	410	ASN	3.4
1	F	443	TYR	3.4
1	E	622	PRO	3.4
2	G	166	ARG	3.4
1	D	496	TYR	3.4
1	D	630	TRP	3.4
1	C	456	LYS	3.4
1	F	275	PHE	3.4
1	A	44	GLU	3.4
1	C	475	VAL	3.4
1	D	399	PRO	3.4
1	D	254	TYR	3.4
1	D	434	SER	3.4
2	G	64	GLU	3.4
1	B	138	LYS	3.4
1	F	49	THR	3.4
2	G	449	MET	3.4
1	B	273	ASP	3.4
1	E	216	GLU	3.4
1	F	133	TYR	3.4
1	F	586	PRO	3.4
1	C	554	ALA	3.4
1	A	461	ASP	3.4
1	B	118	ILE	3.4
1	D	553	ALA	3.4
1	E	403	ASN	3.4
1	B	41	PHE	3.4
1	F	578	LEU	3.4
1	A	702	PRO	3.4
1	D	426	THR	3.4
1	E	683	HIS	3.3
1	A	445	VAL	3.3
1	C	225	LEU	3.3
2	G	95	VAL	3.3
1	D	653	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	670	PHE	3.3
1	F	599	LEU	3.3
1	F	357	ALA	3.3
2	G	78	PHE	3.3
2	G	121	LEU	3.3
2	G	221	LEU	3.3
1	B	508	VAL	3.3
1	E	318	PRO	3.3
1	F	569	ILE	3.3
1	C	436	ALA	3.3
1	F	65	GLY	3.3
1	A	533	LEU	3.3
1	C	653	PHE	3.3
1	F	475	VAL	3.3
1	F	669	ALA	3.3
1	B	504	THR	3.3
1	C	578	LEU	3.3
1	F	355	LEU	3.3
2	G	451	ILE	3.3
1	D	485	ASP	3.3
1	F	41	PHE	3.3
1	E	285	LYS	3.3
1	F	526	PRO	3.3
1	E	488	PHE	3.3
1	F	440	TYR	3.3
1	C	163	ASN	3.3
1	F	279	ARG	3.3
1	A	504	THR	3.3
1	E	197	THR	3.3
2	G	340	VAL	3.3
1	E	569	ILE	3.3
2	G	310	ASP	3.3
1	D	207	PRO	3.3
1	D	116	LEU	3.3
1	A	170	GLY	3.3
1	A	273	ASP	3.3
1	E	612	ILE	3.3
2	G	198	ASP	3.3
1	E	457	LYS	3.3
1	F	501	ARG	3.2
1	E	276	TYR	3.2
1	F	458	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	186	THR	3.2
1	C	255	PHE	3.2
1	C	367	ILE	3.2
1	C	586	PRO	3.2
1	E	506	VAL	3.2
1	F	336	PHE	3.2
1	F	508	VAL	3.2
1	E	350	PRO	3.2
1	C	486	MET	3.2
1	E	55	VAL	3.2
1	A	641	GLU	3.2
1	C	596	PHE	3.2
2	G	286	PHE	3.2
1	C	183	PHE	3.2
2	G	60	PHE	3.2
1	F	630	TRP	3.2
1	E	426	THR	3.2
1	F	185	GLY	3.2
1	E	416	SER	3.2
2	G	129	LEU	3.2
1	F	500	GLU	3.2
1	E	212	MET	3.2
2	G	199	PHE	3.2
1	F	207	PRO	3.2
2	G	91	ILE	3.2
1	B	49	THR	3.2
1	D	460	ALA	3.2
2	G	75	ASP	3.2
1	A	484	ARG	3.2
1	C	310	LEU	3.2
1	F	382	GLU	3.2
1	C	238	HIS	3.2
1	B	615	SER	3.2
1	E	582	VAL	3.2
1	F	671	ARG	3.2
1	A	129	CYS	3.2
1	A	434	SER	3.2
1	B	526	PRO	3.2
1	B	413	LEU	3.2
1	B	626	LEU	3.2
1	C	247	PHE	3.2
1	E	596	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	580	LEU	3.2
1	C	332	GLU	3.2
1	E	497	VAL	3.2
1	C	437	SER	3.2
3	H	62	GLU	3.2
1	F	128	ALA	3.2
1	F	322	LEU	3.2
1	E	339	PHE	3.2
1	F	70	VAL	3.2
1	B	455	LEU	3.2
1	D	484	ARG	3.2
1	E	559	CYS	3.1
1	E	677	TYR	3.1
1	D	115	LYS	3.1
1	F	532	ALA	3.1
1	D	611	VAL	3.1
1	F	138	LYS	3.1
1	C	242	PHE	3.1
1	B	70	VAL	3.1
1	E	309	LEU	3.1
3	H	107	ILE	3.1
1	A	213	LEU	3.1
1	C	363	ILE	3.1
1	E	458	ILE	3.1
1	F	425	TYR	3.1
1	B	670	PHE	3.1
1	C	71	TYR	3.1
1	D	188	VAL	3.1
1	D	586	PRO	3.1
1	F	582	VAL	3.1
1	D	155	LYS	3.1
1	F	298	PHE	3.1
1	E	71	TYR	3.1
2	G	404	ARG	3.1
1	C	227	LYS	3.1
1	D	151	PRO	3.1
2	G	255	GLU	3.1
1	B	498	MET	3.1
1	E	62	VAL	3.1
1	C	484	ARG	3.1
2	G	256	HIS	3.1
2	G	278	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	52	HIS	3.1
2	G	366	TRP	3.1
1	D	527	HIS	3.1
1	A	432	LEU	3.1
1	A	444	SER	3.1
2	G	501	LEU	3.1
1	D	232	THR	3.1
1	F	406	GLY	3.1
1	C	577	LEU	3.1
1	D	495	LEU	3.1
1	A	311	GLN	3.1
1	E	254	TYR	3.1
1	E	118	ILE	3.1
1	D	626	LEU	3.1
1	E	430	ASP	3.1
1	F	203	LEU	3.1
1	F	655	ASN	3.1
2	G	130	TYR	3.1
1	D	166	GLY	3.0
1	D	386	LEU	3.0
1	E	155	LYS	3.0
1	D	185	GLY	3.0
1	D	425	TYR	3.0
1	A	412	PRO	3.0
1	B	159	LEU	3.0
1	B	552	PHE	3.0
2	G	311	VAL	3.0
1	C	588	LEU	3.0
1	A	158	TYR	3.0
1	F	381	LEU	3.0
1	B	151	PRO	3.0
1	C	342	GLY	3.0
1	A	119	ILE	3.0
1	A	155	LYS	3.0
1	E	111	ASN	3.0
1	F	509	GLU	3.0
1	D	299	GLY	3.0
1	A	199	SER	3.0
1	B	444	SER	3.0
1	F	702	PRO	3.0
1	B	346	TYR	3.0
1	B	256	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	280	ILE	3.0
1	D	438	TYR	3.0
2	G	504	GLY	3.0
1	A	501	ARG	3.0
1	E	184	ILE	3.0
1	F	225	LEU	3.0
1	F	315	LEU	3.0
2	G	497	LYS	3.0
1	F	149	VAL	3.0
1	C	344	LYS	3.0
1	F	577	LEU	3.0
1	A	449	GLY	3.0
1	B	295	SER	3.0
1	C	322	LEU	3.0
1	B	573	ASP	3.0
1	C	560	MET	3.0
1	F	150	GLU	3.0
1	A	586	PRO	3.0
1	C	187	ALA	3.0
1	E	181	LYS	3.0
1	F	388	GLY	3.0
1	A	184	ILE	3.0
1	D	127	LEU	3.0
1	D	414	GLY	3.0
1	E	620	ASP	3.0
2	G	69	LEU	3.0
2	G	395	LEU	3.0
1	E	460	ALA	3.0
1	A	469	GLN	3.0
2	G	479	GLU	3.0
1	E	173	VAL	2.9
1	B	342	GLY	2.9
1	D	261	GLU	2.9
1	D	136	VAL	2.9
1	B	260	PRO	2.9
1	C	279	ARG	2.9
1	C	576	ARG	2.9
1	E	449	GLY	2.9
1	E	459	ARG	2.9
1	B	475	VAL	2.9
1	E	419	VAL	2.9
1	E	195	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	461	ASP	2.9
1	C	75	GLY	2.9
1	C	158	TYR	2.9
1	C	426	THR	2.9
2	G	51	LEU	2.9
1	C	231	ASP	2.9
1	F	113	VAL	2.9
1	A	386	LEU	2.9
2	G	431	PHE	2.9
1	C	692	GLU	2.9
1	E	151	PRO	2.9
1	D	182	LEU	2.9
2	G	313	LEU	2.9
1	E	487	ALA	2.9
1	D	609	SER	2.9
1	E	90	ASP	2.9
1	E	539	ARG	2.9
1	F	503	VAL	2.9
3	H	87	VAL	2.9
1	D	308	ARG	2.9
1	A	630	TRP	2.9
1	B	215	TYR	2.9
1	A	526	PRO	2.9
1	A	562	LEU	2.9
1	D	578	LEU	2.9
1	C	556	ILE	2.9
3	H	133	GLY	2.9
1	A	338	ILE	2.9
1	B	434	SER	2.9
1	C	232	THR	2.9
1	E	333	ASP	2.9
1	B	540	ARG	2.9
1	E	242	PHE	2.9
1	B	446	VAL	2.9
1	E	126	LEU	2.9
1	E	142	LEU	2.9
1	F	234	ALA	2.9
1	F	613	CYS	2.9
1	B	227	LYS	2.9
1	A	611	VAL	2.9
1	B	137	CYS	2.9
1	A	349	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	185	GLY	2.9
1	B	116	LEU	2.9
1	E	592	ILE	2.9
1	C	387	LEU	2.9
1	C	165	THR	2.9
1	A	151	PRO	2.9
1	A	477	LYS	2.9
1	B	367	ILE	2.9
1	F	389	LYS	2.9
2	G	291	LEU	2.9
1	A	194	TYR	2.9
1	B	425	TYR	2.9
2	G	288	LYS	2.9
3	H	74	HIS	2.9
1	F	62	VAL	2.9
1	A	95	TYR	2.9
1	E	658	ALA	2.9
1	F	570	SER	2.9
1	B	83	HIS	2.8
1	E	260	PRO	2.8
2	G	373	VAL	2.8
1	D	169	TYR	2.8
1	B	406	GLY	2.8
1	C	321	ALA	2.8
1	C	413	LEU	2.8
1	F	495	LEU	2.8
2	G	308	LEU	2.8
1	A	259	GLN	2.8
1	A	391	VAL	2.8
1	F	457	LYS	2.8
1	B	225	LEU	2.8
2	G	82	LEU	2.8
1	E	473	VAL	2.8
1	A	438	TYR	2.8
1	A	476	PHE	2.8
1	D	437	SER	2.8
1	A	263	PRO	2.8
1	E	52	HIS	2.8
1	A	473	VAL	2.8
1	E	182	LEU	2.8
2	G	489	ILE	2.8
1	A	189	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	201	ARG	2.8
1	E	696	ASN	2.8
1	F	576	ARG	2.8
2	G	356	TYR	2.8
1	F	200	SER	2.8
2	G	80	PHE	2.8
1	B	127	LEU	2.8
1	A	226	ILE	2.8
1	F	215	TYR	2.8
1	E	611	VAL	2.8
1	F	173	VAL	2.8
1	C	394	THR	2.8
1	F	155	LYS	2.8
1	F	292	SER	2.8
1	A	446	VAL	2.8
1	E	132	LEU	2.8
1	F	410	ASN	2.8
1	B	654	TYR	2.8
1	E	345	GLN	2.8
2	G	76	HIS	2.8
3	H	71	PHE	2.8
1	E	72	LYS	2.8
1	C	435	VAL	2.8
1	C	621	VAL	2.8
1	B	254	TYR	2.8
1	C	168	MET	2.8
1	C	336	PHE	2.8
1	F	309	LEU	2.8
1	F	424	LEU	2.8
1	F	633	LEU	2.8
1	E	326	PHE	2.8
1	A	388	GLY	2.8
1	A	201	ARG	2.8
1	C	295	SER	2.8
1	E	676	LYS	2.8
1	A	248	ALA	2.8
1	C	111	ASN	2.8
1	F	430	ASP	2.8
1	F	596	PHE	2.8
1	F	472	MET	2.8
1	F	635	LEU	2.8
2	G	512	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	150	GLU	2.7
2	G	261	THR	2.7
1	C	521	LEU	2.7
1	D	435	VAL	2.7
1	D	218	HIS	2.7
1	E	669	ALA	2.7
1	E	208	GLU	2.7
1	E	386	LEU	2.7
1	A	250	GLY	2.7
1	A	168	MET	2.7
1	A	457	LYS	2.7
1	B	117	LEU	2.7
1	E	470	TYR	2.7
1	F	258	VAL	2.7
1	D	195	PHE	2.7
1	F	290	PHE	2.7
2	G	508	GLY	2.7
1	A	498	MET	2.7
1	E	202	LYS	2.7
1	D	623	VAL	2.7
1	B	258	VAL	2.7
1	C	277	THR	2.7
1	E	249	SER	2.7
1	F	93	ALA	2.7
1	D	238	HIS	2.7
1	D	134	GLN	2.7
2	G	375	TYR	2.7
1	A	404	PHE	2.7
1	B	571	VAL	2.7
1	F	151	PRO	2.7
1	D	487	ALA	2.7
1	E	495	LEU	2.7
1	E	125	ARG	2.7
1	E	238	HIS	2.7
1	C	244	ILE	2.7
1	E	654	TYR	2.7
1	F	610	GLN	2.7
1	C	541	ASP	2.7
1	A	337	ALA	2.7
1	B	596	PHE	2.7
1	F	114	ASN	2.7
2	G	277	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	82	ALA	2.7
1	B	555	SER	2.7
1	B	485	ASP	2.7
1	E	695	ILE	2.7
1	D	475	VAL	2.7
1	A	601	GLU	2.7
1	B	460	ALA	2.7
1	D	668	SER	2.7
1	E	205	ARG	2.7
3	H	40	THR	2.7
1	E	684	ASP	2.7
1	B	149	VAL	2.7
1	E	321	ALA	2.7
1	E	562	LEU	2.7
1	A	241	ILE	2.7
1	E	353	SER	2.7
1	D	646	PHE	2.7
1	E	555	SER	2.7
1	A	508	VAL	2.7
1	D	296	LEU	2.7
1	D	669	ALA	2.6
2	G	408	ALA	2.6
1	A	156	GLU	2.6
1	B	298	PHE	2.6
1	F	318	PRO	2.6
1	D	539	ARG	2.6
1	E	424	LEU	2.6
1	E	526	PRO	2.6
1	E	682	THR	2.6
1	A	594	CYS	2.6
1	E	358	PHE	2.6
1	A	43	SER	2.6
1	B	400	ILE	2.6
2	G	437	ASP	2.6
1	A	225	LEU	2.6
1	B	445	VAL	2.6
1	A	65	GLY	2.6
1	A	111	ASN	2.6
1	D	363	ILE	2.6
1	E	523	SER	2.6
1	D	344	LYS	2.6
2	G	381	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	184	ILE	2.6
1	C	199	SER	2.6
1	A	396	ALA	2.6
1	B	47	ASP	2.6
1	C	326	PHE	2.6
1	C	354	ALA	2.6
1	E	637	LEU	2.6
1	F	637	LEU	2.6
1	A	610	GLN	2.6
1	D	283	LEU	2.6
1	F	120	ASP	2.6
1	A	293	TYR	2.6
2	G	324	VAL	2.6
2	G	345	MET	2.6
1	A	326	PHE	2.6
1	B	344	LYS	2.6
2	G	262	HIS	2.6
1	B	521	LEU	2.6
1	D	229	PRO	2.6
1	B	506	VAL	2.6
1	F	659	HIS	2.6
2	G	279	LEU	2.6
1	C	445	VAL	2.6
1	F	231	ASP	2.6
1	D	152	SER	2.6
1	F	129	CYS	2.6
1	E	297	PRO	2.6
1	B	275	PHE	2.6
1	A	40	THR	2.6
1	B	216	GLU	2.6
1	B	569	ILE	2.6
1	E	503	VAL	2.6
1	D	580	LEU	2.6
2	G	434	ILE	2.6
1	B	158	TYR	2.6
1	D	203	LEU	2.6
2	G	177	THR	2.6
1	E	578	LEU	2.6
2	G	287	LEU	2.6
1	B	152	SER	2.6
1	E	340	SER	2.6
3	H	76	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	2.6
1	D	571	VAL	2.6
1	E	222	VAL	2.6
1	C	254	TYR	2.6
1	D	667	ASN	2.6
1	E	587	ASN	2.6
1	A	350	PRO	2.6
1	D	406	GLY	2.6
1	A	577	LEU	2.5
1	C	213	LEU	2.5
2	G	122	GLU	2.5
2	G	191	ALA	2.5
1	F	131	SER	2.5
2	G	496	THR	2.5
1	E	227	LYS	2.5
2	G	144	ILE	2.5
1	D	449	GLY	2.5
1	A	247	PHE	2.5
2	G	483	PHE	2.5
1	A	413	LEU	2.5
1	A	532	ALA	2.5
1	B	669	ALA	2.5
1	D	290	PHE	2.5
1	F	233	LEU	2.5
1	F	320	GLU	2.5
1	D	114	ASN	2.5
1	F	75	GLY	2.5
1	C	198	LEU	2.5
1	D	670	PHE	2.5
1	C	441	ASN	2.5
1	E	97	PRO	2.5
1	E	415	GLY	2.5
1	C	533	LEU	2.5
1	A	569	ILE	2.5
1	A	653	PHE	2.5
1	D	569	ILE	2.5
1	F	363	ILE	2.5
1	C	320	GLU	2.5
1	A	135	GLY	2.5
1	A	539	ARG	2.5
1	B	58	ARG	2.5
1	E	364	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	196	PRO	2.5
1	C	95	TYR	2.5
1	D	225	LEU	2.5
2	G	132	CYS	2.5
1	A	647	VAL	2.5
1	C	131	SER	2.5
1	E	299	GLY	2.5
1	F	158	TYR	2.5
1	E	702	PRO	2.5
1	F	506	VAL	2.5
2	G	435	VAL	2.5
1	D	354	ALA	2.5
2	G	500	GLN	2.5
1	A	671	ARG	2.5
1	A	322	LEU	2.5
3	H	72	ASN	2.5
1	F	349	PRO	2.5
1	B	336	PHE	2.5
1	D	541	ASP	2.5
1	E	410	ASN	2.5
1	B	437	SER	2.5
1	A	198	LEU	2.5
1	A	312	ALA	2.5
1	C	655	ASN	2.5
1	A	82	ALA	2.5
1	B	426	THR	2.5
1	D	424	LEU	2.5
1	F	483	LEU	2.5
1	F	358	PHE	2.5
1	B	241	ILE	2.5
1	D	455	LEU	2.5
1	C	517	CYS	2.5
1	D	187	ALA	2.5
1	D	305	VAL	2.5
1	B	213	LEU	2.5
1	D	190	GLY	2.5
1	C	207	PRO	2.5
1	C	330	SER	2.5
1	E	653	PHE	2.5
1	A	606	VAL	2.5
1	E	469	GLN	2.5
1	A	260	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	28	ASN	2.5
1	A	52	HIS	2.5
2	G	143	TYR	2.5
1	C	290	PHE	2.5
1	C	431	ARG	2.5
1	F	555	SER	2.5
1	A	687	THR	2.5
1	D	562	LEU	2.5
1	D	608	GLY	2.5
1	F	523	SER	2.4
1	F	587	ASN	2.4
1	B	242	PHE	2.4
1	B	668	SER	2.4
1	C	487	ALA	2.4
1	C	559	CYS	2.4
1	F	47	ASP	2.4
1	D	130	GLY	2.4
1	E	91	ASN	2.4
2	G	175	LEU	2.4
1	A	613	CYS	2.4
1	F	449	GLY	2.4
1	C	630	TRP	2.4
1	A	115	LYS	2.4
1	D	526	PRO	2.4
1	B	470	TYR	2.4
1	F	111	ASN	2.4
3	H	112	VAL	2.4
1	D	181	LYS	2.4
2	G	429	TYR	2.4
1	E	493	LEU	2.4
1	F	580	LEU	2.4
2	G	304	HIS	2.4
2	G	343	TYR	2.4
1	F	648	SER	2.4
1	C	446	VAL	2.4
1	E	253	VAL	2.4
1	F	611	VAL	2.4
1	D	153	HIS	2.4
1	B	244	ILE	2.4
1	F	539	ARG	2.4
1	B	257	THR	2.4
1	E	324	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	212	MET	2.4
1	C	650	GLU	2.4
2	G	61	LEU	2.4
1	B	560	MET	2.4
1	D	168	MET	2.4
2	G	46	ILE	2.4
1	E	613	CYS	2.4
1	B	496	TYR	2.4
2	G	440	ASP	2.4
1	A	459	ARG	2.4
1	D	559	CYS	2.4
2	G	283	TRP	2.4
1	D	659	HIS	2.4
1	A	188	VAL	2.4
2	G	71	VAL	2.4
1	C	539	ARG	2.4
1	E	577	LEU	2.4
1	E	36	PRO	2.4
2	G	276	HIS	2.4
1	C	324	GLN	2.4
1	D	692	GLU	2.4
1	A	325	ALA	2.4
1	F	321	ALA	2.4
1	A	587	ASN	2.4
1	B	274	LEU	2.4
1	F	278	SER	2.4
1	F	541	ASP	2.4
2	G	90	LYS	2.4
1	A	97	PRO	2.4
1	A	321	ALA	2.4
1	F	326	PHE	2.4
2	G	342	MET	2.4
1	B	471	GLU	2.4
1	C	613	CYS	2.4
1	F	529	GLY	2.4
1	E	44	GLU	2.4
2	G	50	GLY	2.4
1	C	164	LYS	2.4
1	A	203	LEU	2.4
1	C	347	HIS	2.4
1	E	93	ALA	2.4
1	B	197	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	343	GLN	2.4
1	E	605	GLN	2.4
1	C	70	VAL	2.4
1	F	653	PHE	2.4
1	F	465	HIS	2.3
1	A	571	VAL	2.3
1	D	212	MET	2.3
2	G	422	MET	2.3
1	B	487	ALA	2.3
1	E	673	HIS	2.3
1	F	193	ASP	2.3
1	A	138	LYS	2.3
1	E	130	GLY	2.3
1	E	328	ILE	2.3
1	B	182	LEU	2.3
1	C	594	CYS	2.3
1	F	419	VAL	2.3
2	G	195	MET	2.3
1	A	336	PHE	2.3
2	G	328	PHE	2.3
1	B	314	TYR	2.3
1	F	276	TYR	2.3
1	D	49	THR	2.3
1	E	549	ALA	2.3
1	B	309	LEU	2.3
1	B	461	ASP	2.3
2	G	201	ILE	2.3
1	E	564	VAL	2.3
1	E	610	GLN	2.3
1	F	296	LEU	2.3
1	B	321	ALA	2.3
1	A	130	GLY	2.3
1	E	524	GLY	2.3
1	E	670	PHE	2.3
1	E	693	GLY	2.3
1	F	99	ILE	2.3
1	B	677	TYR	2.3
1	B	308	ARG	2.3
1	D	167	THR	2.3
1	E	41	PHE	2.3
1	B	414	GLY	2.3
1	E	225	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	441	ASN	2.3
1	D	504	THR	2.3
1	E	472	MET	2.3
1	A	212	MET	2.3
1	A	607	SER	2.3
1	F	687	THR	2.3
1	F	683	HIS	2.3
1	C	384	ASN	2.3
2	G	514	LEU	2.3
1	B	328	ILE	2.3
1	D	356	CYS	2.3
2	G	341	CYS	2.3
2	G	194	PHE	2.3
1	B	621	VAL	2.3
1	A	440	TYR	2.3
1	E	635	LEU	2.3
1	C	236	VAL	2.3
1	F	253	VAL	2.3
1	A	227	LYS	2.3
1	F	571	VAL	2.3
1	A	285	LYS	2.3
1	B	529	GLY	2.3
1	C	63	TYR	2.3
1	F	77	LEU	2.3
1	F	367	ILE	2.3
1	F	573	ASP	2.3
1	D	671	ARG	2.3
1	A	357	ALA	2.3
1	A	592	ILE	2.3
1	B	128	ALA	2.3
1	B	191	LYS	2.3
1	A	474	SER	2.3
1	F	556	ILE	2.3
1	C	433	THR	2.3
2	G	306	ASP	2.3
1	B	173	VAL	2.3
1	D	472	MET	2.3
2	G	363	ASN	2.3
1	F	83	HIS	2.3
1	A	75	GLY	2.3
1	C	64	VAL	2.3
1	A	127	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	594	CYS	2.2
1	D	41	PHE	2.2
1	E	198	LEU	2.2
1	E	483	LEU	2.2
1	A	458	ILE	2.2
1	F	431	ARG	2.2
1	E	322	LEU	2.2
1	A	62	VAL	2.2
1	E	317	LYS	2.2
1	E	598	ASN	2.2
3	H	95	GLU	2.2
1	B	539	ARG	2.2
1	C	215	TYR	2.2
1	D	508	VAL	2.2
1	F	245	TYR	2.2
1	F	415	GLY	2.2
1	D	164	LYS	2.2
1	A	313	ALA	2.2
1	C	599	LEU	2.2
1	F	649	THR	2.2
1	B	430	ASP	2.2
1	D	99	ILE	2.2
3	H	136	ILE	2.2
1	B	194	TYR	2.2
1	B	318	PRO	2.2
1	D	157	HIS	2.2
2	G	406	HIS	2.2
1	F	364	ASN	2.2
1	A	637	LEU	2.2
1	C	371	LEU	2.2
1	C	658	ALA	2.2
1	E	533	LEU	2.2
1	A	684	ASP	2.2
1	D	324	GLN	2.2
1	D	459	ARG	2.2
1	C	166	GLY	2.2
1	D	62	VAL	2.2
1	B	90	ASP	2.2
1	E	573	ASP	2.2
1	C	126	LEU	2.2
1	C	611	VAL	2.2
1	A	353	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	620	ASP	2.2
1	C	99	ILE	2.2
1	C	312	ALA	2.2
1	E	37	GLN	2.2
1	D	498	MET	2.2
2	G	118	ILE	2.2
1	F	213	LEU	2.2
1	A	88	GLU	2.2
1	E	427	THR	2.2
1	D	205	ARG	2.2
1	A	561	SER	2.2
1	D	383	LEU	2.2
1	E	585	ALA	2.2
1	C	155	LYS	2.2
1	F	277	THR	2.2
1	A	183	PHE	2.2
1	E	140	LEU	2.2
1	F	552	PHE	2.2
1	A	408	ASP	2.2
1	F	492	GLN	2.2
3	H	64	TYR	2.2
1	B	371	LEU	2.2
1	E	251	GLY	2.2
1	E	288	PRO	2.2
2	G	27	ASN	2.2
1	C	498	MET	2.2
1	C	391	VAL	2.2
1	A	193	ASP	2.2
1	F	470	TYR	2.2
1	A	197	THR	2.2
1	B	195	PHE	2.2
1	B	459	ARG	2.2
1	E	600	THR	2.2
1	B	405	CYS	2.2
1	C	659	HIS	2.2
1	C	497	VAL	2.2
1	A	347	HIS	2.2
1	B	139	LEU	2.2
2	G	244	TYR	2.2
1	A	113	VAL	2.1
1	A	302	ARG	2.1
1	C	216	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	419	VAL	2.1
1	E	482	ILE	2.1
1	A	500	GLU	2.1
1	E	214	ASP	2.1
1	C	614	ILE	2.1
1	D	122	SER	2.1
1	A	582	VAL	2.1
1	D	113	VAL	2.1
2	G	433	GLN	2.1
1	A	478	ASP	2.1
1	B	77	LEU	2.1
1	F	650	GLU	2.1
1	B	568	SER	2.1
2	G	142	THR	2.1
1	A	333	ASP	2.1
1	C	532	ALA	2.1
1	A	646	PHE	2.1
1	B	599	LEU	2.1
1	C	409	ILE	2.1
1	C	573	ASP	2.1
1	A	344	LYS	2.1
1	A	655	ASN	2.1
1	D	202	LYS	2.1
1	F	538	SER	2.1
1	B	326	PHE	2.1
1	E	218	HIS	2.1
1	F	229	PRO	2.1
2	G	116	ASN	2.1
1	D	274	LEU	2.1
1	B	247	PHE	2.1
1	F	42	HIS	2.1
2	G	246	PHE	2.1
1	D	133	TYR	2.1
2	G	263	ALA	2.1
1	E	550	ASN	2.1
1	F	286	ASP	2.1
2	G	123	ALA	2.1
1	C	702	PRO	2.1
1	E	247	PHE	2.1
1	F	568	SER	2.1
2	G	490	SER	2.1
1	E	671	ARG	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	148	LEU	2.1
3	H	77	LEU	2.1
1	B	111	ASN	2.1
1	D	339	PHE	2.1
2	G	196	GLY	2.1
1	C	455	LEU	2.1
1	D	566	PRO	2.1
1	C	587	ASN	2.1
1	D	42	HIS	2.1
1	F	654	TYR	2.1
1	D	482	ILE	2.1
1	B	386	LEU	2.1
1	C	442	GLY	2.1
1	D	65	GLY	2.1
1	E	368	LYS	2.1
2	G	303	THR	2.1
1	A	654	TYR	2.1
1	B	277	THR	2.1
1	C	353	SER	2.1
2	G	45	VAL	2.1
1	D	367	ILE	2.1
1	F	525	ASP	2.1
1	E	85	THR	2.1
1	E	579	SER	2.1
1	F	43	SER	2.1
1	A	659	HIS	2.1
1	B	660	GLN	2.1
1	C	485	ASP	2.1
1	A	572	SER	2.1
1	C	488	PHE	2.1
1	B	478	ASP	2.1
1	E	471	GLU	2.1
1	D	555	SER	2.1
1	C	507	PRO	2.1
1	E	521	LEU	2.1
1	C	360	ILE	2.1
1	D	75	GLY	2.1
1	F	615	SER	2.1
1	F	314	TYR	2.1
1	D	139	LEU	2.0
1	D	637	LEU	2.0
1	A	650	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	H	106	LYS	2.0
1	C	383	LEU	2.0
1	E	335	LEU	2.0
1	C	197	THR	2.0
1	C	439	VAL	2.0
1	C	564	VAL	2.0
2	G	117	PHE	2.0
1	D	154	LYS	2.0
1	C	424	LEU	2.0
1	C	167	THR	2.0
1	B	352	ASP	2.0
1	B	424	LEU	2.0
1	B	207	PRO	2.0
1	B	488	PHE	2.0
3	H	110	SER	2.0
1	E	42	HIS	2.0
2	G	74	LYS	2.0
1	D	119	ILE	2.0
1	D	440	TYR	2.0
1	E	556	ILE	2.0
1	D	51	ASN	2.0
1	D	353	SER	2.0
1	A	692	GLU	2.0
1	F	44	GLU	2.0
1	A	182	LEU	2.0
1	B	169	TYR	2.0
1	D	126	LEU	2.0
1	F	562	LEU	2.0
2	G	447	ASP	2.0
1	D	52	HIS	2.0
1	F	76	ASN	2.0
1	F	360	ILE	2.0
1	A	253	VAL	2.0
1	B	356	CYS	2.0
1	E	174	ARG	2.0
3	H	89	VAL	2.0
1	E	357	ALA	2.0
1	E	588	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	H	601	1/1	0.84	0.20	-1.61	369,369,369,369	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.