



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:55 PM GMT

PDB ID : 4N5C  
Title : Crystal structure of Ypp1  
Authors : Wu, X.; Chi, R.J.; Baskin, J.M.; Lucast, L.; Burd, C.G.; De Camilli, P.; Reinisch, K.M.  
Deposited on : 2013-10-09  
Resolution : 3.25 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

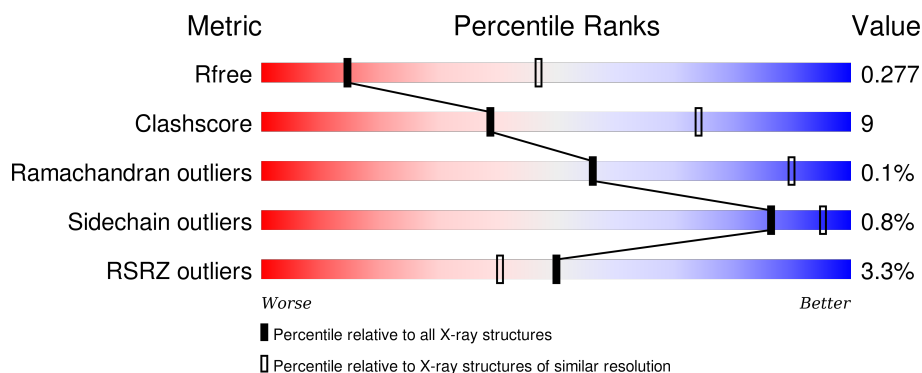
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	802	<div> <div>2%</div> <div>71% 21% 7%</div> </div>
1	B	802	<div> <div>2%</div> <div>72% 20% 8%</div> </div>
1	C	802	<div> <div>2%</div> <div>73% 18% 8%</div> </div>
1	D	802	<div> <div>2%</div> <div>72% 22% 6%</div> </div>
1	E	802	<div> <div>3%</div> <div>69% 21% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	802	<div><div></div><div>3%</div><div>68%</div><div>22%</div><div>9%</div></div>
1	G	802	<div><div></div><div>4%</div><div>70%</div><div>21%</div><div>8%</div></div>
1	H	802	<div><div></div><div>4%</div><div>68%</div><div>23%</div><div>• 8%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 48674 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 Cargo-transport protein YPP1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	745	Total	C	N	O	S	Se	0	0	0
			6138	3963	987	1160	11	17			
1	B	741	Total	C	N	O	S	Se	0	0	0
			6109	3948	982	1151	11	17			
1	C	737	Total	C	N	O	S	Se	0	0	0
			6080	3930	977	1145	11	17			
1	D	757	Total	C	N	O	S	Se	0	0	0
			6241	4031	1003	1179	11	17			
1	E	727	Total	C	N	O	S	Se	0	0	0
			6000	3884	967	1123	11	15			
1	F	727	Total	C	N	O	S	Se	0	0	0
			5993	3872	967	1128	11	15			
1	G	735	Total	C	N	O	S	Se	0	0	0
			6056	3910	977	1143	11	15			
1	H	734	Total	C	N	O	S	Se	0	0	0
			6057	3916	976	1138	11	16			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	EXPRESSION TAG	UNP P46951
A	7	PRO	-	EXPRESSION TAG	UNP P46951
A	8	LEU	-	EXPRESSION TAG	UNP P46951
A	9	GLY	-	EXPRESSION TAG	UNP P46951
A	10	SER	-	EXPRESSION TAG	UNP P46951
A	?	-	LEU	DELETION	UNP P46951
A	?	-	ASP	DELETION	UNP P46951
A	?	-	LYS	DELETION	UNP P46951
A	?	-	LYS	DELETION	UNP P46951
A	?	-	PRO	DELETION	UNP P46951
A	?	-	GLY	DELETION	UNP P46951
A	?	-	LYS	DELETION	UNP P46951
A	?	-	ARG	DELETION	UNP P46951

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	DELETION	UNP P46951
A	?	-	LYS	DELETION	UNP P46951
B	6	GLY	-	EXPRESSION TAG	UNP P46951
B	7	PRO	-	EXPRESSION TAG	UNP P46951
B	8	LEU	-	EXPRESSION TAG	UNP P46951
B	9	GLY	-	EXPRESSION TAG	UNP P46951
B	10	SER	-	EXPRESSION TAG	UNP P46951
B	?	-	LEU	DELETION	UNP P46951
B	?	-	ASP	DELETION	UNP P46951
B	?	-	LYS	DELETION	UNP P46951
B	?	-	LYS	DELETION	UNP P46951
B	?	-	PRO	DELETION	UNP P46951
B	?	-	GLY	DELETION	UNP P46951
B	?	-	LYS	DELETION	UNP P46951
B	?	-	ARG	DELETION	UNP P46951
B	?	-	ALA	DELETION	UNP P46951
B	?	-	LYS	DELETION	UNP P46951
C	6	GLY	-	EXPRESSION TAG	UNP P46951
C	7	PRO	-	EXPRESSION TAG	UNP P46951
C	8	LEU	-	EXPRESSION TAG	UNP P46951
C	9	GLY	-	EXPRESSION TAG	UNP P46951
C	10	SER	-	EXPRESSION TAG	UNP P46951
C	?	-	LEU	DELETION	UNP P46951
C	?	-	ASP	DELETION	UNP P46951
C	?	-	LYS	DELETION	UNP P46951
C	?	-	LYS	DELETION	UNP P46951
C	?	-	PRO	DELETION	UNP P46951
C	?	-	GLY	DELETION	UNP P46951
C	?	-	LYS	DELETION	UNP P46951
C	?	-	ARG	DELETION	UNP P46951
C	?	-	ALA	DELETION	UNP P46951
C	?	-	LYS	DELETION	UNP P46951
D	6	GLY	-	EXPRESSION TAG	UNP P46951
D	7	PRO	-	EXPRESSION TAG	UNP P46951
D	8	LEU	-	EXPRESSION TAG	UNP P46951
D	9	GLY	-	EXPRESSION TAG	UNP P46951
D	10	SER	-	EXPRESSION TAG	UNP P46951
D	?	-	LEU	DELETION	UNP P46951
D	?	-	ASP	DELETION	UNP P46951
D	?	-	LYS	DELETION	UNP P46951
D	?	-	LYS	DELETION	UNP P46951
D	?	-	PRO	DELETION	UNP P46951

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	DELETION	UNP P46951
D	?	-	LYS	DELETION	UNP P46951
D	?	-	ARG	DELETION	UNP P46951
D	?	-	ALA	DELETION	UNP P46951
D	?	-	LYS	DELETION	UNP P46951
E	6	GLY	-	EXPRESSION TAG	UNP P46951
E	7	PRO	-	EXPRESSION TAG	UNP P46951
E	8	LEU	-	EXPRESSION TAG	UNP P46951
E	9	GLY	-	EXPRESSION TAG	UNP P46951
E	10	SER	-	EXPRESSION TAG	UNP P46951
E	?	-	LEU	DELETION	UNP P46951
E	?	-	ASP	DELETION	UNP P46951
E	?	-	LYS	DELETION	UNP P46951
E	?	-	LYS	DELETION	UNP P46951
E	?	-	PRO	DELETION	UNP P46951
E	?	-	GLY	DELETION	UNP P46951
E	?	-	LYS	DELETION	UNP P46951
E	?	-	ARG	DELETION	UNP P46951
E	?	-	ALA	DELETION	UNP P46951
E	?	-	LYS	DELETION	UNP P46951
F	6	GLY	-	EXPRESSION TAG	UNP P46951
F	7	PRO	-	EXPRESSION TAG	UNP P46951
F	8	LEU	-	EXPRESSION TAG	UNP P46951
F	9	GLY	-	EXPRESSION TAG	UNP P46951
F	10	SER	-	EXPRESSION TAG	UNP P46951
F	?	-	LEU	DELETION	UNP P46951
F	?	-	ASP	DELETION	UNP P46951
F	?	-	LYS	DELETION	UNP P46951
F	?	-	LYS	DELETION	UNP P46951
F	?	-	PRO	DELETION	UNP P46951
F	?	-	GLY	DELETION	UNP P46951
F	?	-	LYS	DELETION	UNP P46951
F	?	-	ARG	DELETION	UNP P46951
F	?	-	ALA	DELETION	UNP P46951
F	?	-	LYS	DELETION	UNP P46951
G	6	GLY	-	EXPRESSION TAG	UNP P46951
G	7	PRO	-	EXPRESSION TAG	UNP P46951
G	8	LEU	-	EXPRESSION TAG	UNP P46951
G	9	GLY	-	EXPRESSION TAG	UNP P46951
G	10	SER	-	EXPRESSION TAG	UNP P46951
G	?	-	LEU	DELETION	UNP P46951
G	?	-	ASP	DELETION	UNP P46951

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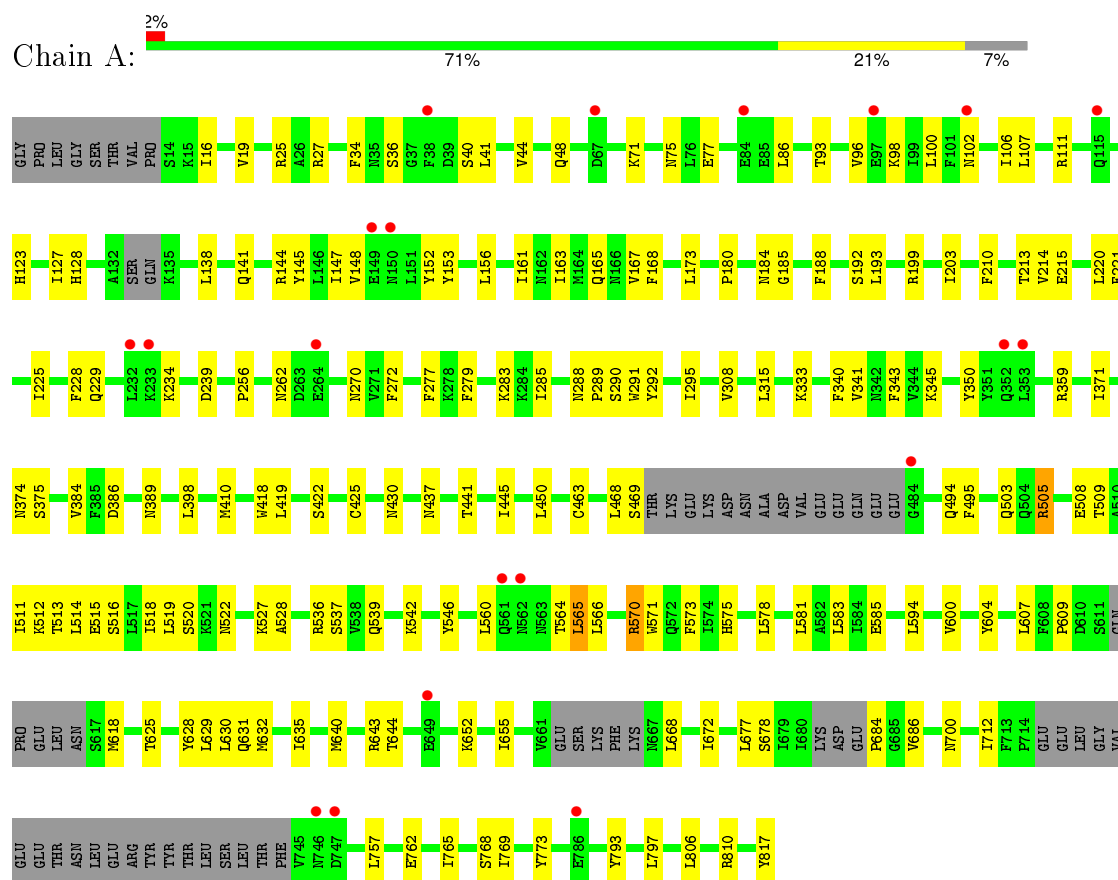
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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	DELETION	UNP P46951
G	?	-	LYS	DELETION	UNP P46951
G	?	-	PRO	DELETION	UNP P46951
G	?	-	GLY	DELETION	UNP P46951
G	?	-	LYS	DELETION	UNP P46951
G	?	-	ARG	DELETION	UNP P46951
G	?	-	ALA	DELETION	UNP P46951
G	?	-	LYS	DELETION	UNP P46951
H	6	GLY	-	EXPRESSION TAG	UNP P46951
H	7	PRO	-	EXPRESSION TAG	UNP P46951
H	8	LEU	-	EXPRESSION TAG	UNP P46951
H	9	GLY	-	EXPRESSION TAG	UNP P46951
H	10	SER	-	EXPRESSION TAG	UNP P46951
H	?	-	LEU	DELETION	UNP P46951
H	?	-	ASP	DELETION	UNP P46951
H	?	-	LYS	DELETION	UNP P46951
H	?	-	LYS	DELETION	UNP P46951
H	?	-	PRO	DELETION	UNP P46951
H	?	-	GLY	DELETION	UNP P46951
H	?	-	LYS	DELETION	UNP P46951
H	?	-	ARG	DELETION	UNP P46951
H	?	-	ALA	DELETION	UNP P46951
H	?	-	LYS	DELETION	UNP P46951

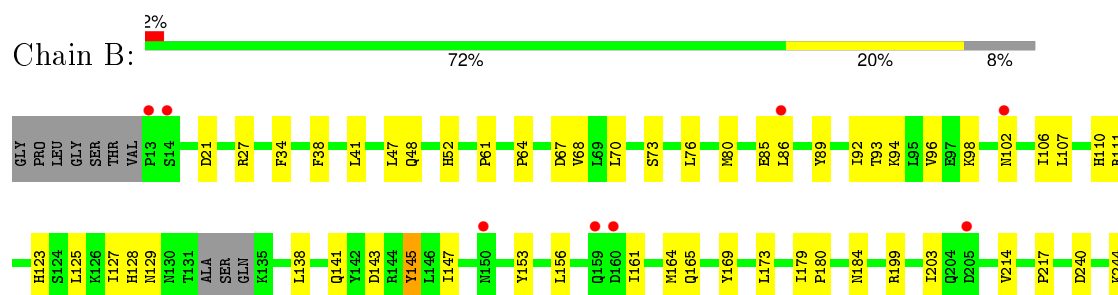
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

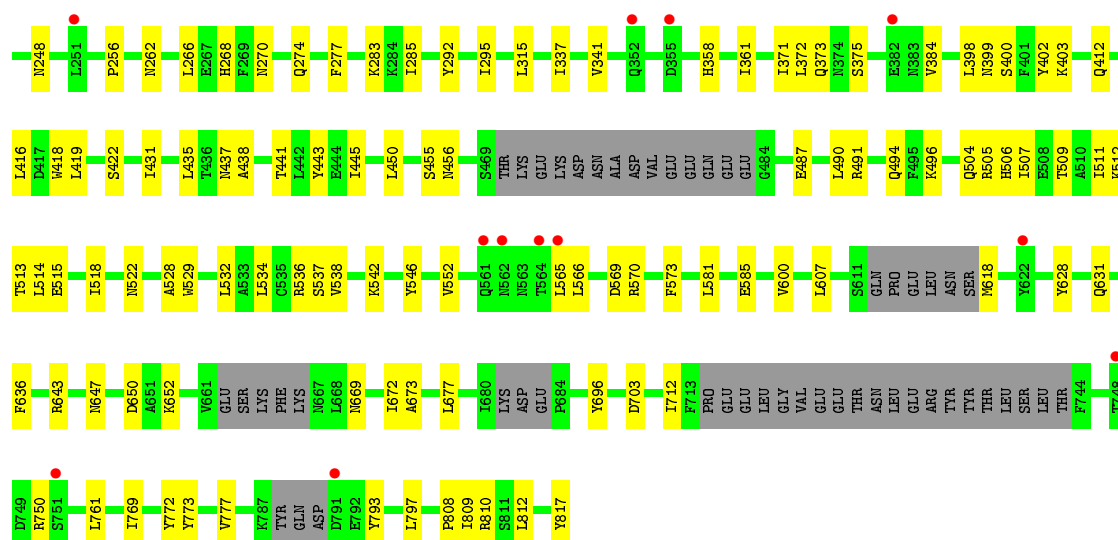
#### • Molecule 1: Cargo-transport protein YPP1



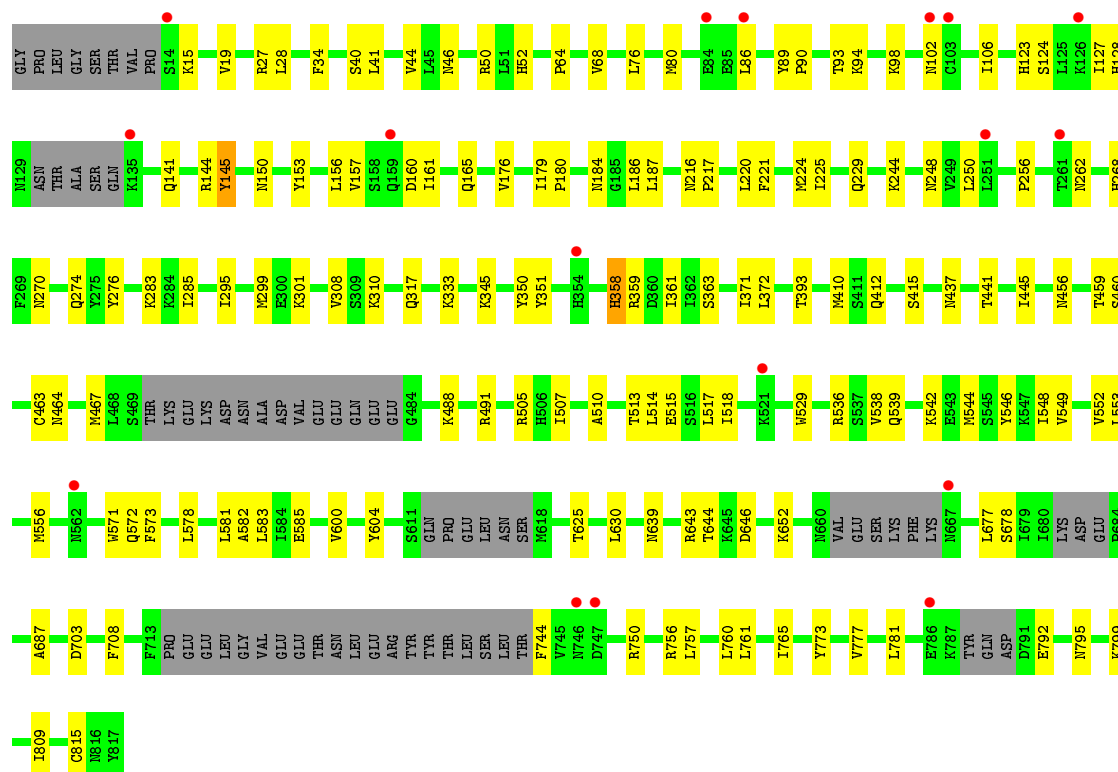
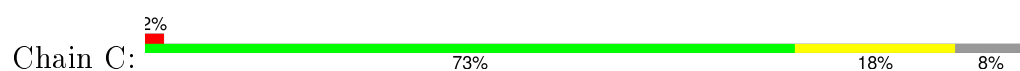
#### • Molecule 1: Cargo-transport protein YPP1



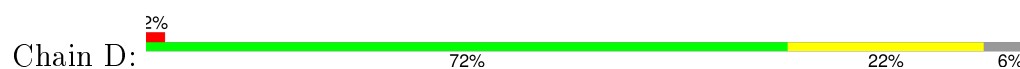


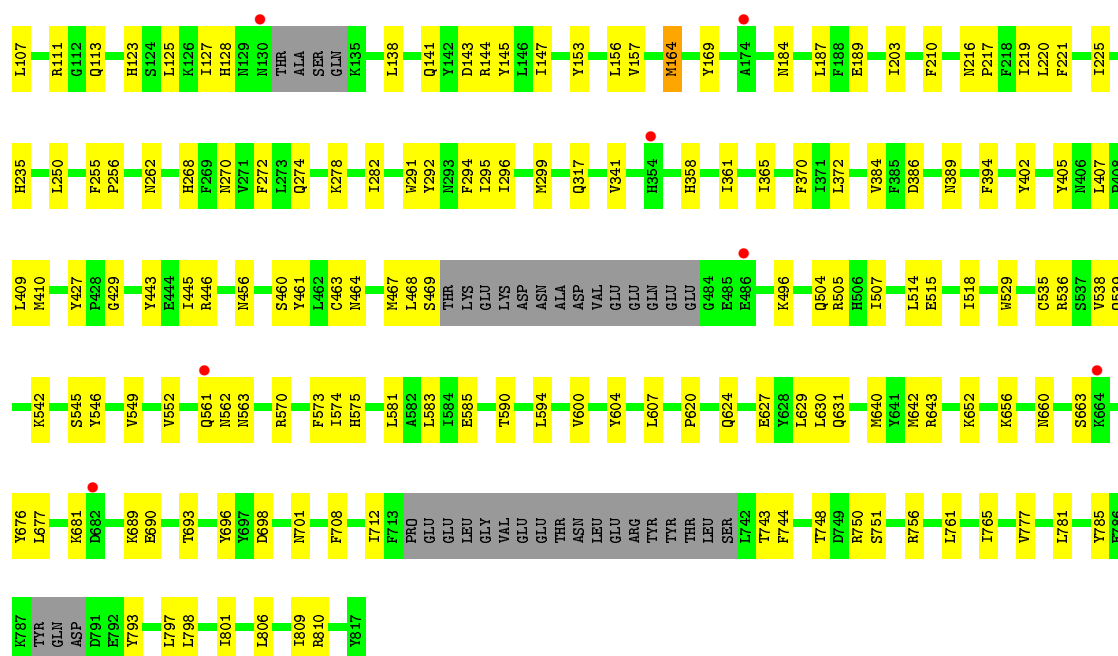


• Molecule 1: Cargo-transport protein YPP1



• Molecule 1: Cargo-transport protein YPP1

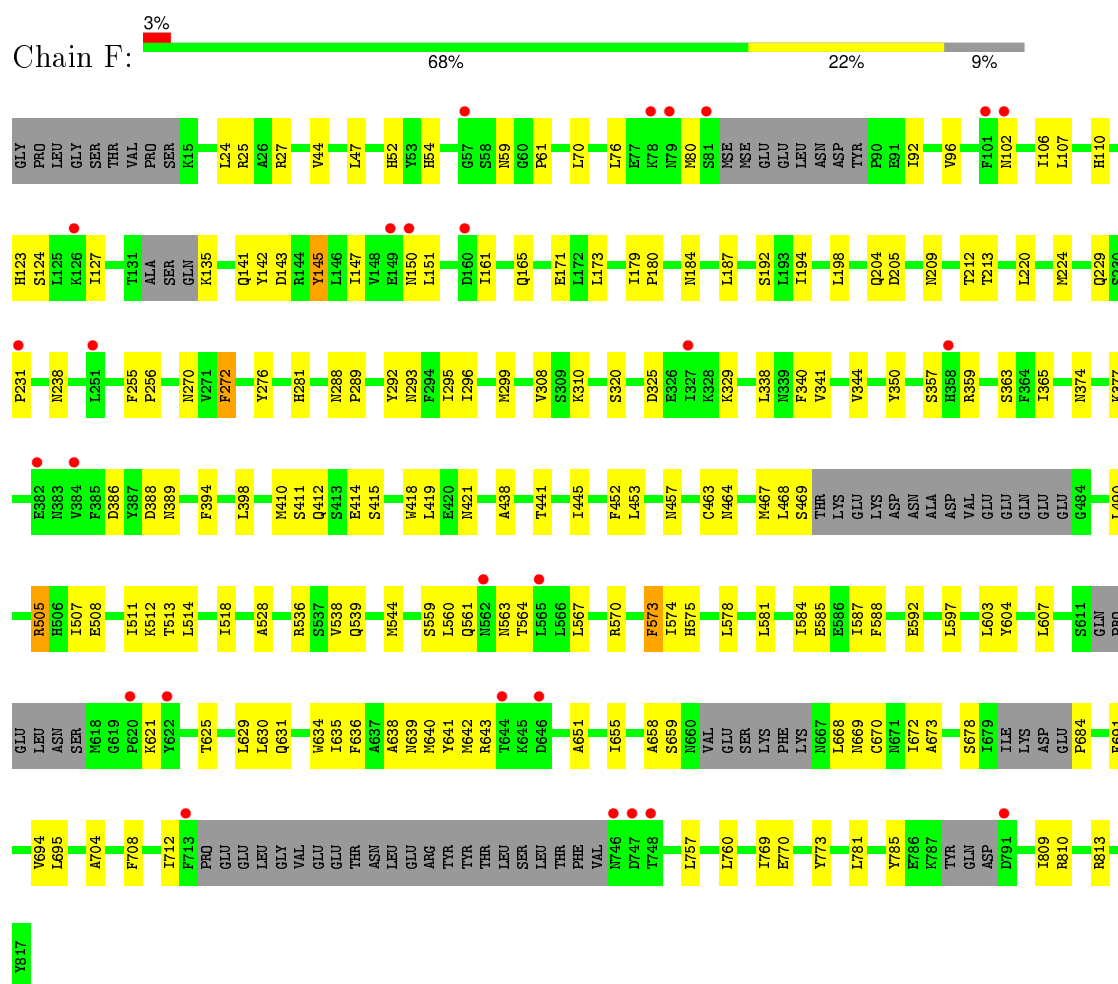




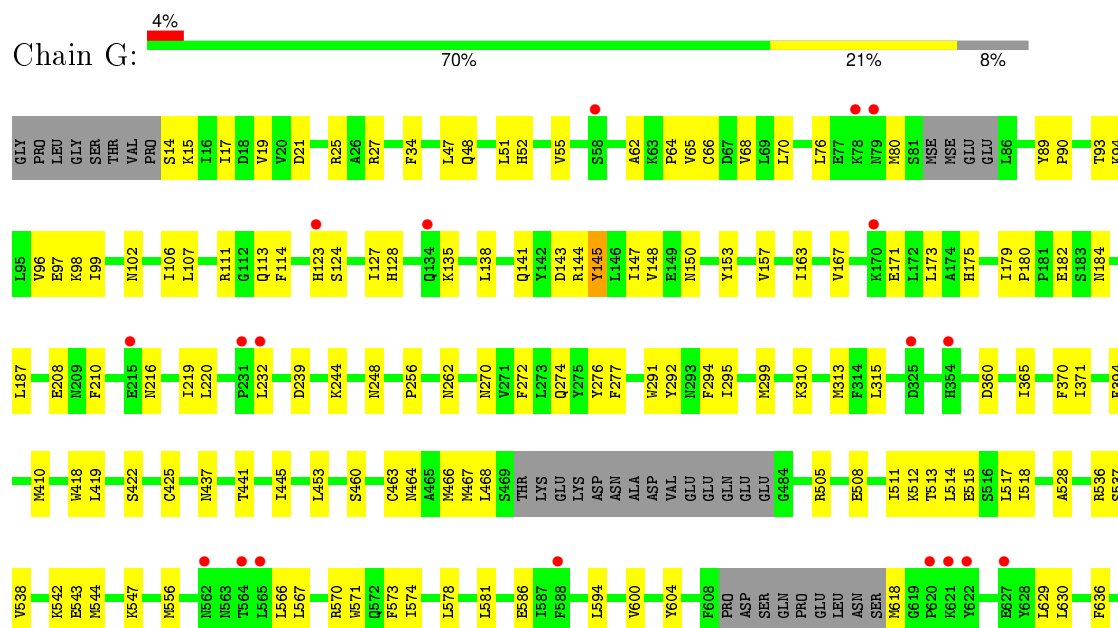
• Molecule 1: Cargo-transport protein YPP1

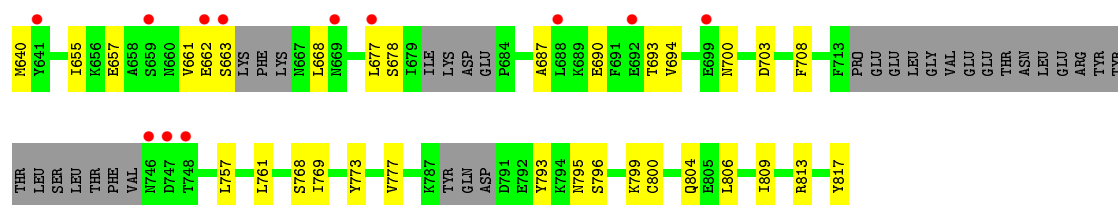


• Molecule 1: Cargo-transport protein YPP1

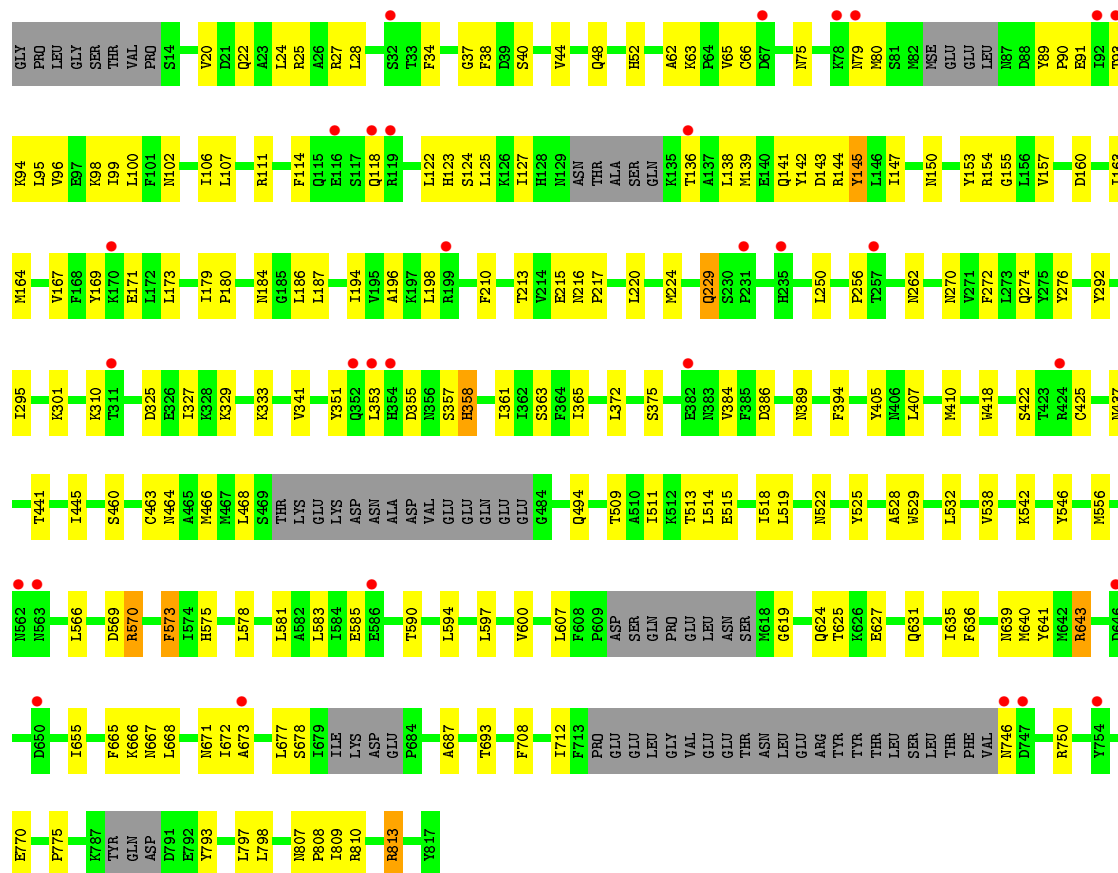


- Molecule 1: Cargo-transport protein YPP1





• Molecule 1: Cargo-transport protein YPP1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.55Å 136.65Å 154.12Å 76.69° 85.67° 72.74°	Depositor
Resolution (Å)	25.00 – 3.25 25.12 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-3.25) 86.2 (25.12-3.25)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.23Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.240 , 0.277 0.239 , 0.277	Depositor DCC
$R_{free}$ test set	1850 reflections (1.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 20.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 114807 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	48674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.18 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.8092e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

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	0.28	0/6252	0.49	1/8423 (0.0%)
1	B	0.28	0/6223	0.49	0/8382
1	C	0.28	0/6193	0.49	1/8340 (0.0%)
1	D	0.29	0/6359	0.51	1/8569 (0.0%)
1	E	0.27	0/6114	0.48	0/8234
1	F	0.27	0/6105	0.49	0/8223
1	G	0.29	0/6169	0.49	0/8312
1	H	0.29	0/6171	0.52	1/8310 (0.0%)
All	All	0.28	0/49586	0.49	4/66793 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	663	SER	N-CA-C	-5.50	96.14	111.00
1	C	756	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	565	LEU	CA-CB-CG	5.31	127.51	115.30
1	H	353	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	LYS	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	6138	0	6060	112	0
1	B	6109	0	6038	101	1
1	C	6080	0	6008	99	0
1	D	6241	0	6171	115	0
1	E	6000	0	5943	104	1
1	F	5993	0	5927	114	0
1	G	6056	0	5984	115	0
1	H	6057	0	5993	124	0
All	All	48674	0	48124	873	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (873) 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:581:LEU:HD11	1:A:600:VAL:HG21	1.63	0.79
1:C:514:LEU:HD12	1:C:518:ILE:HD11	1.64	0.79
1:D:189:GLU:OE2	1:D:429:GLY:N	2.15	0.78
1:D:402:TYR:HB3	1:D:409:LEU:HD11	1.66	0.77
1:C:581:LEU:HD11	1:C:600:VAL:HG21	1.66	0.75
1:G:27:ARG:HH12	1:G:52:HIS:HD2	1.33	0.75
1:E:50:ARG:NH2	1:E:72:GLU:OE2	2.20	0.75
1:H:770:GLU:OE1	1:H:813:ARG:NH2	2.17	0.75
1:A:570:ARG:HG3	1:A:607:LEU:HD22	1.69	0.74
1:D:581:LEU:HD11	1:D:600:VAL:HG21	1.69	0.74
1:D:642:MSE:HE1	1:D:676:TYR:HB3	1.71	0.73
1:H:124:SER:OG	1:H:150:ASN:ND2	2.22	0.73
1:B:669:ASN:HA	1:B:672:ILE:HG12	1.69	0.73
1:E:71:LYS:O	1:E:75:ASN:ND2	2.20	0.72
1:B:507:ILE:HD13	1:B:538:VAL:HG21	1.71	0.72
1:A:652:LYS:HG2	1:A:677:LEU:HD21	1.71	0.72
1:H:25:ARG:HB2	1:H:138:LEU:HD21	1.71	0.71
1:E:672:ILE:HD11	1:E:694:VAL:HG11	1.73	0.71
1:H:27:ARG:HH12	1:H:52:HIS:HD2	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:GLU:OE2	1:D:536:ARG:NH2	2.23	0.71
1:G:111:ARG:NH1	1:G:113:GLN:OE1	2.24	0.70
1:F:570:ARG:HB3	1:F:607:LEU:HD22	1.73	0.70
1:E:526:TYR:HB3	1:E:556:MSE:HE2	1.72	0.70
1:E:574:ILE:HD12	1:E:629:LEU:HD13	1.74	0.70
1:D:570:ARG:NH1	1:D:607:LEU:O	2.25	0.70
1:F:770:GLU:OE1	1:F:813:ARG:NH2	2.23	0.70
1:E:27:ARG:HH12	1:E:52:HIS:HD2	1.40	0.70
1:B:514:LEU:HA	1:B:518:ILE:HD13	1.74	0.69
1:A:27:ARG:HD3	1:A:48:GLN:HE21	1.56	0.69
1:B:27:ARG:HH12	1:B:52:HIS:HD2	1.38	0.69
1:E:95:LEU:HA	1:E:98:LYS:HE2	1.74	0.69
1:D:98:LYS:HE2	1:D:128:HIS:HA	1.75	0.69
1:E:581:LEU:HD11	1:E:600:VAL:HG21	1.74	0.69
1:E:700:ASN:HB3	1:E:768:SER:HB2	1.75	0.68
1:D:690:GLU:O	1:D:693:THR:OG1	2.09	0.68
1:B:509:THR:HA	1:B:512:LYS:HE2	1.74	0.68
1:C:393:THR:OG1	1:G:208:GLU:OE2	2.11	0.68
1:D:574:ILE:HG21	1:D:629:LEU:HD21	1.76	0.68
1:E:286:LYS:HE3	1:E:322:ASN:HB3	1.74	0.68
1:G:542:LYS:HZ2	1:G:586:GLU:HG2	1.57	0.68
1:C:412:GLN:O	1:C:456:ASN:ND2	2.27	0.68
1:E:25:ARG:HB2	1:E:138:LEU:HD21	1.76	0.68
1:D:456:ASN:OD1	1:D:504:GLN:NE2	2.27	0.67
1:F:124:SER:OG	1:F:150:ASN:ND2	2.28	0.67
1:D:696:TYR:OH	1:H:667:ASN:O	2.13	0.67
1:F:560:LEU:HD23	1:F:561:GLN:HG3	1.76	0.67
1:G:542:LYS:NZ	1:G:586:GLU:HG2	2.10	0.67
1:A:594:LEU:HD11	1:A:644:THR:HG21	1.77	0.66
1:A:505:ARG:HD3	1:A:773:TYR:HB3	1.78	0.66
1:D:712:ILE:O	1:D:750:ARG:NH1	2.27	0.66
1:G:453:LEU:HD13	1:G:769:ILE:HD13	1.77	0.66
1:A:77:GLU:HB2	1:A:100:LEU:HD21	1.78	0.66
1:H:460:SER:O	1:H:464:ASN:ND2	2.28	0.66
1:C:124:SER:OG	1:C:150:ASN:ND2	2.29	0.66
1:B:518:ILE:O	1:B:522:ASN:ND2	2.29	0.66
1:B:647:ASN:HB2	1:B:650:ASP:HB2	1.76	0.66
1:B:98:LYS:HE2	1:B:128:HIS:HA	1.77	0.65
1:F:205:ASP:O	1:F:209:ASN:ND2	2.28	0.65
1:G:566:LEU:H	1:G:566:LEU:HD23	1.61	0.65
1:G:574:ILE:HG21	1:G:629:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:566:LEU:O	1:G:570:ARG:NE	2.30	0.65
1:A:604:TYR:CZ	1:A:630:LEU:HG	2.32	0.65
1:H:372:LEU:HB3	1:H:445:ILE:HD11	1.78	0.65
1:G:514:LEU:HD11	1:G:528:ALA:HB1	1.79	0.64
1:B:570:ARG:HB3	1:B:607:LEU:HD22	1.80	0.64
1:E:144:ARG:HA	1:E:147:ILE:HD12	1.78	0.64
1:H:154:ARG:NH2	1:H:171:GLU:OE1	2.31	0.64
1:C:244:LYS:O	1:C:248:ASN:ND2	2.25	0.64
1:H:386:ASP:HB3	1:H:389:ASN:HB2	1.79	0.64
1:D:410:MSE:HG3	1:D:463:CYS:HB3	1.80	0.64
1:E:27:ARG:HD3	1:E:48:GLN:HE21	1.63	0.64
1:A:594:LEU:HD23	1:A:640:MSE:HE2	1.81	0.63
1:B:505:ARG:HH12	1:B:808:PRO:HD3	1.62	0.63
1:H:196:ALA:HA	1:H:229:GLN:HE22	1.62	0.63
1:H:655:ILE:HG23	1:H:673:ALA:HB1	1.79	0.63
1:H:635:ILE:O	1:H:639:ASN:ND2	2.31	0.63
1:C:515:GLU:OE2	1:C:536:ARG:NH2	2.26	0.63
1:G:581:LEU:HD11	1:G:600:VAL:HG21	1.81	0.63
1:D:652:LYS:HG2	1:D:677:LEU:HD21	1.79	0.63
1:F:44:VAL:HG21	1:F:96:VAL:HG13	1.80	0.63
1:H:27:ARG:HE	1:H:34:PHE:HZ	1.46	0.63
1:F:639:ASN:O	1:F:643:ARG:HG3	1.99	0.63
1:B:244:LYS:O	1:B:248:ASN:ND2	2.23	0.62
1:C:46:ASN:OD1	1:C:50:ARG:NH1	2.32	0.62
1:A:141:GLN:HG3	1:A:184:ASN:ND2	2.15	0.62
1:F:141:GLN:HG3	1:F:184:ASN:ND2	2.14	0.62
1:E:491:ARG:NH1	1:E:522:ASN:OD1	2.28	0.62
1:D:141:GLN:HG3	1:D:184:ASN:ND2	2.15	0.62
1:E:655:ILE:HG23	1:E:673:ALA:HB1	1.80	0.62
1:A:536:ARG:O	1:A:539:GLN:HG2	1.99	0.62
1:E:712:ILE:HD13	1:E:757:LEU:HD22	1.82	0.62
1:C:460:SER:O	1:C:464:ASN:ND2	2.34	0.61
1:G:594:LEU:HD23	1:G:640:MSE:HE2	1.82	0.61
1:H:62:ALA:HB3	1:H:65:VAL:HG22	1.82	0.61
1:C:542:LYS:HD3	1:C:809:ILE:HD11	1.83	0.61
1:F:414:GLU:HB3	1:F:421:ASN:HD22	1.65	0.61
1:G:538:VAL:HG11	1:G:806:LEU:HA	1.83	0.61
1:D:256:PRO:HG3	1:D:262:ASN:HA	1.80	0.61
1:D:696:TYR:OH	1:H:671:ASN:OD1	2.09	0.61
1:D:681:LYS:HG3	1:H:327:ILE:HG13	1.81	0.61
1:C:744:PHE:HZ	1:C:750:ARG:HG3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:460:SER:O	1:G:464:ASN:ND2	2.34	0.61
1:C:40:SER:OG	1:C:86:LEU:HD21	2.01	0.61
1:B:761:LEU:HD22	1:B:777:VAL:HG13	1.82	0.61
1:G:27:ARG:HE	1:G:34:PHE:HZ	1.49	0.60
1:F:597:LEU:HD21	1:F:640:MSE:HE1	1.82	0.60
1:A:98:LYS:HE2	1:A:128:HIS:HA	1.83	0.60
1:D:460:SER:O	1:D:464:ASN:ND2	2.33	0.60
1:H:95:LEU:HD22	1:H:139:MSE:HE1	1.84	0.60
1:H:793:TYR:CZ	1:H:797:LEU:HD11	2.36	0.60
1:E:604:TYR:CZ	1:E:630:LEU:HG	2.36	0.60
1:D:756:ARG:HH22	1:H:693:THR:HG22	1.66	0.60
1:G:657:GLU:O	1:G:661:VAL:HG23	2.02	0.60
1:B:450:LEU:HD13	1:B:769:ILE:HA	1.82	0.60
1:D:141:GLN:HG3	1:D:184:ASN:HD22	1.67	0.60
1:B:86:LEU:O	1:B:93:THR:OG1	2.20	0.60
1:E:534:LEU:HD23	1:E:812:LEU:HD23	1.83	0.60
1:H:125:LEU:HD11	1:H:154:ARG:NE	2.16	0.60
1:G:700:ASN:HB3	1:G:768:SER:HB2	1.84	0.60
1:D:514:LEU:HD23	1:D:518:ILE:HD12	1.82	0.60
1:B:21:ASP:HB3	1:B:138:LEU:HD12	1.84	0.59
1:G:708:PHE:HD2	1:G:757:LEU:HD13	1.66	0.59
1:A:192:SER:O	1:A:229:GLN:NE2	2.32	0.59
1:C:86:LEU:HB3	1:C:93:THR:HG22	1.84	0.59
1:D:407:LEU:HD23	1:D:427:TYR:CZ	2.38	0.59
1:E:655:ILE:HG21	1:E:677:LEU:HB2	1.85	0.59
1:B:283:LYS:HD3	1:B:285:ILE:HD11	1.84	0.59
1:E:180:PRO:HB3	1:E:187:LEU:HD23	1.85	0.59
1:H:515:GLU:HG3	1:H:532:LEU:HD11	1.83	0.59
1:F:145:TYR:HA	1:F:187:LEU:HD13	1.85	0.59
1:D:594:LEU:HD23	1:D:640:MSE:HE3	1.84	0.59
1:F:559:SER:O	1:F:564:THR:N	2.36	0.59
1:H:809:ILE:HG22	1:H:810:ARG:HG3	1.85	0.59
1:C:536:ARG:O	1:C:539:GLN:HG2	2.03	0.58
1:F:514:LEU:HD23	1:F:518:ILE:HD12	1.85	0.58
1:H:655:ILE:HG21	1:H:677:LEU:HB2	1.84	0.58
1:D:278:LYS:HE3	1:D:282:ILE:HD11	1.85	0.58
1:F:708:PHE:HD1	1:F:757:LEU:HD13	1.68	0.58
1:D:72:GLU:O	1:D:76:LEU:HG	2.03	0.58
1:B:67:ASP:OD1	1:B:111:ARG:NE	2.35	0.58
1:F:635:ILE:HD12	1:F:673:ALA:HB2	1.86	0.58
1:A:518:ILE:O	1:A:522:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:PHE:HB3	1:G:157:VAL:HG13	1.84	0.58
1:B:581:LEU:HD11	1:B:600:VAL:HG21	1.85	0.58
1:B:618:MSE:HE1	1:B:817:TYR:HD1	1.69	0.58
1:F:505:ARG:NH1	1:F:773:TYR:O	2.37	0.58
1:E:92:ILE:O	1:E:95:LEU:HB3	2.04	0.57
1:B:456:ASN:OD1	1:B:504:GLN:NE2	2.36	0.57
1:G:21:ASP:HB3	1:G:138:LEU:HD12	1.87	0.57
1:A:509:THR:O	1:A:513:THR:HG23	2.03	0.57
1:D:386:ASP:HB3	1:D:389:ASN:HB2	1.86	0.57
1:G:70:LEU:HD22	1:G:111:ARG:HD2	1.86	0.57
1:D:25:ARG:HB2	1:D:138:LEU:HD21	1.87	0.57
1:C:217:PRO:HA	1:C:220:LEU:HD12	1.87	0.57
1:A:27:ARG:HE	1:A:34:PHE:HZ	1.50	0.57
1:G:244:LYS:O	1:G:248:ASN:ND2	2.28	0.57
1:H:514:LEU:O	1:H:519:LEU:HD12	2.05	0.56
1:G:571:TRP:CD1	1:G:629:LEU:HD12	2.40	0.56
1:H:410:MSE:HG2	1:H:463:CYS:HB3	1.87	0.56
1:D:13:PRO:HB3	1:D:17:ILE:HD12	1.86	0.56
1:B:652:LYS:HG2	1:B:677:LEU:HD21	1.88	0.56
1:G:70:LEU:HA	1:G:107:LEU:HD13	1.86	0.56
1:G:141:GLN:HG3	1:G:184:ASN:ND2	2.21	0.56
1:D:27:ARG:HH12	1:D:52:HIS:HD2	1.54	0.56
1:H:118:GLN:HG3	1:H:157:VAL:HG11	1.88	0.56
1:G:690:GLU:O	1:G:694:VAL:HG23	2.06	0.56
1:G:514:LEU:HA	1:G:518:ILE:HD13	1.88	0.56
1:B:505:ARG:HE	1:B:773:TYR:HB3	1.70	0.56
1:A:419:LEU:HD23	1:A:513:THR:HG22	1.87	0.56
1:G:124:SER:OG	1:G:150:ASN:ND2	2.39	0.56
1:A:350:TYR:CE1	1:A:359:ARG:HG2	2.41	0.56
1:C:678:SER:HB2	1:C:687:ALA:HB2	1.86	0.56
1:C:507:ILE:HD13	1:C:538:VAL:HG11	1.86	0.56
1:D:529:TRP:HB3	1:D:552:VAL:HG21	1.88	0.56
1:D:536:ARG:O	1:D:539:GLN:HG2	2.05	0.56
1:A:519:LEU:HD21	1:A:528:ALA:HB3	1.85	0.56
1:E:514:LEU:HD23	1:E:518:ILE:HD12	1.86	0.56
1:B:141:GLN:HG3	1:B:184:ASN:ND2	2.21	0.56
1:A:256:PRO:HG3	1:A:262:ASN:HA	1.87	0.56
1:D:443:TYR:HE2	1:D:496:LYS:HD3	1.70	0.56
1:H:775:PRO:HG3	1:H:807:ASN:ND2	2.21	0.56
1:C:546:TYR:HA	1:C:583:LEU:HD13	1.87	0.56
1:E:386:ASP:HB3	1:E:389:ASN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:MSE:HE2	1:G:370:PHE:HD2	1.70	0.56
1:D:102:ASN:O	1:D:106:ILE:HG12	2.05	0.56
1:G:574:ILE:HD13	1:G:629:LEU:HD11	1.88	0.55
1:H:511:ILE:O	1:H:515:GLU:HB2	2.06	0.55
1:C:217:PRO:HB2	1:C:268:HIS:CE1	2.41	0.55
1:A:239:ASP:OD1	1:A:291:TRP:NE1	2.30	0.55
1:A:386:ASP:HB3	1:A:389:ASN:HB2	1.88	0.55
1:E:348:ASP:HA	1:E:351:TYR:CD2	2.41	0.55
1:H:566:LEU:HD13	1:H:570:ARG:HG2	1.86	0.55
1:C:644:THR:HG22	1:C:646:ASP:H	1.71	0.55
1:G:655:ILE:HD12	1:G:677:LEU:HD22	1.88	0.55
1:G:14:SER:N	1:G:17:ILE:HD13	2.22	0.55
1:F:691:PHE:O	1:F:695:LEU:HD13	2.06	0.55
1:H:570:ARG:HB3	1:H:607:LEU:HD22	1.87	0.55
1:F:25:ARG:HH12	1:F:357:SER:HB2	1.70	0.55
1:A:570:ARG:NH2	1:D:562:ASN:O	2.40	0.55
1:G:25:ARG:HE	1:G:138:LEU:HD11	1.72	0.55
1:C:529:TRP:HB3	1:C:552:VAL:HG21	1.89	0.55
1:D:54:HIS:HB3	1:D:61:PRO:HB3	1.87	0.55
1:C:27:ARG:HH12	1:C:52:HIS:HD2	1.53	0.55
1:B:106:ILE:HG23	1:B:153:TYR:CE2	2.42	0.55
1:H:333:LYS:NZ	1:H:375:SER:HB3	2.21	0.55
1:B:511:ILE:O	1:B:515:GLU:HB2	2.07	0.55
1:G:537:SER:O	1:G:542:LYS:HE2	2.07	0.54
1:G:567:LEU:O	1:G:570:ARG:HG3	2.06	0.54
1:F:411:SER:O	1:F:415:SER:OG	2.24	0.54
1:D:748:THR:O	1:D:751:SER:OG	2.20	0.54
1:H:141:GLN:HG3	1:H:184:ASN:ND2	2.23	0.54
1:B:372:LEU:HB3	1:B:445:ILE:HD11	1.89	0.54
1:F:695:LEU:HD23	1:F:760:LEU:HD13	1.89	0.54
1:C:224:MSE:HE2	1:C:276:TYR:HA	1.88	0.54
1:H:358:HIS:CD2	1:H:361:ILE:HG12	2.42	0.54
1:F:640:MSE:HA	1:F:643:ARG:HD2	1.90	0.54
1:H:145:TYR:HA	1:H:187:LEU:HD13	1.90	0.54
1:A:564:THR:HG22	1:D:561:GLN:HA	1.90	0.54
1:D:156:LEU:HD23	1:D:164:MSE:HE1	1.89	0.54
1:H:144:ARG:HA	1:H:147:ILE:HD12	1.89	0.54
1:H:160:ASP:O	1:H:164:MSE:HG3	2.08	0.54
1:H:75:ASN:O	1:H:79:ASN:ND2	2.31	0.54
1:C:441:THR:O	1:C:445:ILE:HG12	2.08	0.54
1:F:270:ASN:HD22	1:F:308:VAL:HG22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:LYS:HD3	1:E:285:ILE:HD11	1.90	0.54
1:B:92:ILE:O	1:B:96:VAL:HG23	2.08	0.54
1:A:25:ARG:HB2	1:A:138:LEU:HD21	1.89	0.54
1:B:156:LEU:HD23	1:B:164:MSE:HE1	1.90	0.54
1:A:213:THR:HG22	1:A:215:GLU:H	1.73	0.54
1:A:511:ILE:O	1:A:515:GLU:HB2	2.08	0.53
1:A:333:LYS:NZ	1:A:374:ASN:O	2.41	0.53
1:G:256:PRO:HG3	1:G:262:ASN:HA	1.90	0.53
1:C:90:PRO:O	1:C:93:THR:OG1	2.22	0.53
1:F:508:GLU:O	1:F:512:LYS:HG3	2.08	0.53
1:B:76:LEU:O	1:B:80:MSE:HG3	2.08	0.53
1:E:217:PRO:HB2	1:E:268:HIS:CE1	2.42	0.53
1:D:689:LYS:O	1:D:693:THR:HG23	2.08	0.53
1:F:27:ARG:HH12	1:F:52:HIS:HD2	1.57	0.53
1:C:283:LYS:HG2	1:C:285:ILE:HG13	1.90	0.53
1:H:538:VAL:HG13	1:H:807:ASN:O	2.09	0.53
1:H:102:ASN:O	1:H:106:ILE:HG12	2.09	0.53
1:B:125:LEU:O	1:B:129:ASN:ND2	2.40	0.53
1:A:450:LEU:HD13	1:A:769:ILE:HA	1.90	0.53
1:B:809:ILE:HG23	1:B:810:ARG:H	1.72	0.53
1:G:505:ARG:NH1	1:G:773:TYR:O	2.41	0.53
1:G:437:ASN:O	1:G:441:THR:HG23	2.09	0.53
1:C:505:ARG:NH1	1:C:773:TYR:O	2.42	0.53
1:A:71:LYS:O	1:A:75:ASN:ND2	2.36	0.53
1:G:419:LEU:HD11	1:G:513:THR:HA	1.92	0.52
1:A:141:GLN:HG3	1:A:184:ASN:HD22	1.74	0.52
1:G:310:LYS:O	1:G:313:MSE:HG2	2.09	0.52
1:E:793:TYR:O	1:E:796:SER:OG	2.19	0.52
1:H:566:LEU:HB2	1:H:569:ASP:HB2	1.91	0.52
1:G:578:LEU:HD22	1:G:636:PHE:HD2	1.75	0.52
1:A:628:TYR:CE2	1:A:632:MSE:HE2	2.45	0.52
1:C:437:ASN:O	1:C:441:THR:HG23	2.09	0.52
1:C:708:PHE:HD2	1:C:757:LEU:HD23	1.74	0.52
1:H:98:LYS:NZ	1:H:143:ASP:OD1	2.42	0.52
1:A:16:ILE:O	1:A:19:VAL:HG12	2.08	0.52
1:C:161:ILE:O	1:C:165:GLN:HG3	2.08	0.52
1:H:107:LEU:O	1:H:111:ARG:HG3	2.09	0.52
1:G:145:TYR:HA	1:G:187:LEU:HD13	1.92	0.52
1:A:86:LEU:HB3	1:A:93:THR:HG22	1.90	0.52
1:G:274:GLN:OE1	1:G:310:LYS:NZ	2.32	0.52
1:C:317:GLN:HE22	1:C:333:LYS:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:579:THR:HA	1:E:810:ARG:HD2	1.91	0.52
1:B:358:HIS:HB2	1:B:361:ILE:HG13	1.92	0.51
1:D:64:PRO:O	1:D:68:VAL:HG23	2.10	0.51
1:H:494:GLN:HB3	1:H:518:ILE:HD11	1.92	0.51
1:E:515:GLU:OE1	1:E:536:ARG:NH2	2.39	0.51
1:F:641:TYR:HB2	1:F:651:ALA:HB2	1.93	0.51
1:E:220:LEU:HB3	1:E:272:PHE:CE1	2.46	0.51
1:D:123:HIS:CE1	1:D:127:ILE:HD11	2.46	0.51
1:B:256:PRO:HG3	1:B:262:ASN:HA	1.92	0.51
1:F:588:PHE:HB3	1:F:592:GLU:HG3	1.93	0.51
1:G:441:THR:O	1:G:445:ILE:HG12	2.11	0.51
1:D:92:ILE:O	1:D:96:VAL:HG23	2.11	0.51
1:F:604:TYR:CZ	1:F:630:LEU:HG	2.46	0.51
1:A:441:THR:O	1:A:445:ILE:HG12	2.10	0.51
1:A:123:HIS:CE1	1:A:127:ILE:HD11	2.46	0.51
1:A:578:LEU:HA	1:A:581:LEU:HD12	1.93	0.51
1:D:507:ILE:HD13	1:D:538:VAL:HG11	1.93	0.51
1:E:224:MSE:HE2	1:E:276:TYR:HA	1.93	0.51
1:F:584:ILE:HA	1:F:587:ILE:HG22	1.93	0.50
1:A:270:ASN:ND2	1:A:308:VAL:HG22	2.25	0.50
1:F:192:SER:OG	1:F:229:GLN:OE1	2.26	0.50
1:F:452:PHE:HD1	1:F:457:ASN:HD22	1.59	0.50
1:H:28:LEU:HD23	1:H:186:LEU:HD12	1.93	0.50
1:B:337:ILE:HD13	1:B:371:ILE:HD11	1.93	0.50
1:F:47:LEU:HD22	1:F:76:LEU:HD12	1.94	0.50
1:C:270:ASN:O	1:C:274:GLN:HG3	2.11	0.50
1:H:250:LEU:HD22	1:H:301:LYS:HD2	1.93	0.50
1:G:511:ILE:HD12	1:G:536:ARG:NH2	2.25	0.50
1:F:70:LEU:HA	1:F:107:LEU:HD13	1.94	0.50
1:B:494:GLN:HB3	1:B:518:ILE:HD11	1.93	0.50
1:H:155:GLY:O	1:H:164:MSE:HG2	2.12	0.50
1:B:537:SER:O	1:B:542:LYS:HE2	2.11	0.50
1:C:351:TYR:HE2	1:C:358:HIS:CD2	2.29	0.50
1:F:511:ILE:HG21	1:F:536:ARG:HH21	1.75	0.50
1:G:93:THR:O	1:G:97:GLU:HG3	2.12	0.50
1:H:270:ASN:O	1:H:274:GLN:HG3	2.12	0.50
1:B:487:GLU:OE1	1:B:491:ARG:NH2	2.45	0.50
1:B:27:ARG:NH1	1:B:52:HIS:HD2	2.07	0.50
1:G:418:TRP:O	1:G:422:SER:HB3	2.11	0.50
1:C:744:PHE:CZ	1:C:750:ARG:HG3	2.44	0.50
1:D:123:HIS:O	1:D:127:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:ILE:HG21	1:F:536:ARG:NH2	2.26	0.50
1:H:123:HIS:CE1	1:H:127:ILE:HD11	2.47	0.50
1:E:546:TYR:HA	1:E:583:LEU:HD13	1.94	0.50
1:A:585:GLU:OE2	1:A:643:ARG:HD2	2.11	0.50
1:B:270:ASN:O	1:B:274:GLN:HG3	2.12	0.50
1:G:47:LEU:HD22	1:G:76:LEU:HD12	1.93	0.50
1:D:585:GLU:OE2	1:D:640:MSE:HG3	2.12	0.50
1:F:539:GLN:HE22	1:F:544:MSE:HE1	1.77	0.50
1:F:464:ASN:HA	1:F:467:MSE:HE2	1.93	0.50
1:E:567:LEU:O	1:E:570:ARG:HG3	2.12	0.50
1:E:571:TRP:CH2	1:E:618:MSE:HB2	2.47	0.50
1:F:669:ASN:HA	1:F:672:ILE:HG12	1.94	0.50
1:E:545:SER:O	1:E:549:VAL:HG13	2.12	0.49
1:F:575:HIS:O	1:F:810:ARG:NH1	2.45	0.49
1:C:27:ARG:NH1	1:C:52:HIS:HD2	2.09	0.49
1:F:270:ASN:ND2	1:F:308:VAL:HG22	2.27	0.49
1:H:63:LYS:HA	1:H:66:CYS:HB3	1.94	0.49
1:E:418:TRP:O	1:E:422:SER:HB3	2.11	0.49
1:D:545:SER:O	1:D:549:VAL:HG13	2.12	0.49
1:G:102:ASN:O	1:G:106:ILE:HG12	2.12	0.49
1:G:313:MSE:HE1	1:G:371:ILE:HB	1.94	0.49
1:A:437:ASN:O	1:A:441:THR:HG23	2.12	0.49
1:D:13:PRO:HB3	1:D:17:ILE:CD1	2.42	0.49
1:A:618:MSE:HE1	1:A:817:TYR:HD1	1.78	0.49
1:H:310:LYS:NZ	1:H:363:SER:OG	2.38	0.49
1:C:145:TYR:HA	1:C:187:LEU:HD13	1.95	0.49
1:G:463:CYS:HA	1:G:466:MSE:HE3	1.94	0.49
1:H:538:VAL:HG22	1:H:808:PRO:HA	1.94	0.49
1:G:295:ILE:HB	1:G:315:LEU:HD23	1.94	0.49
1:A:684:PRO:HG2	1:A:686:VAL:HG12	1.95	0.49
1:C:578:LEU:HA	1:C:581:LEU:HD12	1.95	0.49
1:F:350:TYR:CZ	1:F:359:ARG:HB3	2.47	0.49
1:C:792:GLU:HA	1:C:795:ASN:HD21	1.77	0.49
1:A:571:TRP:HH2	1:A:625:THR:O	1.95	0.49
1:G:123:HIS:CE1	1:G:127:ILE:HD11	2.48	0.49
1:H:581:LEU:HD11	1:H:600:VAL:HG11	1.95	0.49
1:B:585:GLU:OE2	1:B:643:ARG:HD2	2.12	0.49
1:B:515:GLU:HG3	1:B:532:LEU:HD11	1.94	0.48
1:H:24:LEU:HD22	1:H:142:TYR:CD2	2.47	0.48
1:A:41:LEU:HA	1:A:44:VAL:HG12	1.95	0.48
1:D:203:ILE:HD11	1:D:219:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:355:ASP:C	1:H:357:SER:H	2.16	0.48
1:F:123:HIS:O	1:F:127:ILE:HG13	2.13	0.48
1:A:514:LEU:HD12	1:A:518:ILE:HD12	1.94	0.48
1:D:27:ARG:HE	1:D:34:PHE:HZ	1.61	0.48
1:G:578:LEU:HD22	1:G:636:PHE:CD2	2.47	0.48
1:G:292:TYR:O	1:G:295:ILE:HG22	2.13	0.48
1:E:365:ILE:HG23	1:E:394:PHE:HE1	1.78	0.48
1:D:296:ILE:HA	1:D:299:MSE:HE3	1.93	0.48
1:B:581:LEU:HB2	1:B:636:PHE:HE2	1.78	0.48
1:H:463:CYS:HA	1:H:466:MSE:HE3	1.94	0.48
1:D:97:GLU:HB3	1:D:127:ILE:HD13	1.96	0.48
1:A:270:ASN:HD22	1:A:308:VAL:HG22	1.78	0.48
1:D:295:ILE:HG13	1:D:299:MSE:HE2	1.96	0.48
1:E:639:ASN:HB3	1:E:643:ARG:HH12	1.78	0.48
1:H:37:GLY:C	1:H:38:PHE:HD1	2.17	0.48
1:A:102:ASN:O	1:A:106:ILE:HG12	2.13	0.48
1:D:270:ASN:O	1:D:274:GLN:HG3	2.13	0.48
1:H:173:LEU:HD23	1:H:173:LEU:HA	1.63	0.48
1:G:98:LYS:HE2	1:G:128:HIS:HA	1.96	0.48
1:G:542:LYS:NZ	1:G:809:ILE:HD11	2.28	0.48
1:F:631:GLN:O	1:F:635:ILE:HG12	2.14	0.48
1:B:240:ASP:O	1:B:244:LYS:HG3	2.13	0.48
1:F:536:ARG:HD3	1:F:544:MSE:HB3	1.95	0.48
1:B:431:ILE:O	1:B:435:LEU:HD23	2.14	0.48
1:D:220:LEU:HB3	1:D:272:PHE:CE1	2.48	0.48
1:E:556:MSE:HE3	1:E:576:LEU:HD22	1.95	0.48
1:A:546:TYR:HA	1:A:583:LEU:HD13	1.95	0.48
1:D:575:HIS:O	1:D:810:ARG:NH1	2.46	0.48
1:D:809:ILE:HG22	1:D:810:ARG:HG3	1.95	0.48
1:D:144:ARG:HD2	1:D:187:LEU:HD11	1.95	0.48
1:E:628:TYR:HE1	1:E:669:ASN:HD21	1.61	0.48
1:G:106:ILE:HG23	1:G:153:TYR:CE2	2.48	0.48
1:C:256:PRO:HG3	1:C:262:ASN:HA	1.94	0.48
1:G:123:HIS:O	1:G:127:ILE:HG13	2.13	0.48
1:G:800:CYS:O	1:G:804:GLN:HB2	2.14	0.48
1:B:94:LYS:O	1:B:98:LYS:HG3	2.14	0.48
1:C:27:ARG:HE	1:C:34:PHE:HZ	1.62	0.48
1:D:317:GLN:HG3	1:D:370:PHE:CE2	2.48	0.48
1:A:516:SER:O	1:A:520:SER:HB2	2.13	0.48
1:D:405:TYR:HB2	1:D:407:LEU:HD11	1.95	0.48
1:H:22:GLN:OE1	1:H:25:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:GLY:HA3	1:E:624:GLN:NE2	2.29	0.48
1:F:585:GLU:OE2	1:F:643:ARG:HD3	2.14	0.47
1:C:795:ASN:O	1:C:799:LYS:HD2	2.14	0.47
1:H:597:LEU:O	1:H:600:VAL:HG22	2.13	0.47
1:A:537:SER:O	1:A:542:LYS:NZ	2.44	0.47
1:C:15:LYS:O	1:C:19:VAL:HG23	2.14	0.47
1:H:425:CYS:HB2	1:H:468:LEU:HD23	1.96	0.47
1:C:141:GLN:HG3	1:C:184:ASN:ND2	2.29	0.47
1:H:94:LYS:O	1:H:98:LYS:HG3	2.15	0.47
1:E:292:TYR:O	1:E:295:ILE:HG22	2.14	0.47
1:E:54:HIS:HB3	1:E:61:PRO:HB3	1.97	0.47
1:G:62:ALA:O	1:G:66:CYS:N	2.36	0.47
1:G:64:PRO:O	1:G:68:VAL:HG23	2.13	0.47
1:H:635:ILE:HG13	1:H:672:ILE:HD11	1.97	0.47
1:G:661:VAL:O	1:G:663:SER:N	2.47	0.47
1:A:36:SER:HB3	1:A:41:LEU:HD23	1.94	0.47
1:E:41:LEU:HA	1:E:44:VAL:HG12	1.95	0.47
1:E:15:LYS:O	1:E:19:VAL:HG23	2.15	0.47
1:C:464:ASN:HA	1:C:467:MSE:HE2	1.97	0.47
1:H:256:PRO:HG3	1:H:262:ASN:HA	1.96	0.47
1:A:514:LEU:HD11	1:A:528:ALA:HB1	1.97	0.47
1:F:151:LEU:HD13	1:F:171:GLU:HB2	1.97	0.47
1:H:341:VAL:HG21	1:H:384:VAL:HG12	1.96	0.47
1:H:437:ASN:O	1:H:441:THR:HG23	2.15	0.47
1:G:761:LEU:HD22	1:G:777:VAL:HG13	1.96	0.47
1:D:365:ILE:HG23	1:D:394:PHE:HE1	1.80	0.47
1:E:700:ASN:CB	1:E:768:SER:HB2	2.45	0.47
1:A:40:SER:OG	1:A:86:LEU:HD21	2.15	0.47
1:H:256:PRO:HD3	1:H:301:LYS:O	2.15	0.47
1:H:213:THR:HG22	1:H:215:GLU:H	1.79	0.47
1:F:574:ILE:HG13	1:F:629:LEU:HD21	1.96	0.47
1:A:762:GLU:O	1:A:765:ILE:HG12	2.14	0.47
1:F:92:ILE:O	1:F:96:VAL:HG23	2.15	0.47
1:D:27:ARG:NH1	1:D:52:HIS:HD2	2.11	0.47
1:G:270:ASN:O	1:G:274:GLN:HG3	2.14	0.47
1:D:546:TYR:HA	1:D:583:LEU:HD13	1.96	0.47
1:H:44:VAL:HG22	1:H:100:LEU:HD21	1.97	0.47
1:E:705:LEU:HD11	1:E:760:LEU:HB3	1.96	0.47
1:F:338:LEU:O	1:F:341:VAL:HG22	2.15	0.47
1:G:618:MSE:HE1	1:G:817:TYR:HD1	1.78	0.47
1:H:509:THR:O	1:H:513:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:LYS:HD3	1:F:238:ASN:HD21	1.79	0.47
1:H:627:GLU:O	1:H:631:GLN:HG3	2.15	0.47
1:B:266:LEU:O	1:B:270:ASN:ND2	2.35	0.47
1:G:678:SER:HB3	1:G:687:ALA:HB2	1.96	0.47
1:A:288:ASN:OD1	1:A:290:SER:OG	2.22	0.47
1:F:651:ALA:O	1:F:655:ILE:HG13	2.15	0.47
1:H:24:LEU:HD22	1:H:142:TYR:CE2	2.50	0.47
1:G:508:GLU:O	1:G:512:LYS:HG3	2.15	0.47
1:F:621:LYS:O	1:F:625:THR:HG23	2.14	0.47
1:B:418:TRP:O	1:B:422:SER:HB3	2.14	0.47
1:D:761:LEU:HD22	1:D:777:VAL:HG13	1.95	0.47
1:E:123:HIS:O	1:E:127:ILE:HG13	2.15	0.47
1:H:122:LEU:HD23	1:H:125:LEU:HD12	1.96	0.47
1:D:443:TYR:CE2	1:D:496:LYS:HD3	2.49	0.47
1:B:793:TYR:CZ	1:B:797:LEU:HD11	2.49	0.47
1:F:143:ASP:O	1:F:147:ILE:HG12	2.15	0.47
1:E:213:THR:HG22	1:E:215:GLU:H	1.80	0.47
1:C:144:ARG:HD3	1:C:176:VAL:HG12	1.96	0.47
1:E:507:ILE:HD13	1:E:538:VAL:HG21	1.96	0.47
1:C:604:TYR:CE2	1:C:630:LEU:HD13	2.50	0.47
1:G:80:MSE:HE2	1:G:96:VAL:HG21	1.97	0.46
1:H:365:ILE:HG23	1:H:394:PHE:HE1	1.80	0.46
1:F:668:LEU:HD21	1:F:694:VAL:HG13	1.96	0.46
1:A:560:LEU:HD13	1:A:566:LEU:HD12	1.96	0.46
1:A:575:HIS:O	1:A:810:ARG:NH1	2.48	0.46
1:C:180:PRO:HB3	1:C:187:LEU:HD23	1.98	0.46
1:D:468:LEU:O	1:D:469:SER:OG	2.24	0.46
1:E:369:SER:O	1:E:373:GLN:HB2	2.14	0.46
1:C:76:LEU:O	1:C:80:MSE:HG3	2.16	0.46
1:G:171:GLU:OE1	1:G:175:HIS:NE2	2.47	0.46
1:F:411:SER:HB2	1:F:414:GLU:HG3	1.97	0.46
1:G:700:ASN:CB	1:G:768:SER:HB2	2.45	0.46
1:D:372:LEU:HB3	1:D:445:ILE:HD11	1.97	0.46
1:C:488:LYS:HG2	1:C:491:ARG:HH21	1.80	0.46
1:E:566:LEU:HB2	1:E:569:ASP:HB2	1.96	0.46
1:F:281:HIS:CE1	1:F:374:ASN:HD21	2.33	0.46
1:A:425:CYS:HB2	1:A:468:LEU:HD23	1.97	0.46
1:F:560:LEU:CD2	1:F:561:GLN:HG3	2.42	0.46
1:C:123:HIS:O	1:C:127:ILE:HG13	2.16	0.46
1:B:534:LEU:HD23	1:B:812:LEU:HD23	1.96	0.46
1:A:77:GLU:CB	1:A:100:LEU:HD21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:CYS:O	1:D:538:VAL:HG22	2.15	0.46
1:E:341:VAL:HG21	1:E:384:VAL:HG12	1.98	0.46
1:H:292:TYR:O	1:H:295:ILE:HG22	2.15	0.46
1:D:405:TYR:HB2	1:D:407:LEU:CD1	2.46	0.46
1:C:351:TYR:CE2	1:C:358:HIS:CD2	3.03	0.46
1:E:102:ASN:O	1:E:106:ILE:HG12	2.15	0.46
1:F:24:LEU:HD22	1:F:142:TYR:CD2	2.51	0.46
1:E:803:TYR:HA	1:E:806:LEU:HD12	1.98	0.46
1:C:295:ILE:O	1:C:299:MSE:HG3	2.16	0.46
1:H:546:TYR:HA	1:H:583:LEU:HD13	1.97	0.46
1:D:402:TYR:CB	1:D:409:LEU:HD11	2.41	0.46
1:B:203:ILE:HG22	1:B:214:VAL:HG13	1.96	0.46
1:H:220:LEU:HB3	1:H:272:PHE:CE1	2.51	0.46
1:C:604:TYR:CE2	1:C:630:LEU:HB2	2.51	0.46
1:A:144:ARG:O	1:A:148:VAL:HG23	2.16	0.46
1:D:590:THR:HG21	1:D:643:ARG:HB2	1.98	0.46
1:C:571:TRP:HH2	1:C:625:THR:C	2.19	0.46
1:H:678:SER:HB2	1:H:687:ALA:HB2	1.97	0.46
1:G:419:LEU:HD21	1:G:517:LEU:HG	1.98	0.45
1:F:708:PHE:O	1:F:712:ILE:HD12	2.16	0.45
1:H:410:MSE:HG2	1:H:463:CYS:CB	2.46	0.45
1:G:313:MSE:HE3	1:G:371:ILE:HD13	1.98	0.45
1:E:28:LEU:HD23	1:E:186:LEU:HD12	1.98	0.45
1:A:185:GLY:HA2	1:A:430:ASN:HD21	1.80	0.45
1:G:153:TYR:O	1:G:157:VAL:HG23	2.15	0.45
1:B:123:HIS:CE1	1:B:127:ILE:HD11	2.51	0.45
1:G:220:LEU:HB3	1:G:272:PHE:CE1	2.52	0.45
1:H:668:LEU:HA	1:H:668:LEU:HD23	1.82	0.45
1:E:668:LEU:HD11	1:E:694:VAL:HA	1.99	0.45
1:A:123:HIS:O	1:A:127:ILE:HG13	2.17	0.45
1:C:102:ASN:O	1:C:106:ILE:HG12	2.16	0.45
1:D:341:VAL:HG11	1:D:384:VAL:HG13	1.97	0.45
1:D:656:LYS:O	1:D:660:ASN:HB2	2.17	0.45
1:F:161:ILE:O	1:F:165:GLN:HG2	2.16	0.45
1:F:296:ILE:HD12	1:F:299:MSE:SE	2.66	0.45
1:E:221:PHE:CZ	1:E:225:ILE:HD11	2.52	0.45
1:H:40:SER:HB3	1:H:96:VAL:HG11	1.98	0.45
1:D:698:ASP:CB	1:D:701:ASN:HB2	2.47	0.45
1:A:668:LEU:O	1:A:672:ILE:HG13	2.16	0.45
1:D:627:GLU:O	1:D:631:GLN:HG3	2.17	0.45
1:D:12:VAL:HB	1:D:13:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ILE:HG23	1:D:153:TYR:CE2	2.52	0.45
1:D:546:TYR:O	1:D:549:VAL:HG22	2.16	0.45
1:A:152:TYR:CZ	1:A:193:LEU:HB3	2.52	0.45
1:B:143:ASP:O	1:B:147:ILE:HG12	2.16	0.45
1:A:161:ILE:HG21	1:A:199:ARG:NH1	2.31	0.45
1:F:54:HIS:HB3	1:F:61:PRO:HG3	1.99	0.45
1:C:250:LEU:HA	1:C:250:LEU:HD23	1.85	0.45
1:E:693:THR:O	1:E:697:TYR:HD1	1.99	0.45
1:F:220:LEU:HB3	1:F:272:PHE:CE1	2.52	0.45
1:H:631:GLN:O	1:H:635:ILE:HG12	2.17	0.45
1:H:114:PHE:HB3	1:H:157:VAL:HG13	1.98	0.45
1:G:76:LEU:O	1:G:80:MSE:HG2	2.17	0.45
1:D:217:PRO:HB2	1:D:268:HIS:CE1	2.51	0.45
1:C:415:SER:HB2	1:C:459:THR:HG22	1.98	0.45
1:B:217:PRO:HB2	1:B:268:HIS:CE1	2.51	0.45
1:A:283:LYS:HG2	1:A:285:ILE:HG23	1.98	0.45
1:B:277:PHE:CZ	1:B:315:LEU:HD13	2.51	0.45
1:E:277:PHE:CZ	1:E:315:LEU:HD13	2.51	0.45
1:B:536:ARG:HD3	1:B:536:ARG:HA	1.81	0.45
1:E:443:TYR:OH	1:E:447:LYS:NZ	2.46	0.45
1:F:635:ILE:O	1:F:639:ASN:ND2	2.47	0.45
1:C:179:ILE:HA	1:C:180:PRO:HD3	1.82	0.45
1:G:239:ASP:OD2	1:G:276:TYR:OH	2.29	0.45
1:F:410:MSE:HE3	1:F:418:TRP:HZ3	1.80	0.45
1:C:94:LYS:O	1:C:98:LYS:HG3	2.17	0.45
1:D:221:PHE:CZ	1:D:225:ILE:HD11	2.52	0.45
1:F:365:ILE:HG23	1:F:394:PHE:HE1	1.82	0.45
1:A:25:ARG:NH2	1:A:138:LEU:HD22	2.32	0.45
1:C:98:LYS:HE2	1:C:128:HIS:HA	1.99	0.45
1:B:529:TRP:HB3	1:B:552:VAL:HG21	1.99	0.45
1:D:781:LEU:HG	1:D:785:TYR:CE2	2.52	0.45
1:B:64:PRO:O	1:B:68:VAL:HG23	2.17	0.45
1:B:703:ASP:OD1	1:B:703:ASP:N	2.50	0.45
1:B:672:ILE:HG13	1:B:673:ALA:N	2.31	0.45
1:H:27:ARG:NH1	1:H:52:HIS:HD2	2.10	0.45
1:B:514:LEU:HD12	1:B:518:ILE:HD13	1.98	0.45
1:B:27:ARG:HE	1:B:34:PHE:HZ	1.65	0.45
1:G:708:PHE:HE2	1:G:757:LEU:HB2	1.82	0.45
1:E:145:TYR:HA	1:E:187:LEU:HD13	1.98	0.45
1:B:361:ILE:HD12	1:B:361:ILE:H	1.81	0.45
1:B:400:SER:HA	1:B:403:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:LEU:O	1:D:765:ILE:HG12	2.17	0.45
1:A:418:TRP:O	1:A:422:SER:HB3	2.17	0.45
1:A:678:SER:HB3	1:A:686:VAL:HG13	1.99	0.45
1:G:793:TYR:O	1:G:796:SER:OG	2.27	0.45
1:F:634:TRP:HB3	1:F:658:ALA:HB2	1.99	0.45
1:B:443:TYR:HE2	1:B:496:LYS:HD3	1.82	0.45
1:F:587:ILE:HG23	1:F:588:PHE:CD1	2.52	0.44
1:H:590:THR:O	1:H:594:LEU:HG	2.16	0.44
1:F:224:MSE:HE2	1:F:276:TYR:HA	1.99	0.44
1:C:703:ASP:N	1:C:703:ASP:OD1	2.49	0.44
1:E:635:ILE:HD11	1:E:673:ALA:HB2	1.98	0.44
1:B:542:LYS:O	1:B:546:TYR:HB3	2.17	0.44
1:D:292:TYR:O	1:D:295:ILE:HG22	2.17	0.44
1:D:698:ASP:HB3	1:D:701:ASN:HB2	1.99	0.44
1:C:761:LEU:HD22	1:C:777:VAL:HG13	1.98	0.44
1:D:169:TYR:HA	1:D:210:PHE:CE1	2.52	0.44
1:G:182:GLU:N	1:G:360:ASP:OD2	2.51	0.44
1:B:292:TYR:O	1:B:295:ILE:HG22	2.18	0.44
1:H:514:LEU:HD11	1:H:528:ALA:HB1	2.00	0.44
1:H:28:LEU:HD21	1:H:142:TYR:HD1	1.82	0.44
1:B:399:ASN:OD1	1:F:204:GLN:NE2	2.50	0.44
1:B:373:GLN:NE2	1:B:437:ASN:OD1	2.49	0.44
1:B:102:ASN:O	1:B:106:ILE:HG13	2.17	0.44
1:H:89:TYR:CE2	1:H:91:GLU:HB2	2.53	0.44
1:H:325:ASP:O	1:H:329:LYS:HG3	2.18	0.44
1:A:173:LEU:HG	1:A:210:PHE:CD1	2.52	0.44
1:B:165:GLN:O	1:B:169:TYR:HD1	2.00	0.44
1:H:556:MSE:SE	1:H:573:PHE:HA	2.67	0.44
1:G:604:TYR:CZ	1:G:630:LEU:HB2	2.53	0.44
1:E:304:GLN:HG3	1:E:346:TYR:CE1	2.52	0.44
1:B:566:LEU:HB2	1:B:569:ASP:HB2	2.00	0.44
1:G:277:PHE:CZ	1:G:315:LEU:HD13	2.53	0.44
1:H:594:LEU:HD22	1:H:641:TYR:CE1	2.53	0.44
1:C:64:PRO:O	1:C:68:VAL:HG23	2.18	0.44
1:E:765:ILE:HG23	1:E:772:TYR:HD2	1.83	0.44
1:D:693:THR:HA	1:H:666:LYS:HE3	1.99	0.44
1:E:44:VAL:HG11	1:E:96:VAL:HG13	1.99	0.44
1:F:507:ILE:HD13	1:F:538:VAL:HG21	1.98	0.44
1:H:514:LEU:HD12	1:H:518:ILE:HG13	1.98	0.44
1:D:216:ASN:HD22	1:D:219:ILE:HG12	1.83	0.44
1:G:62:ALA:HB3	1:G:65:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HA	1:B:107:LEU:HD13	1.99	0.44
1:A:153:TYR:HA	1:A:156:LEU:HB2	2.00	0.44
1:C:572:GLN:OE1	1:C:815:CYS:HA	2.16	0.44
1:E:765:ILE:HD12	1:E:781:LEU:HD22	2.00	0.44
1:G:144:ARG:HA	1:G:147:ILE:HD12	1.99	0.44
1:E:270:ASN:O	1:E:274:GLN:HG3	2.17	0.44
1:B:416:LEU:HD23	1:B:506:HIS:CD2	2.53	0.44
1:H:619:GLY:HA3	1:H:624:GLN:OE1	2.18	0.44
1:C:153:TYR:HA	1:C:156:LEU:HB2	2.00	0.44
1:G:365:ILE:HG23	1:G:394:PHE:HE1	1.83	0.44
1:E:441:THR:O	1:E:445:ILE:HG12	2.17	0.44
1:C:514:LEU:CD1	1:C:518:ILE:HD11	2.43	0.43
1:D:402:TYR:HA	1:D:407:LEU:HD13	2.00	0.43
1:D:464:ASN:HA	1:D:467:MSE:HE2	1.99	0.43
1:H:153:TYR:O	1:H:157:VAL:HG23	2.17	0.43
1:G:148:VAL:HG21	1:G:187:LEU:HD11	1.99	0.43
1:B:123:HIS:O	1:B:127:ILE:HG13	2.17	0.43
1:F:165:GLN:HE22	1:F:198:LEU:HA	1.83	0.43
1:B:566:LEU:O	1:B:566:LEU:HD12	2.19	0.43
1:E:64:PRO:O	1:E:68:VAL:HG23	2.18	0.43
1:E:203:ILE:HG22	1:E:214:VAL:HG13	1.99	0.43
1:B:628:TYR:O	1:B:631:GLN:HG2	2.18	0.43
1:D:798:LEU:O	1:D:801:ILE:HG22	2.18	0.43
1:E:698:ASP:HB3	1:E:701:ASN:HB2	2.00	0.43
1:D:708:PHE:O	1:D:712:ILE:HG12	2.18	0.43
1:C:604:TYR:HE2	1:C:630:LEU:HB2	1.84	0.43
1:A:161:ILE:HD13	1:A:199:ARG:HH22	1.83	0.43
1:A:161:ILE:O	1:A:165:GLN:HG3	2.18	0.43
1:F:678:SER:O	1:F:684:PRO:HD2	2.17	0.43
1:E:71:LYS:HE3	1:E:71:LYS:HB3	1.82	0.43
1:C:792:GLU:HA	1:C:795:ASN:ND2	2.34	0.43
1:G:94:LYS:O	1:G:98:LYS:HG3	2.17	0.43
1:C:28:LEU:HD23	1:C:186:LEU:HD12	2.00	0.43
1:H:89:TYR:O	1:H:93:THR:HG23	2.18	0.43
1:C:41:LEU:HA	1:C:44:VAL:HG12	2.00	0.43
1:A:371:ILE:O	1:A:375:SER:OG	2.20	0.43
1:D:48:GLN:NE2	1:D:99:ILE:HG23	2.32	0.43
1:H:418:TRP:O	1:H:422:SER:HB3	2.18	0.43
1:D:89:TYR:HA	1:D:90:PRO:HD3	1.62	0.43
1:G:52:HIS:HA	1:G:55:VAL:HG22	2.01	0.43
1:D:125:LEU:O	1:D:128:HIS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:CYS:O	1:C:467:MSE:HG3	2.18	0.43
1:G:536:ARG:HD3	1:G:544:MSE:SE	2.69	0.43
1:E:684:PRO:HB2	1:E:685:GLY:H	1.70	0.43
1:B:61:PRO:HD2	1:B:110:HIS:CE1	2.54	0.43
1:H:625:THR:HG21	1:H:665:PHE:CE2	2.54	0.43
1:A:655:ILE:HD12	1:A:677:LEU:HD22	1.99	0.43
1:E:25:ARG:NH2	1:E:357:SER:HB2	2.33	0.43
1:H:575:HIS:O	1:H:810:ARG:NH1	2.51	0.43
1:H:123:HIS:O	1:H:127:ILE:HG13	2.18	0.43
1:A:44:VAL:HG11	1:A:96:VAL:HG13	2.00	0.43
1:A:410:MSE:HG2	1:A:463:CYS:SG	2.58	0.43
1:B:179:ILE:HA	1:B:180:PRO:HD3	1.79	0.43
1:B:341:VAL:HG21	1:B:384:VAL:HG12	2.01	0.43
1:F:173:LEU:HA	1:F:173:LEU:HD23	1.49	0.43
1:B:419:LEU:HG	1:B:513:THR:HG22	2.01	0.43
1:H:594:LEU:HD23	1:H:640:MSE:HE3	2.01	0.43
1:H:89:TYR:CD1	1:H:90:PRO:HD2	2.54	0.43
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.76	0.43
1:F:453:LEU:HD22	1:F:769:ILE:HD13	2.01	0.43
1:F:59:ASN:O	1:F:110:HIS:NE2	2.52	0.43
1:E:125:LEU:O	1:E:129:ASN:ND2	2.46	0.43
1:F:398:LEU:HD11	1:F:438:ALA:HB1	2.01	0.43
1:H:578:LEU:HD22	1:H:636:PHE:CD2	2.53	0.43
1:E:708:PHE:CE1	1:E:712:ILE:HD11	2.54	0.43
1:D:255:PHE:HA	1:D:256:PRO:HD3	1.88	0.43
1:F:514:LEU:HD22	1:F:528:ALA:HB1	2.00	0.43
1:B:161:ILE:O	1:B:165:GLN:HG3	2.18	0.43
1:H:216:ASN:HA	1:H:217:PRO:HD3	1.90	0.43
1:A:508:GLU:O	1:A:512:LYS:HG3	2.18	0.43
1:F:102:ASN:O	1:F:106:ILE:HG13	2.18	0.43
1:F:578:LEU:HA	1:F:581:LEU:HD12	2.01	0.43
1:C:371:ILE:HA	1:C:371:ILE:HD12	1.91	0.43
1:G:703:ASP:OD1	1:G:703:ASP:N	2.51	0.43
1:H:169:TYR:HA	1:H:210:PHE:CE1	2.54	0.43
1:B:509:THR:O	1:B:513:THR:HG23	2.19	0.43
1:C:552:VAL:O	1:C:556:MSE:HG3	2.19	0.43
1:F:194:ILE:O	1:F:198:LEU:HG	2.18	0.43
1:A:793:TYR:CZ	1:A:797:LEU:HD11	2.54	0.43
1:F:419:LEU:HD11	1:F:513:THR:HA	2.00	0.43
1:F:320:SER:O	1:F:329:LYS:HG2	2.19	0.43
1:F:386:ASP:OD2	1:F:389:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:THR:HG22	1:F:213:THR:N	2.34	0.43
1:D:361:ILE:H	1:D:361:ILE:HD12	1.84	0.43
1:A:220:LEU:HB3	1:A:272:PHE:CE1	2.54	0.43
1:A:221:PHE:CZ	1:A:225:ILE:HD11	2.53	0.43
1:E:27:ARG:NH1	1:E:52:HIS:HD2	2.12	0.43
1:B:618:MSE:HE1	1:B:817:TYR:CD1	2.51	0.43
1:E:337:ILE:HD11	1:E:379:ASP:HB3	2.01	0.43
1:A:292:TYR:O	1:A:295:ILE:HG22	2.19	0.43
1:F:76:LEU:O	1:F:80:MSE:HG2	2.18	0.42
1:B:402:TYR:CE1	1:B:435:LEU:HD12	2.54	0.42
1:F:441:THR:O	1:F:445:ILE:HG13	2.19	0.42
1:H:585:GLU:OE1	1:H:643:ARG:HD3	2.18	0.42
1:D:28:LEU:HD22	1:D:184:ASN:OD1	2.18	0.42
1:G:15:LYS:O	1:G:19:VAL:HG23	2.18	0.42
1:G:295:ILE:O	1:G:299:MSE:HG3	2.20	0.42
1:H:522:ASN:HB3	1:H:525:TYR:HB2	2.01	0.42
1:C:350:TYR:CE1	1:C:359:ARG:HB2	2.54	0.42
1:B:41:LEU:HD13	1:B:96:VAL:HG22	2.00	0.42
1:A:288:ASN:HA	1:A:289:PRO:HD3	1.87	0.42
1:F:255:PHE:HA	1:F:256:PRO:HD3	1.89	0.42
1:G:216:ASN:HD21	1:G:219:ILE:HG12	1.85	0.42
1:H:194:ILE:O	1:H:198:LEU:HG	2.20	0.42
1:D:446:ARG:NH1	1:D:461:TYR:OH	2.53	0.42
1:F:92:ILE:H	1:F:92:ILE:HD12	1.84	0.42
1:A:494:GLN:HB3	1:A:518:ILE:HG12	2.01	0.42
1:G:313:MSE:HE2	1:G:370:PHE:CD2	2.52	0.42
1:G:463:CYS:O	1:G:467:MSE:HG3	2.19	0.42
1:D:743:THR:OG1	1:D:744:PHE:N	2.52	0.42
1:E:313:MSE:HE3	1:E:371:ILE:HD13	2.01	0.42
1:E:291:TRP:O	1:E:294:PHE:HB3	2.19	0.42
1:D:77:GLU:HB2	1:D:100:LEU:HD21	2.02	0.42
1:A:180:PRO:HG2	1:A:188:PHE:CE2	2.55	0.42
1:D:604:TYR:CZ	1:D:630:LEU:HB2	2.55	0.42
1:G:14:SER:OG	1:G:15:LYS:N	2.52	0.42
1:F:809:ILE:HG22	1:F:810:ARG:HG3	2.01	0.42
1:F:293:ASN:O	1:F:296:ILE:HG22	2.19	0.42
1:C:765:ILE:HD11	1:C:781:LEU:HD22	2.01	0.42
1:F:325:ASP:O	1:F:329:LYS:HG3	2.19	0.42
1:G:163:ILE:O	1:G:167:VAL:HG12	2.20	0.42
1:H:542:LYS:HE2	1:H:809:ILE:HD11	2.00	0.42
1:G:690:GLU:O	1:G:693:THR:OG1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:LYS:NZ	1:F:143:ASP:OD2	2.45	0.42
1:E:802:LYS:O	1:E:806:LEU:HG	2.19	0.42
1:F:179:ILE:HA	1:F:180:PRO:HD3	1.85	0.42
1:F:468:LEU:O	1:F:469:SER:OG	2.26	0.42
1:E:590:THR:O	1:E:594:LEU:HG	2.19	0.42
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.66	0.42
1:D:94:LYS:O	1:D:98:LYS:HG3	2.20	0.42
1:H:519:LEU:HD23	1:H:529:TRP:CE2	2.55	0.42
1:C:153:TYR:O	1:C:157:VAL:HG23	2.19	0.42
1:D:111:ARG:NH1	1:D:113:GLN:OE1	2.51	0.42
1:A:340:PHE:O	1:A:343:PHE:HB3	2.20	0.42
1:G:48:GLN:NE2	1:G:99:ILE:HG23	2.34	0.42
1:D:143:ASP:O	1:D:147:ILE:HG12	2.18	0.42
1:H:136:THR:OG1	1:H:139:MSE:HB3	2.20	0.42
1:A:161:ILE:HD13	1:A:199:ARG:HH12	1.84	0.42
1:H:224:MSE:HE2	1:H:276:TYR:HA	2.02	0.42
1:G:291:TRP:O	1:G:294:PHE:HB3	2.20	0.42
1:F:781:LEU:HG	1:F:785:TYR:CE2	2.53	0.42
1:G:795:ASN:O	1:G:799:LYS:HD2	2.20	0.42
1:C:513:THR:HG23	1:C:517:LEU:HD12	2.01	0.42
1:D:250:LEU:HA	1:D:250:LEU:HD23	1.87	0.42
1:B:450:LEU:HD21	1:B:772:TYR:CD2	2.55	0.42
1:E:546:TYR:O	1:E:549:VAL:HG22	2.18	0.42
1:A:468:LEU:O	1:A:469:SER:HB2	2.20	0.42
1:G:543:GLU:HB3	1:G:547:LYS:NZ	2.35	0.42
1:A:631:GLN:O	1:A:635:ILE:HG12	2.20	0.42
1:F:292:TYR:O	1:F:295:ILE:HG22	2.20	0.42
1:C:310:LYS:NZ	1:C:363:SER:OG	2.40	0.42
1:F:640:MSE:HA	1:F:643:ARG:CD	2.50	0.41
1:G:668:LEU:HD11	1:G:694:VAL:HA	2.02	0.41
1:C:270:ASN:OD1	1:C:308:VAL:HG22	2.20	0.41
1:H:405:TYR:HB2	1:H:407:LEU:HG	2.01	0.41
1:C:221:PHE:CZ	1:C:225:ILE:HD11	2.54	0.41
1:D:793:TYR:CZ	1:D:797:LEU:HD11	2.55	0.41
1:H:746:ASN:O	1:H:750:ARG:HG3	2.20	0.41
1:C:410:MSE:HB2	1:C:410:MSE:HE2	1.78	0.41
1:C:361:ILE:HD12	1:C:361:ILE:H	1.84	0.41
1:E:708:PHE:O	1:E:712:ILE:HD12	2.21	0.41
1:D:255:PHE:CD1	1:D:256:PRO:HD2	2.55	0.41
1:D:153:TYR:O	1:D:157:VAL:HG23	2.20	0.41
1:C:283:LYS:HD3	1:C:285:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:TRP:CE3	1:A:629:LEU:HG	2.55	0.41
1:F:638:ALA:O	1:F:642:MSE:HG3	2.20	0.41
1:A:712:ILE:HD12	1:A:757:LEU:HG	2.02	0.41
1:B:490:LEU:HA	1:B:490:LEU:HD23	1.84	0.41
1:G:90:PRO:O	1:G:94:LYS:HG3	2.20	0.41
1:E:313:MSE:HE1	1:E:371:ILE:HB	2.03	0.41
1:D:291:TRP:O	1:D:294:PHE:HB3	2.20	0.41
1:B:712:ILE:O	1:B:750:ARG:NH1	2.53	0.41
1:A:495:PHE:CE2	1:A:527:LYS:HE2	2.55	0.41
1:F:659:SER:HA	1:F:670:CYS:SG	2.60	0.41
1:C:510:ALA:O	1:C:514:LEU:HB2	2.21	0.41
1:E:143:ASP:O	1:E:147:ILE:HG13	2.21	0.41
1:H:106:ILE:HG23	1:H:153:TYR:CE2	2.56	0.41
1:E:280:THR:HG22	1:E:285:ILE:O	2.20	0.41
1:C:160:ASP:OD1	1:C:161:ILE:N	2.53	0.41
1:A:371:ILE:HA	1:A:371:ILE:HD12	1.91	0.41
1:F:340:PHE:O	1:F:344:VAL:HG23	2.20	0.41
1:E:278:LYS:O	1:E:282:ILE:HG13	2.20	0.41
1:B:398:LEU:HD11	1:B:438:ALA:HB1	2.02	0.41
1:A:203:ILE:HG22	1:A:214:VAL:HG23	2.01	0.41
1:C:639:ASN:O	1:C:643:ARG:HG3	2.20	0.41
1:B:441:THR:O	1:B:445:ILE:HG13	2.20	0.41
1:E:507:ILE:HD13	1:E:538:VAL:HG11	2.02	0.41
1:D:107:LEU:O	1:D:111:ARG:HG3	2.20	0.41
1:E:463:CYS:O	1:E:467:MSE:HG3	2.21	0.41
1:A:163:ILE:O	1:A:167:VAL:HG12	2.20	0.41
1:G:179:ILE:HA	1:G:180:PRO:HD3	1.79	0.41
1:H:708:PHE:O	1:H:712:ILE:HD12	2.21	0.41
1:C:549:VAL:O	1:C:553:LEU:HB2	2.21	0.41
1:D:620:PRO:HD2	1:D:624:GLN:NE2	2.36	0.41
1:B:505:ARG:NE	1:B:773:TYR:HB3	2.35	0.41
1:A:350:TYR:CD1	1:A:359:ARG:HG2	2.56	0.41
1:B:371:ILE:O	1:B:375:SER:OG	2.29	0.41
1:A:571:TRP:CZ3	1:A:629:LEU:HG	2.55	0.41
1:C:28:LEU:HD22	1:C:184:ASN:OD1	2.21	0.41
1:A:152:TYR:HA	1:A:168:PHE:CE1	2.56	0.41
1:B:161:ILE:HD13	1:B:199:ARG:HH12	1.86	0.41
1:B:412:GLN:HG2	1:B:455:SER:O	2.20	0.41
1:G:232:LEU:HA	1:G:232:LEU:HD23	1.81	0.41
1:B:89:TYR:O	1:B:93:THR:OG1	2.39	0.41
1:E:639:ASN:HA	1:E:642:MSE:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:578:LEU:HD22	1:F:636:PHE:HD2	1.86	0.41
1:G:135:LYS:NZ	1:G:143:ASP:OD2	2.38	0.41
1:D:581:LEU:HD11	1:D:600:VAL:CG2	2.45	0.41
1:C:582:ALA:O	1:C:585:GLU:HB3	2.21	0.41
1:F:310:LYS:NZ	1:F:363:SER:OG	2.38	0.41
1:G:173:LEU:HB2	1:G:210:PHE:HD2	1.86	0.41
1:E:101:PHE:HA	1:E:104:LEU:HD12	2.02	0.41
1:D:505:ARG:HB3	1:D:806:LEU:HD13	2.03	0.41
1:E:256:PRO:HG2	1:E:262:ASN:OD1	2.20	0.41
1:C:544:MSE:HE3	1:C:548:ILE:HD11	2.02	0.41
1:C:760:LEU:HD23	1:C:760:LEU:HA	1.94	0.41
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.95	0.41
1:G:51:LEU:O	1:G:55:VAL:HG22	2.20	0.41
1:E:630:LEU:HD23	1:E:630:LEU:HA	1.95	0.41
1:H:542:LYS:CE	1:H:809:ILE:HD11	2.51	0.41
1:F:695:LEU:CD1	1:F:704:ALA:HB1	2.50	0.41
1:F:350:TYR:CE1	1:F:359:ARG:HB3	2.56	0.41
1:G:678:SER:CB	1:G:687:ALA:HB2	2.50	0.41
1:F:634:TRP:CB	1:F:658:ALA:HB2	2.51	0.41
1:E:255:PHE:HA	1:E:256:PRO:HD3	1.84	0.41
1:H:179:ILE:HA	1:H:180:PRO:HD3	1.83	0.41
1:A:341:VAL:HG21	1:A:384:VAL:HG12	2.02	0.41
1:E:702:LEU:O	1:E:706:VAL:HG23	2.20	0.41
1:F:377:LYS:HE2	1:F:388:ASP:OD1	2.21	0.41
1:H:163:ILE:O	1:H:167:VAL:HG12	2.21	0.41
1:C:372:LEU:HA	1:C:372:LEU:HD23	1.92	0.41
1:D:570:ARG:HB3	1:D:607:LEU:HD22	2.03	0.41
1:A:27:ARG:HD3	1:A:48:GLN:NE2	2.30	0.41
1:F:44:VAL:HG21	1:F:96:VAL:CG1	2.49	0.41
1:C:216:ASN:HA	1:C:217:PRO:HD3	1.81	0.41
1:A:503:GLN:OE1	1:A:769:ILE:HG21	2.20	0.41
1:C:225:ILE:HG22	1:C:229:GLN:HE21	1.86	0.41
1:E:256:PRO:HG3	1:E:262:ASN:HA	2.03	0.41
1:B:48:GLN:OE1	1:B:145:TYR:OH	2.18	0.41
1:E:656:LYS:HB2	1:E:656:LYS:HE3	1.87	0.41
1:F:490:LEU:HD23	1:F:490:LEU:HA	1.98	0.41
1:F:573:PHE:CD1	1:F:603:LEU:HD21	2.56	0.41
1:A:228:PHE:CE1	1:A:279:PHE:HD1	2.39	0.41
1:F:559:SER:HA	1:F:563:ASN:HB2	2.03	0.40
1:E:536:ARG:O	1:E:539:GLN:HG2	2.21	0.40
1:F:463:CYS:O	1:F:467:MSE:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:O	1:A:147:ILE:HG22	2.21	0.40
1:A:609:PRO:HG3	1:D:563:ASN:OD1	2.21	0.40
1:G:425:CYS:HB2	1:G:468:LEU:HD23	2.03	0.40
1:B:38:PHE:HD1	1:B:85:GLU:CD	2.25	0.40
1:E:317:GLN:HE22	1:E:333:LYS:HE2	1.86	0.40
1:H:25:ARG:HH11	1:H:25:ARG:HD3	1.78	0.40
1:B:514:LEU:HD11	1:B:528:ALA:HB1	2.02	0.40
1:C:652:LYS:HG2	1:C:677:LEU:HD21	2.02	0.40
1:H:48:GLN:NE2	1:H:99:ILE:HG23	2.36	0.40
1:A:700:ASN:HB3	1:A:768:SER:OG	2.21	0.40
1:C:345:LYS:HB2	1:C:345:LYS:HE3	1.90	0.40
1:B:47:LEU:HD21	1:B:73:SER:HB3	2.03	0.40
1:H:20:VAL:O	1:H:24:LEU:HG	2.20	0.40
1:C:250:LEU:O	1:C:301:LYS:NZ	2.46	0.40
1:C:777:VAL:O	1:C:781:LEU:HB2	2.22	0.40
1:H:80:MSE:HE2	1:H:80:MSE:HB2	1.98	0.40
1:F:567:LEU:O	1:F:570:ARG:HG3	2.21	0.40
1:G:517:LEU:HB2	1:G:518:ILE:HD12	2.03	0.40
1:H:635:ILE:HD11	1:H:673:ALA:HB2	2.03	0.40
1:E:348:ASP:O	1:E:352:GLN:HG3	2.21	0.40
1:F:412:GLN:NE2	1:F:457:ASN:OD1	2.32	0.40
1:A:410:MSE:HE3	1:A:463:CYS:SG	2.61	0.40
1:F:288:ASN:HA	1:F:289:PRO:HD3	1.81	0.40
1:E:63:LYS:HA	1:E:66:CYS:HB2	2.03	0.40
1:A:107:LEU:O	1:A:111:ARG:HG3	2.21	0.40
1:H:798:LEU:HD23	1:H:798:LEU:HA	1.91	0.40
1:A:277:PHE:CE2	1:A:315:LEU:HB2	2.57	0.40
1:A:505:ARG:HB3	1:A:806:LEU:HD13	2.03	0.40
1:G:418:TRP:HE3	1:G:517:LEU:HD11	1.87	0.40
1:C:507:ILE:HD13	1:C:538:VAL:HG21	2.03	0.40
1:G:511:ILE:O	1:G:515:GLU:HG3	2.22	0.40
1:G:618:MSE:HE1	1:G:817:TYR:CD1	2.57	0.40
1:A:341:VAL:HG12	1:A:345:LYS:HE3	2.03	0.40
1:E:412:GLN:O	1:E:415:SER:OG	2.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:TYR:OH	1:E:671:ASN:OD1[1_655]	2.17	0.03

## 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	731/802 (91%)	714 (98%)	17 (2%)	0	100	100
1	B	725/802 (90%)	704 (97%)	21 (3%)	0	100	100
1	C	721/802 (90%)	701 (97%)	20 (3%)	0	100	100
1	D	747/802 (93%)	727 (97%)	19 (2%)	1 (0%)	56	90
1	E	709/802 (88%)	691 (98%)	18 (2%)	0	100	100
1	F	709/802 (88%)	688 (97%)	20 (3%)	1 (0%)	56	90
1	G	719/802 (90%)	699 (97%)	19 (3%)	1 (0%)	56	90
1	H	718/802 (90%)	700 (98%)	18 (2%)	0	100	100
All	All	5779/6416 (90%)	5624 (97%)	152 (3%)	3 (0%)	56	90

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	662	GLU
1	D	90	PRO
1	F	231	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	688/724 (95%)	683 (99%)	5 (1%)	88	96
1	B	685/724 (95%)	682 (100%)	3 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	681/724 (94%)	677 (99%)	4 (1%)	90	96
1	D	701/724 (97%)	695 (99%)	6 (1%)	84	94
1	E	671/724 (93%)	664 (99%)	7 (1%)	82	93
1	F	671/724 (93%)	667 (99%)	4 (1%)	90	96
1	G	678/724 (94%)	672 (99%)	6 (1%)	84	94
1	H	678/724 (94%)	670 (99%)	8 (1%)	78	92
All	All	5453/5792 (94%)	5410 (99%)	43 (1%)	86	95

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	TYR
1	A	505	ARG
1	A	565	LEU
1	A	570	ARG
1	A	573	PHE
1	B	145	TYR
1	B	565	LEU
1	B	573	PHE
1	C	89	TYR
1	C	145	TYR
1	C	358	HIS
1	C	573	PHE
1	D	145	TYR
1	D	164	MSE
1	D	235	HIS
1	D	358	HIS
1	D	542	LYS
1	D	573	PHE
1	E	145	TYR
1	E	351	TYR
1	E	358	HIS
1	E	505	ARG
1	E	573	PHE
1	E	806	LEU
1	E	810	ARG
1	F	145	TYR
1	F	272	PHE
1	F	505	ARG
1	F	573	PHE

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Mol	Chain	Res	Type
1	G	89	TYR
1	G	145	TYR
1	G	410	MSE
1	G	556	MSE
1	G	573	PHE
1	G	813	ARG
1	H	145	TYR
1	H	229	GLN
1	H	351	TYR
1	H	358	HIS
1	H	570	ARG
1	H	573	PHE
1	H	643	ARG
1	H	813	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	318	ASN
1	B	141	GLN
1	C	141	GLN
1	C	150	ASN
1	D	110	HIS
1	F	202	GLN
1	F	238	ASN
1	G	412	GLN
1	H	141	GLN
1	H	150	ASN
1	H	229	GLN
1	H	358	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	728/802 (90%)	-0.02	20 (2%) 58 48	26, 69, 112, 156	0
1	B	724/802 (90%)	-0.01	20 (2%) 56 47	35, 67, 107, 142	0
1	C	720/802 (89%)	0.01	17 (2%) 62 52	30, 68, 106, 140	0
1	D	740/802 (92%)	-0.05	15 (2%) 68 58	27, 61, 102, 144	0
1	E	712/802 (88%)	0.01	28 (3%) 43 33	30, 62, 101, 131	0
1	F	712/802 (88%)	0.07	27 (3%) 44 34	25, 69, 117, 155	0
1	G	720/802 (89%)	0.11	31 (4%) 39 29	27, 75, 116, 144	0
1	H	718/802 (89%)	0.16	30 (4%) 40 30	34, 77, 126, 152	0
All	All	5774/6416 (89%)	0.03	188 (3%) 50 40	25, 68, 112, 156	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	14	SER	6.2
1	D	130	ASN	5.6
1	G	746	ASN	5.5
1	F	160	ASP	5.5
1	E	79	ASN	5.3
1	B	562	ASN	5.1
1	C	747	ASP	4.9
1	C	14	SER	4.7
1	B	159	GLN	4.4
1	C	562	ASN	4.4
1	B	565	LEU	4.2
1	G	565	LEU	4.2
1	B	14	SER	4.2
1	E	645	LYS	4.1
1	C	786	GLU	4.0
1	E	665	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	149	GLU	3.9
1	F	565	LEU	3.9
1	G	699	GLU	3.8
1	G	641	TYR	3.8
1	F	791	ASP	3.8
1	G	692	GLU	3.8
1	D	84	GLU	3.7
1	H	650	ASP	3.7
1	F	747	ASP	3.7
1	F	79	ASN	3.6
1	A	746	ASN	3.6
1	H	119	ARG	3.6
1	H	747	ASP	3.6
1	F	382	GLU	3.6
1	C	103	CYS	3.6
1	G	659	SER	3.5
1	H	382	GLU	3.5
1	H	646	ASP	3.4
1	E	674	ASN	3.4
1	G	232	LEU	3.4
1	F	78	LYS	3.4
1	E	795	ASN	3.4
1	B	622	TYR	3.4
1	F	713	PHE	3.3
1	H	746	ASN	3.3
1	H	78	LYS	3.3
1	H	67	ASP	3.3
1	H	424	ARG	3.2
1	C	667	ASN	3.2
1	B	102	ASN	3.1
1	F	562	ASN	3.1
1	H	79	ASN	3.1
1	F	358	HIS	3.1
1	F	81	SER	3.1
1	G	621	LYS	3.1
1	G	622	TYR	3.0
1	E	232	LEU	3.0
1	F	251	LEU	3.0
1	H	231	PRO	3.0
1	G	78	LYS	3.0
1	C	521	LYS	2.9
1	D	561	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	235	HIS	2.9
1	F	746	ASN	2.9
1	A	353	LEU	2.9
1	A	561	GLN	2.9
1	E	424	ARG	2.9
1	F	102	ASN	2.9
1	H	673	ALA	2.9
1	A	562	ASN	2.8
1	E	677	LEU	2.8
1	F	57	GLY	2.8
1	D	15	LYS	2.8
1	G	170	LYS	2.8
1	E	231	PRO	2.8
1	H	562	ASN	2.8
1	G	662	GLU	2.8
1	D	18	ASP	2.8
1	G	354	HIS	2.8
1	B	751	SER	2.7
1	B	791	ASP	2.7
1	E	382	GLU	2.7
1	F	101	PHE	2.7
1	B	160	ASP	2.7
1	E	562	ASN	2.7
1	A	649	GLU	2.6
1	E	798	LEU	2.6
1	H	586	GLU	2.6
1	C	746	ASN	2.6
1	G	747	ASP	2.6
1	A	786	GLU	2.6
1	E	646	ASP	2.6
1	D	174	ALA	2.6
1	G	79	ASN	2.6
1	E	644	THR	2.6
1	G	663	SER	2.6
1	D	97	GLU	2.6
1	H	352	GLN	2.6
1	G	669	ASN	2.6
1	D	87	ASN	2.6
1	D	102	ASN	2.6
1	B	748	THR	2.6
1	F	748	THR	2.6
1	E	750	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	352	GLN	2.6
1	F	126	LYS	2.5
1	A	232	LEU	2.5
1	G	215	GLU	2.5
1	B	13	PRO	2.5
1	B	86	LEU	2.5
1	A	747	ASP	2.5
1	H	92	ILE	2.5
1	H	199	ARG	2.5
1	E	354	HIS	2.4
1	H	257	THR	2.4
1	H	354	HIS	2.4
1	A	102	ASN	2.4
1	G	627	GLU	2.4
1	C	251	LEU	2.4
1	A	264	GLU	2.4
1	G	562	ASN	2.4
1	G	688	LEU	2.4
1	F	150	ASN	2.4
1	D	354	HIS	2.4
1	H	32	SER	2.3
1	G	325	ASP	2.3
1	H	170	LYS	2.3
1	B	564	THR	2.3
1	F	622	TYR	2.3
1	B	561	GLN	2.3
1	F	646	ASP	2.3
1	G	620	PRO	2.3
1	H	93	THR	2.3
1	H	353	LEU	2.3
1	E	679	ILE	2.3
1	E	61	PRO	2.2
1	G	677	LEU	2.2
1	B	382	GLU	2.2
1	A	38	PHE	2.2
1	A	233	LYS	2.2
1	E	540	GLU	2.2
1	H	754	TYR	2.2
1	E	163	ILE	2.2
1	G	58	SER	2.2
1	H	118	GLN	2.2
1	C	126	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	150	ASN	2.2
1	G	231	PRO	2.2
1	A	84	GLU	2.2
1	A	115	GLN	2.2
1	C	102	ASN	2.2
1	G	588	PHE	2.2
1	C	84	GLU	2.2
1	F	327	ILE	2.2
1	G	748	THR	2.2
1	H	563	ASN	2.2
1	C	354	HIS	2.2
1	A	149	GLU	2.2
1	E	162	ASN	2.2
1	D	682	ASP	2.2
1	E	754	TYR	2.1
1	D	664	LYS	2.1
1	C	135	LYS	2.1
1	E	649	GLU	2.1
1	H	311	THR	2.1
1	G	123	HIS	2.1
1	B	352	GLN	2.1
1	A	97	GLU	2.1
1	D	486	GLU	2.1
1	H	116	GLU	2.1
1	B	251	LEU	2.1
1	C	86	LEU	2.1
1	E	60	GLY	2.1
1	C	159	GLN	2.1
1	C	261	THR	2.1
1	F	644	THR	2.1
1	E	78	LYS	2.1
1	E	149	GLU	2.1
1	F	384	VAL	2.1
1	A	67	ASP	2.1
1	A	150	ASN	2.0
1	F	231	PRO	2.0
1	B	205	ASP	2.0
1	D	79	ASN	2.0
1	E	609	PRO	2.0
1	A	484	GLY	2.0
1	H	136	THR	2.0
1	F	620	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	115	GLN	2.0
1	G	564	THR	2.0
1	G	134	GLN	2.0
1	B	355	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.