



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 02:50 AM EDT

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

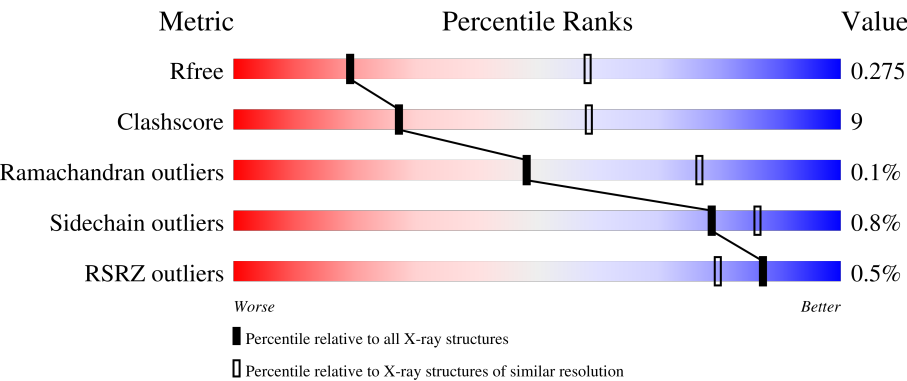
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	164625	1482 (3.30-3.22)
Clashscore	180529	1546 (3.30-3.22)
Ramachandran outliers	177936	1536 (3.30-3.22)
Sidechain outliers	177891	1535 (3.30-3.22)
RSRZ outliers	164620	1483 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	802	<div><div></div><div>71%21%7%</div></div>
1	B	802	<div><div></div><div>72%20%8%</div></div>
1	C	802	<div><div></div><div>73%18%8%</div></div>
1	D	802	<div><div></div><div>72%22%6%</div></div>
1	E	802	<div><div></div><div>69%21%9%</div></div>

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

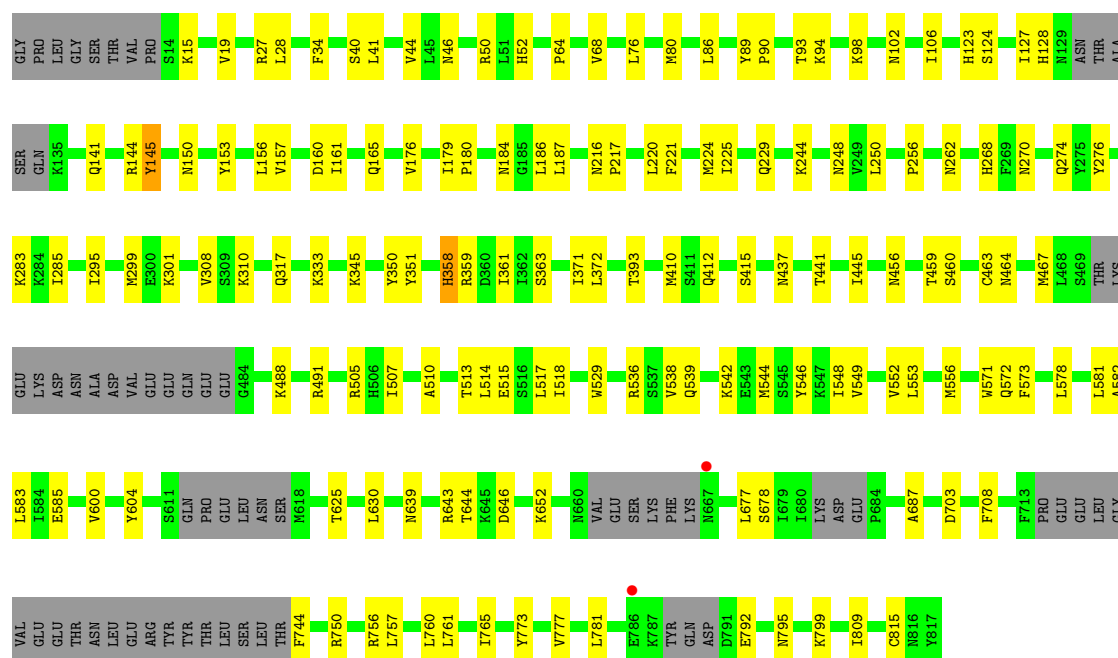






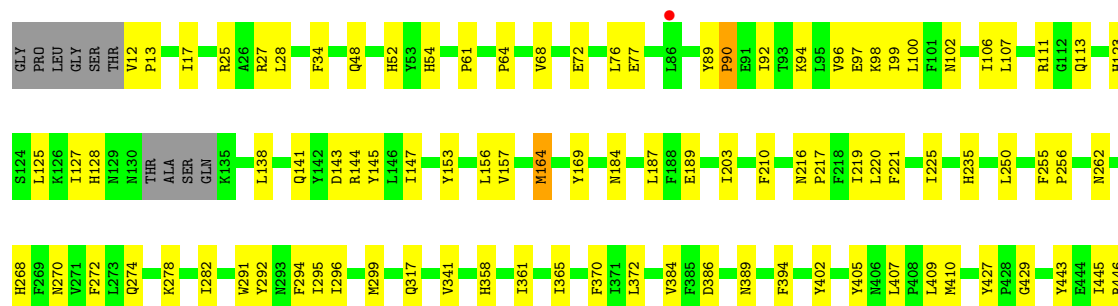
● Molecule 1: Cargo-transport protein YPP1

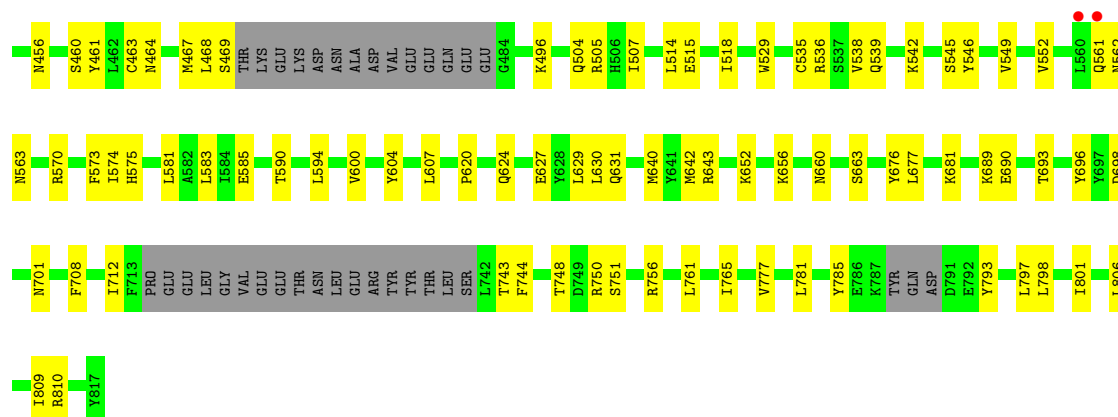
Chain C: 73% 18% 8%



● Molecule 1: Cargo-transport protein YPP1

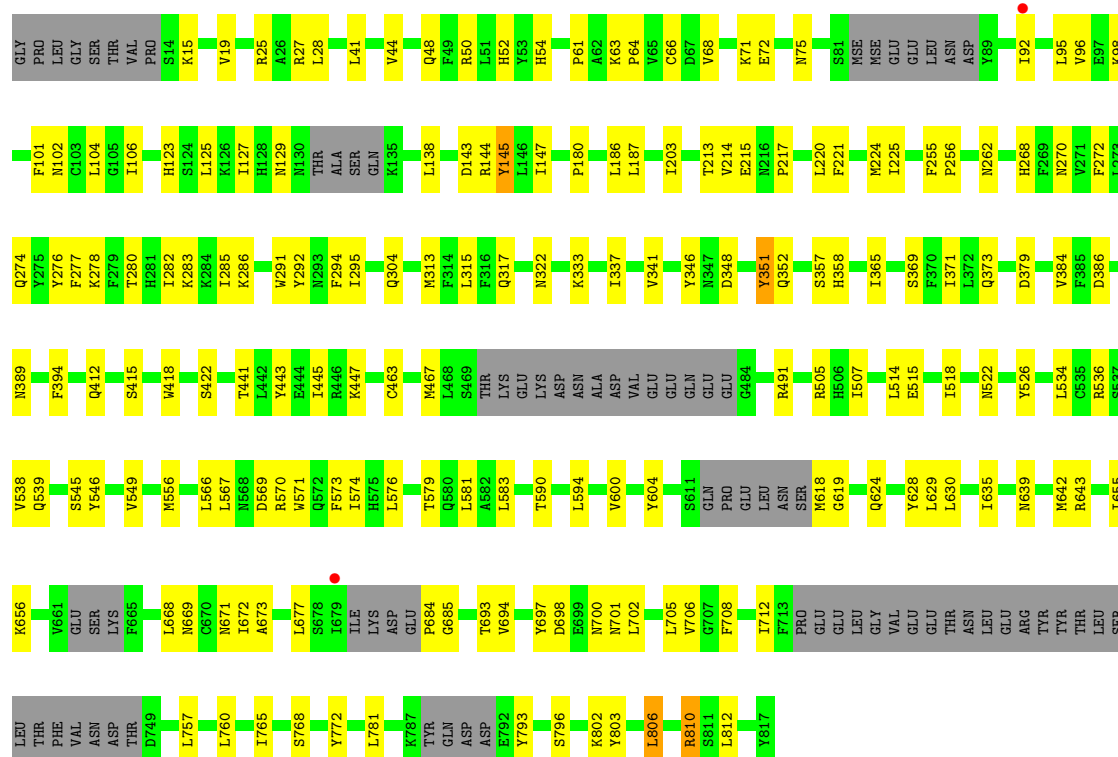
Chain D: 72% 22% 6%





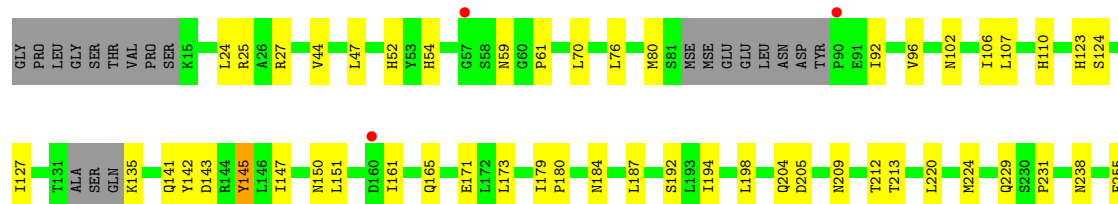
• Molecule 1: Cargo-transport protein YPP1

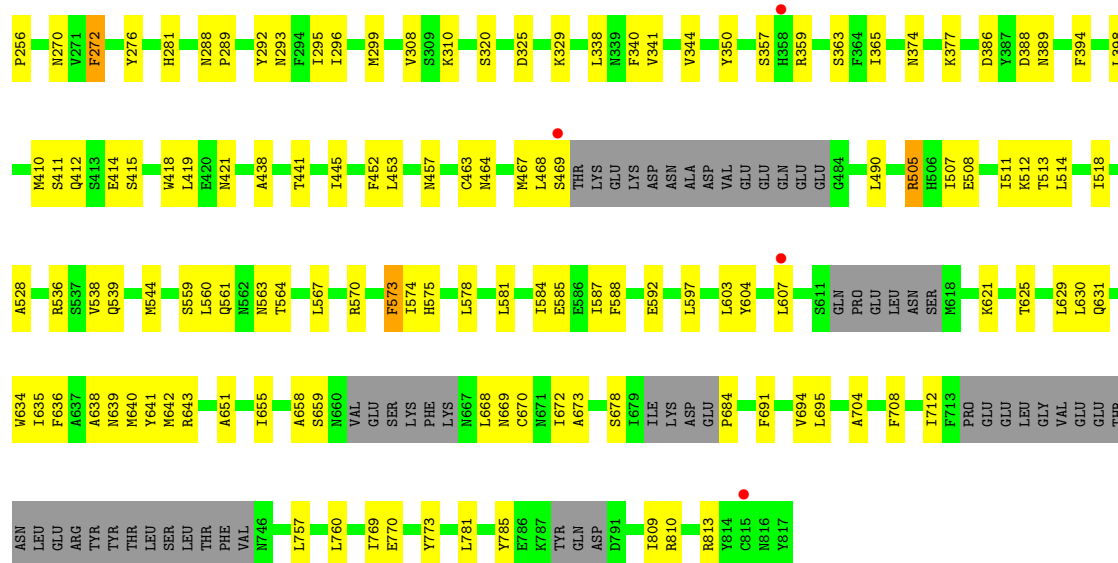
Chain E: 69% 21% 9%



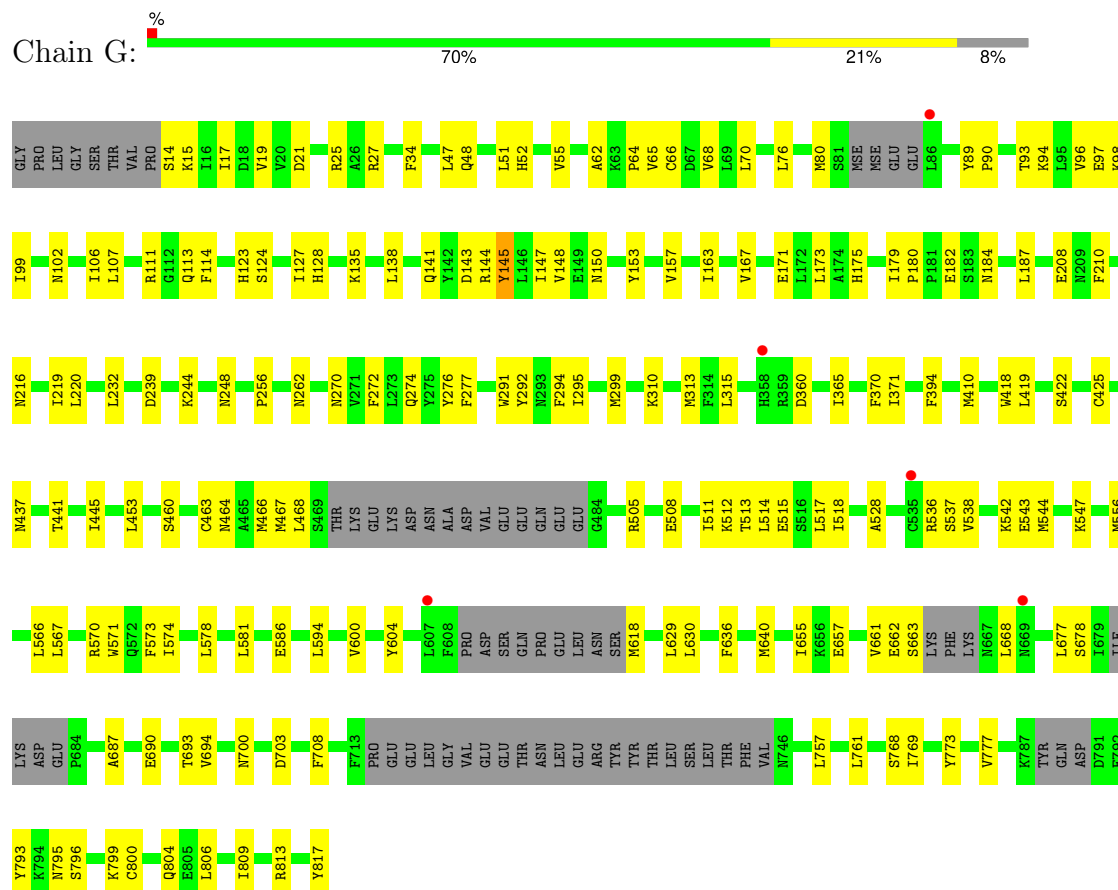
• Molecule 1: Cargo-transport protein YPP1

Chain F: 68% 22% 9%





- Molecule 1: Cargo-transport protein YPP1



- Molecule 1: Cargo-transport protein YPP1



GLY	PRO	LEU	GLY	SER	THR	VAL	PRO	S14	V20	D21	Q22	A23	L24	R25	A26	R27	L28	F34	G37	F38	D39	S40	V44	Q48	H52	A62	K63	P64	V65	C66	N75	N79	M80	S81	M82	MSE	GLU	GLU	LEU	N87	D88	Y89	P90	E91	I92	T93	K94	L95	V96	E97	
K98	I99	L100	F101	N102	I106	L107	R111	F114	Q118	L122	H123	S124	L125	K126	I127	H128	N129	ASN	THR	ALA	SER	GLN	K135	T136	A137	L138	M139	E140	Q141	Y142	D143	R144	Y145	L146	I147	N150	Y153	R154	G155	L156	V157	D160	I163	M164	V167	F168	K94	L95	Y169	K170	E171
L172	L173	I179	P180	N184	G185	L186	L187	I194	V195	A196	K197	L198	F210	T213	V214	E215	N216	P217	L220	M224	Q229	L250	P256	T257	N262	N270	V271	L272	L273	Q274	Y275	Y276	Y292	I295	K301	K310	A465	N466	N467	F325	I327	K328	K329								
K333	V341	Y351	Q352	L353	H354	D355	N356	S357	H358	I361	S362	S363	F364	I365	L372	S375	N389	F394	Y405	N406	L407	N410	N418	S422	C425	N437	T441	I445	S460	C463	N464	N465	N466	N467	L468	S469	THR	LYS													
GLU	LYS	ASP	ASN	ALA	ASP	VAL	GLU	GLN	G484	Q494	T509	A510	I511	K512	T513	L514	E515	I518	L519	N522	Y525	A528	N529	L532	V538	K542	Y546	M556	L566	D569	R570	F573	I574	H575	L578	L581	A582	L583	I584	E585											
T590	L594	L597	V600	L607	F608	P609	ASP	SER	GLN	PRO	GLU	GLU	LEU	ASN	SER	M618	G619	Q624	T625	K626	E627	Q631	I635	F636	N639	M640	Y641	M642	R643	D650	I655	F665	K666	N667	L668	N671	I672	A673	L677	S678	I679	ILE	LYS	ASP	GLU	P684					
A687	T693	F708	A709	I712	F713	PRO	GLU	GLU	LEU	GLY	VAL	GLU	GLU	THR	ASN	LEU	GLU	ARG	TYR	THR	THR	LEU	SER	LEU	THR	PHE	VAL	N746	R750	E770	P775	K787	TYR	GLN	ASP	D791	E792	Y793	L797	L798	N807	P808	I809	R810	R813	Y817					

## 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 25.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (25.00-3.25) 91.9 (25.00-3.25)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.23Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.240 , 0.277 0.239 , 0.275	Depositor DCC
$R_{free}$ test set	1973 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 29.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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 32.33 % 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 9.5695e-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, 0.333 respectively for untwinned datasets, and 0.375, 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:A:27:ARG:HD3	1:A:48:GLN:HE21	1.56	0.69
1:B:514:LEU:HA	1:B:518:ILE:HD13	1.74	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:C:412:GLN:O	1:C:456:ASN:ND2	2.27	0.68
1:G:542:LYS:HZ2	1:G:586:GLU:HG2	1.57	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:A:77:GLU:HB2	1:A:100:LEU:HD21	1.78	0.66
1:G:453:LEU:HD13	1:G:769:ILE:HD13	1.77	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:C:244:LYS:O	1:C:248:ASN:ND2	2.25	0.64
1:H:154:ARG:NH2	1:H:171:GLU:OE1	2.31	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:C:515:GLU:OE2	1:C:536:ARG:NH2	2.26	0.63
1:H:635:ILE:O	1:H:639:ASN:ND2	2.31	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:G:581:LEU:HD11	1:G:600:VAL:HG21	1.81	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:D:141:GLN:HG3	1:D:184:ASN:ND2	2.15	0.62
1:E:491:ARG:NH1	1:E:522:ASN:OD1	2.28	0.62
1:A:536:ARG:O	1:A:539:GLN:HG2	1.99	0.62
1:E:655:ILE:HG23	1:E:673:ALA:HB1	1.80	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: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: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:D:256:PRO:HG3	1:D:262:ASN:HA	1.80	0.61
1:G:538:VAL:HG11	1:G:806:LEU:HA	1.83	0.61
1:D:681:LYS:HG3	1:H:327:ILE:HG13	1.81	0.61
1:D:696:TYR:OH	1:H:671:ASN:OD1	2.09	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:B:761:LEU:HD22	1:B:777:VAL:HG13	1.82	0.61
1:C:40:SER:OG	1:C:86:LEU:HD21	2.01	0.61
1:A:98:LYS:HE2	1:A:128:HIS:HA	1.83	0.60
1:F:597:LEU:HD21	1:F:640:MSE:HE1	1.82	0.60
1:G:27:ARG:HE	1:G:34:PHE:HZ	1.49	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:B:450:LEU:HD13	1:B:769:ILE:HA	1.82	0.60
1:D:756:ARG:HH22	1:H:693:THR:HG22	1.66	0.60
1:E:604:TYR:CZ	1:E:630:LEU:HG	2.36	0.60
1:G:657:GLU:O	1:G:661:VAL:HG23	2.02	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:G:700:ASN:HB3	1:G:768:SER:HB2	1.84	0.60
1:H:125:LEU:HD11	1:H:154:ARG:NE	2.16	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:B:283:LYS:HD3	1:B:285:ILE:HD11	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:D:594:LEU:HD23	1:D:640:MSE:HE3	1.84	0.59
1:E:180:PRO:HB3	1:E:187:LEU:HD23	1.85	0.59
1:F:145:TYR:HA	1:F:187:LEU:HD13	1.85	0.59
1:H:515:GLU:HG3	1:H:532:LEU:HD11	1.83	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:D:278:LYS:HE3	1:D:282:ILE:HD11	1.85	0.58
1:H:655:ILE:HG21	1:H:677:LEU:HB2	1.84	0.58
1:B:67:ASP:OD1	1:B:111:ARG:NE	2.35	0.58
1:D:72:GLU:O	1:D:76:LEU:HG	2.03	0.58
1:F:708:PHE:HD1	1:F:757:LEU:HD13	1.68	0.58
1:A:518:ILE:O	1:A:522:ASN:HB2	2.03	0.58
1:F:635:ILE:HD12	1:F:673:ALA:HB2	1.86	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:C:217:PRO:HA	1:C:220:LEU:HD12	1.87	0.57
1:D:25:ARG:HB2	1:D:138:LEU:HD21	1.87	0.57
1:G:70:LEU:HD22	1:G:111:ARG:HD2	1.86	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:B:652:LYS:HG2	1:B:677:LEU:HD21	1.88	0.56
1:D:13:PRO:HB3	1:D:17:ILE:HD12	1.86	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:27:ARG:HH12	1:D:52:HIS:HD2	1.54	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:G:690:GLU:O	1:G:694:VAL:HG23	2.06	0.56
1:H:118:GLN:HG3	1:H:157:VAL:HG11	1.88	0.56
1:A:350:TYR:CE1	1:A:359:ARG:HG2	2.41	0.56
1:A:419:LEU:HD23	1:A:513:THR:HG22	1.87	0.56
1:B:505:ARG:HE	1:B:773:TYR:HB3	1.70	0.56
1:G:124:SER:OG	1:G:150:ASN:ND2	2.39	0.56
1:G:514:LEU:HA	1:G:518:ILE:HD13	1.88	0.56
1:C:507:ILE:HD13	1:C:538:VAL:HG11	1.86	0.56
1:C:678:SER:HB2	1:C:687:ALA:HB2	1.86	0.56
1:D:529:TRP:HB3	1:D:552:VAL:HG21	1.88	0.56
1:A:519:LEU:HD21	1:A:528:ALA:HB3	1.85	0.56
1:D:536:ARG:O	1:D:539:GLN:HG2	2.05	0.56
1:E:514:LEU:HD23	1:E:518:ILE:HD12	1.86	0.56
1:A:256:PRO:HG3	1:A:262:ASN:HA	1.87	0.56
1:B:141:GLN:HG3	1:B:184:ASN:ND2	2.21	0.56
1:D:443:TYR:HE2	1:D:496:LYS:HD3	1.70	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
1:G:313:MSE:HE2	1:G:370:PHE:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:775:PRO:HG3	1:H:807:ASN:ND2	2.21	0.56
1:D:102:ASN:O	1:D:106:ILE:HG12	2.05	0.56
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:C:217:PRO:HB2	1:C:268:HIS:CE1	2.41	0.55
1:E:348:ASP:HA	1:E:351:TYR:CD2	2.41	0.55
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:644:THR:HG22	1:C:646:ASP:H	1.71	0.55
1:H:566:LEU:HD13	1:H:570:ARG:HG2	1.86	0.55
1:G:655:ILE:HD12	1:G:677:LEU:HD22	1.88	0.55
1:F:691:PHE:O	1:F:695:LEU:HD13	2.06	0.55
1:G:14:SER:N	1:G:17:ILE:HD13	2.22	0.55
1:F:25:ARG:HH12	1:F:357:SER:HB2	1.70	0.55
1:H:570:ARG:HB3	1:H:607:LEU:HD22	1.87	0.55
1:A:570:ARG:NH2	1:D:562:ASN:O	2.40	0.55
1:C:27:ARG:HH12	1:C:52:HIS:HD2	1.53	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:G:25:ARG:HE	1:G:138:LEU:HD11	1.72	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:B:372:LEU:HB3	1:B:445:ILE:HD11	1.89	0.54
1:D:748:THR:O	1:D:751:SER:OG	2.20	0.54
1:F:411:SER:O	1:F:415:SER:OG	2.24	0.54
1:G:567:LEU:O	1:G:570:ARG:HG3	2.06	0.54
1:H:141:GLN:HG3	1:H:184:ASN:ND2	2.23	0.54
1:C:224:MSE:HE2	1:C:276:TYR:HA	1.88	0.54
1:F:695:LEU:HD23	1:F:760:LEU:HD13	1.89	0.54
1:H:358:HIS:CD2	1:H:361:ILE:HG12	2.42	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: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:H:75:ASN:O	1:H:79:ASN:ND2	2.31	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: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:A:25:ARG:HB2	1:A:138:LEU:HD21	1.89	0.54
1:B:92:ILE:O	1:B:96:VAL:HG23	2.08	0.54
1:E:283:LYS:HD3	1:E:285:ILE:HD11	1.90	0.54
1:A:213:THR:HG22	1:A:215:GLU:H	1.73	0.54
1:B:156:LEU:HD23	1:B:164:MSE:HE1	1.90	0.54
1:A:333:LYS:NZ	1:A:374:ASN:O	2.41	0.53
1:A:511:ILE:O	1:A:515:GLU:HB2	2.08	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:C:283:LYS:HG2	1:C:285:ILE:HG13	1.90	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:H:538:VAL:HG13	1:H:807:ASN:O	2.09	0.53
1:B:125:LEU:O	1:B:129:ASN:ND2	2.40	0.53
1:H:102:ASN:O	1:H:106:ILE:HG12	2.09	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:A:71:LYS:O	1:A:75:ASN:ND2	2.36	0.53
1:C:505:ARG:NH1	1:C:773:TYR:O	2.42	0.53
1:G:437:ASN:O	1:G:441:THR:HG23	2.09	0.53
1:G:505:ARG:NH1	1:G:773:TYR:O	2.41	0.53
1:A:141:GLN:HG3	1:A:184:ASN:HD22	1.74	0.52
1:G:419:LEU:HD11	1:G:513:THR:HA	1.92	0.52
1:E:793:TYR:O	1:E:796:SER:OG	2.19	0.52
1:G:310:LYS:O	1:G:313:MSE:HG2	2.09	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: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: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:H:107:LEU:O	1:H:111:ARG:HG3	2.09	0.52
1:A:86:LEU:HB3	1:A:93:THR:HG22	1.90	0.52
1:G:145:TYR:HA	1:G:187:LEU:HD13	1.92	0.52
1:C:317:GLN:HE22	1:C:333:LYS:HE2	1.73	0.52
1:G:274:GLN:OE1	1:G:310:LYS:NZ	2.32	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:E:515:GLU:OE1	1:E:536:ARG:NH2	2.39	0.51
1:H:494:GLN:HB3	1:H:518:ILE:HD11	1.92	0.51
1:E:220:LEU:HB3	1:E:272:PHE:CE1	2.46	0.51
1:F:641:TYR:HB2	1:F:651:ALA:HB2	1.93	0.51
1:B:256:PRO:HG3	1:B:262:ASN:HA	1.92	0.51
1:D:123:HIS:CE1	1:D:127:ILE:HD11	2.46	0.51
1:F:588:PHE:HB3	1:F:592:GLU:HG3	1.93	0.51
1:D:92:ILE:O	1:D:96:VAL:HG23	2.11	0.51
1:G:441:THR:O	1:G:445:ILE:HG12	2.11	0.51
1:A:123:HIS:CE1	1:A:127:ILE:HD11	2.46	0.51
1:A:441:THR:O	1:A:445:ILE:HG12	2.10	0.51
1:F:604:TYR:CZ	1:F:630:LEU:HG	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: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:584:ILE:HA	1:F:587:ILE:HG22	1.93	0.50
1:B:337:ILE:HD13	1:B:371:ILE:HD11	1.93	0.50
1:C:270:ASN:O	1:C:274:GLN:HG3	2.11	0.50
1:F:47:LEU:HD22	1:F:76:LEU:HD12	1.94	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:H:250:LEU:HD22	1:H:301:LYS:HD2	1.93	0.50
1:F:70:LEU:HA	1:F:107:LEU:HD13	1.94	0.50
1:G:511:ILE:HD12	1:G:536:ARG:NH2	2.25	0.50
1:B:494:GLN:HB3	1:B:518:ILE:HD11	1.93	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:155:GLY:O	1:H:164:MSE:HG2	2.12	0.50
1:B:487:GLU:OE1	1:B:491:ARG:NH2	2.45	0.50
1:H:270:ASN:O	1:H:274:GLN:HG3	2.12	0.50
1:A:585:GLU:OE2	1:A:643:ARG:HD2	2.11	0.50
1:B:27:ARG:NH1	1:B:52:HIS:HD2	2.07	0.50
1:B:270:ASN:O	1:B:274:GLN:HG3	2.12	0.50
1:C:744:PHE:CZ	1:C:750:ARG:HG3	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:HIS:O	1:D:127:ILE:HG13	2.12	0.50
1:E:546:TYR:HA	1:E:583:LEU:HD13	1.94	0.50
1:F:511:ILE:HG21	1:F:536:ARG:NH2	2.26	0.50
1:G:47:LEU:HD22	1:G:76:LEU:HD12	1.93	0.50
1:G:418:TRP:O	1:G:422:SER:HB3	2.11	0.50
1:H:123:HIS:CE1	1:H:127:ILE:HD11	2.47	0.50
1:D:585:GLU:OE2	1:D:640:MSE:HG3	2.12	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:464:ASN:HA	1:F:467:MSE:HE2	1.93	0.50
1:F:539:GLN:HE22	1:F:544:MSE:HE1	1.77	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:D:545:SER:O	1:D:549:VAL:HG13	2.12	0.49
1:E:418:TRP:O	1:E:422:SER:HB3	2.11	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:A:437:ASN:O	1:A:441:THR:HG23	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:618:MSE:HE1	1:A:817:TYR:HD1	1.78	0.49
1:C:145:TYR:HA	1:C:187:LEU:HD13	1.95	0.49
1:D:13:PRO:HB3	1:D:17:ILE:CD1	2.42	0.49
1:H:310:LYS:NZ	1:H:363:SER:OG	2.38	0.49
1:G:463:CYS:HA	1:G:466:MSE:HE3	1.94	0.49
1:A:684:PRO:HG2	1:A:686:VAL:HG12	1.95	0.49
1:G:295:ILE:HB	1:G:315:LEU:HD23	1.94	0.49
1:H:538:VAL:HG22	1:H:808:PRO:HA	1.94	0.49
1:C:578:LEU:HA	1:C:581:LEU:HD12	1.95	0.49
1:C:792:GLU:HA	1:C:795:ASN:HD21	1.77	0.49
1:F:350:TYR:CZ	1:F:359:ARG:HB3	2.47	0.49
1:A:571:TRP:HH2	1:A:625:THR:O	1.95	0.49
1:B:585:GLU:OE2	1:B:643:ARG:HD2	2.12	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:A:41:LEU:HA	1:A:44:VAL:HG12	1.95	0.48
1:B:515:GLU:HG3	1:B:532:LEU:HD11	1.94	0.48
1:D:203:ILE:HD11	1:D:219:ILE:HG22	1.94	0.48
1:F:123:HIS:O	1:F:127:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:LEU:HD22	1:H:142:TYR:CD2	2.47	0.48
1:H:355:ASP:C	1:H:357:SER:H	2.16	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:D:296:ILE:HA	1:D:299:MSE:HE3	1.93	0.48
1:E:365:ILE:HG23	1:E:394:PHE:HE1	1.78	0.48
1:G:292:TYR:O	1:G:295:ILE:HG22	2.13	0.48
1:G:578:LEU:HD22	1:G:636:PHE:CD2	2.47	0.48
1:A:102:ASN:O	1:A:106:ILE:HG12	2.13	0.48
1:A:270:ASN:HD22	1:A:308:VAL:HG22	1.78	0.48
1:B:581:LEU:HB2	1:B:636:PHE:HE2	1.78	0.48
1:D:97:GLU:HB3	1:D:127:ILE:HD13	1.96	0.48
1:D:270:ASN:O	1:D:274:GLN:HG3	2.13	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:G:98:LYS:HE2	1:G:128:HIS:HA	1.96	0.48
1:H:37:GLY:C	1:H:38:PHE:HD1	2.17	0.48
1:H:173:LEU:HA	1:H:173:LEU:HD23	1.63	0.48
1:H:463:CYS:HA	1:H:466:MSE:HE3	1.94	0.48
1:B:240:ASP:O	1:B:244:LYS:HG3	2.13	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:F:536:ARG:HD3	1:F:544:MSE:HB3	1.95	0.48
1:F:631:GLN:O	1:F:635:ILE:HG12	2.14	0.48
1:G:542:LYS:NZ	1:G:809:ILE:HD11	2.28	0.48
1:A:546:TYR:HA	1:A:583:LEU:HD13	1.95	0.48
1:D:144:ARG:HD2	1:D:187:LEU:HD11	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:E:556:MSE:HE3	1:E:576:LEU:HD22	1.95	0.48
1:E:628:TYR:HE1	1:E:669:ASN:HD21	1.61	0.48
1:C:256:PRO:HG3	1:C:262:ASN:HA	1.94	0.48
1:G:106:ILE:HG23	1:G:153:TYR:CE2	2.48	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:A:516:SER:O	1:A:520:SER:HB2	2.13	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:D:405:TYR:HB2	1:D:407:LEU:HD11	1.95	0.48
1:E:619:GLY:HA3	1:E:624:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:GLN:OE1	1:H:25:ARG:NH1	2.45	0.48
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:C:141:GLN:HG3	1:C:184:ASN:ND2	2.29	0.47
1:C:795:ASN:O	1:C:799:LYS:HD2	2.14	0.47
1:F:585:GLU:OE2	1:F:643:ARG:HD3	2.14	0.47
1:H:425:CYS:HB2	1:H:468:LEU:HD23	1.96	0.47
1:H:597:LEU:O	1:H:600:VAL:HG22	2.13	0.47
1:E:54:HIS:HB3	1:E:61:PRO:HB3	1.97	0.47
1:E:292:TYR:O	1:E:295:ILE:HG22	2.14	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:94:LYS:O	1:H:98:LYS:HG3	2.15	0.47
1:A:36:SER:HB3	1:A:41:LEU:HD23	1.94	0.47
1:E:15:LYS:O	1:E:19:VAL:HG23	2.15	0.47
1:E:41:LEU:HA	1:E:44:VAL:HG12	1.95	0.47
1:G:661:VAL:O	1:G:663:SER:N	2.47	0.47
1:H:635:ILE:HG13	1:H:672:ILE:HD11	1.97	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:D:365:ILE:HG23	1:D:394:PHE:HE1	1.80	0.47
1:F:151:LEU:HD13	1:F:171:GLU:HB2	1.97	0.47
1:G:761:LEU:HD22	1:G:777:VAL:HG13	1.96	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:A:40:SER:OG	1:A:86:LEU:HD21	2.15	0.47
1:A:762:GLU:O	1:A:765:ILE:HG12	2.14	0.47
1:E:700:ASN:CB	1:E:768:SER:HB2	2.45	0.47
1:F:574:ILE:HG13	1:F:629:LEU:HD21	1.96	0.47
1:H:213:THR:HG22	1:H:215:GLU:H	1.79	0.47
1:H:256:PRO:HD3	1:H:301:LYS:O	2.15	0.47
1:B:403:LYS:HD3	1:F:238:ASN:HD21	1.79	0.47
1:D:27:ARG:NH1	1:D:52:HIS:HD2	2.11	0.47
1:D:546:TYR:HA	1:D:583:LEU:HD13	1.96	0.47
1:E:705:LEU:HD11	1:E:760:LEU:HB3	1.96	0.47
1:F:92:ILE:O	1:F:96:VAL:HG23	2.15	0.47
1:F:338:LEU:O	1:F:341:VAL:HG22	2.15	0.47
1:G:270:ASN:O	1:G:274:GLN:HG3	2.14	0.47
1:G:618:MSE:HE1	1:G:817:TYR:HD1	1.78	0.47
1:H:44:VAL:HG22	1:H:100:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:509:THR:O	1:H:513:THR:HG23	2.15	0.47
1:A:288:ASN:OD1	1:A:290:SER:OG	2.22	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:H:627:GLU:O	1:H:631:GLN:HG3	2.15	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:F:621:LYS:O	1:F:625:THR:HG23	2.14	0.47
1:F:651:ALA:O	1:F:655:ILE:HG13	2.15	0.47
1:G:508:GLU:O	1:G:512:LYS:HG3	2.15	0.47
1:H:24:LEU:HD22	1:H:142:TYR:CE2	2.50	0.47
1:B:793:TYR:CZ	1:B:797:LEU:HD11	2.49	0.47
1:C:144:ARG:HD3	1:C:176:VAL:HG12	1.96	0.47
1:C:604:TYR:CE2	1:C:630:LEU:HD13	2.50	0.47
1:D:443:TYR:CE2	1:D:496:LYS:HD3	2.49	0.47
1:E:213:THR:HG22	1:E:215:GLU:H	1.80	0.47
1:E:507:ILE:HD13	1:E:538:VAL:HG21	1.96	0.47
1:F:143:ASP:O	1:F:147:ILE:HG12	2.15	0.47
1:H:122:LEU:HD23	1:H:125:LEU:HD12	1.96	0.47
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:F:668:LEU:HD21	1:F:694:VAL:HG13	1.96	0.46
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:C:76:LEU:O	1:C:80:MSE:HG3	2.16	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:G:171:GLU:OE1	1:G:175:HIS:NE2	2.47	0.46
1:A:425:CYS:HB2	1:A:468:LEU:HD23	1.97	0.46
1:C:488:LYS:HG2	1:C:491:ARG:HH21	1.80	0.46
1:D:372:LEU:HB3	1:D:445:ILE:HD11	1.97	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: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:B:534:LEU:HD23	1:B:812:LEU:HD23	1.96	0.46
1:C:123:HIS:O	1:C:127:ILE:HG13	2.16	0.46
1:F:560:LEU:CD2	1:F:561:GLN:HG3	2.42	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:C:295:ILE:O	1:C:299:MSE:HG3	2.16	0.46
1:C:351:TYR:CE2	1:C:358:HIS:CD2	3.03	0.46
1:D:405:TYR:HB2	1:D:407:LEU:CD1	2.46	0.46
1:E:102:ASN:O	1:E:106:ILE:HG12	2.15	0.46
1:E:803:TYR:HA	1:E:806:LEU:HD12	1.98	0.46
1:F:24:LEU:HD22	1:F:142:TYR:CD2	2.51	0.46
1:H:546:TYR:HA	1:H:583:LEU:HD13	1.97	0.46
1:B:203:ILE:HG22	1:B:214:VAL:HG13	1.96	0.46
1:D:402:TYR:CB	1:D:409:LEU:HD11	2.41	0.46
1:H:220:LEU:HB3	1:H:272:PHE:CE1	2.51	0.46
1:A:144:ARG:O	1:A:148:VAL:HG23	2.16	0.46
1:C:571:TRP:HH2	1:C:625:THR:C	2.19	0.46
1:C:604:TYR:CE2	1:C:630:LEU:HB2	2.51	0.46
1:D:590:THR:HG21	1:D:643:ARG:HB2	1.98	0.46
1:H:678:SER:HB2	1:H:687:ALA:HB2	1.97	0.46
1:A:185:GLY:HA2	1:A:430:ASN:HD21	1.80	0.45
1:E:28:LEU:HD23	1:E:186:LEU:HD12	1.98	0.45
1:F:708:PHE:O	1:F:712:ILE:HD12	2.16	0.45
1:G:313:MSE:HE3	1:G:371:ILE:HD13	1.98	0.45
1:G:419:LEU:HD21	1:G:517:LEU:HG	1.98	0.45
1:H:410:MSE:HG2	1:H:463:CYS:CB	2.46	0.45
1:B:123:HIS:CE1	1:B:127:ILE:HD11	2.51	0.45
1:G:153:TYR:O	1:G:157:VAL:HG23	2.15	0.45
1:G:220:LEU:HB3	1:G:272:PHE:CE1	2.52	0.45
1:H:668:LEU:HD23	1:H:668:LEU:HA	1.82	0.45
1:A:123:HIS:O	1:A:127:ILE:HG13	2.17	0.45
1:A:668:LEU:O	1:A:672:ILE:HG13	2.16	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:627:GLU:O	1:D:631:GLN:HG3	2.17	0.45
1:D:656:LYS:O	1:D:660:ASN:HB2	2.17	0.45
1:D:698:ASP:CB	1:D:701:ASN:HB2	2.47	0.45
1:E:221:PHE:CZ	1:E:225:ILE:HD11	2.52	0.45
1:E:668:LEU:HD11	1:E:694:VAL:HA	1.99	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:H:40:SER:HB3	1:H:96:VAL:HG11	1.98	0.45
1:A:152:TYR:CZ	1:A:193:LEU:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG21	1:A:199:ARG:NH1	2.31	0.45
1:B:143:ASP:O	1:B:147:ILE:HG12	2.16	0.45
1:C:250:LEU:HD23	1:C:250:LEU:HA	1.85	0.45
1:D:12:VAL:HB	1:D:13:PRO:HD3	1.98	0.45
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:E:693:THR:O	1:E:697:TYR:HD1	1.99	0.45
1:F:54:HIS:HB3	1:F:61:PRO:HG3	1.99	0.45
1:F:220:LEU:HB3	1:F:272:PHE:CE1	2.52	0.45
1:A:283:LYS:HG2	1:A:285:ILE:HG23	1.98	0.45
1:B:217:PRO:HB2	1:B:268:HIS:CE1	2.51	0.45
1:B:277:PHE:CZ	1:B:315:LEU:HD13	2.51	0.45
1:B:536:ARG:HA	1:B:536:ARG:HD3	1.81	0.45
1:C:415:SER:HB2	1:C:459:THR:HG22	1.98	0.45
1:D:217:PRO:HB2	1:D:268:HIS:CE1	2.51	0.45
1:E:277:PHE:CZ	1:E:315:LEU:HD13	2.51	0.45
1:E:443:TYR:OH	1:E:447:LYS:NZ	2.46	0.45
1:G:76:LEU:O	1:G:80:MSE:HG2	2.17	0.45
1:H:114:PHE:HB3	1:H:157:VAL:HG13	1.98	0.45
1:H:631:GLN:O	1:H:635:ILE:HG12	2.17	0.45
1:C:94:LYS:O	1:C:98:LYS:HG3	2.17	0.45
1:C:179:ILE:HA	1:C:180:PRO:HD3	1.82	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:F:410:MSE:HE3	1:F:418:TRP:HZ3	1.80	0.45
1:F:635:ILE:O	1:F:639:ASN:ND2	2.47	0.45
1:G:239:ASP:OD2	1:G:276:TYR:OH	2.29	0.45
1:A:25:ARG:NH2	1:A:138:LEU:HD22	2.32	0.45
1:B:64:PRO:O	1:B:68:VAL:HG23	2.17	0.45
1:B:529:TRP:HB3	1:B:552:VAL:HG21	1.99	0.45
1:B:703:ASP:OD1	1:B:703:ASP:N	2.50	0.45
1:C:98:LYS:HE2	1:C:128:HIS:HA	1.99	0.45
1:D:781:LEU:HG	1:D:785:TYR:CE2	2.52	0.45
1:A:418:TRP:O	1:A:422:SER:HB3	2.17	0.45
1:B:27:ARG:HE	1:B:34:PHE:HZ	1.65	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
1:B:514:LEU:HD12	1:B:518:ILE:HD13	1.98	0.45
1:B:672:ILE:HG13	1:B:673:ALA:N	2.31	0.45
1:D:761:LEU:O	1:D:765:ILE:HG12	2.17	0.45
1:E:145:TYR:HA	1:E:187:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:708:PHE:HE2	1:G:757:LEU:HB2	1.82	0.45
1:H:27:ARG:NH1	1:H:52:HIS:HD2	2.10	0.45
1:A:678:SER:HB3	1:A:686:VAL:HG13	1.99	0.45
1:B:443:TYR:HE2	1:B:496:LYS:HD3	1.82	0.45
1:F:634:TRP:HB3	1:F:658:ALA:HB2	1.99	0.45
1:G:793:TYR:O	1:G:796:SER:OG	2.27	0.45
1:C:703:ASP:OD1	1:C:703:ASP:N	2.49	0.44
1:F:224:MSE:HE2	1:F:276:TYR:HA	1.99	0.44
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:B:292:TYR:O	1:B:295:ILE:HG22	2.18	0.44
1:B:542:LYS:O	1:B:546:TYR:HB3	2.17	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: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:E:635:ILE:HD11	1:E:673:ALA:HB2	1.98	0.44
1:G:182:GLU:N	1:G:360:ASP:OD2	2.51	0.44
1:B:373:GLN:NE2	1:B:437:ASN:OD1	2.49	0.44
1:B:399:ASN:OD1	1:F:204:GLN:NE2	2.50	0.44
1:H:28:LEU:HD21	1:H:142:TYR:HD1	1.82	0.44
1:H:514:LEU:HD11	1:H:528:ALA:HB1	2.00	0.44
1:A:173:LEU:HG	1:A:210:PHE:CD1	2.52	0.44
1:B:102:ASN:O	1:B:106:ILE:HG13	2.17	0.44
1:B:165:GLN:O	1:B:169:TYR:HD1	2.00	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:B:566:LEU:HB2	1:B:569:ASP:HB2	2.00	0.44
1:E:304:GLN:HG3	1:E:346:TYR:CE1	2.52	0.44
1:G:604:TYR:CZ	1:G:630:LEU:HB2	2.53	0.44
1:H:556:MSE:SE	1:H:573:PHE:HA	2.67	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: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: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:A:153:TYR:HA	1:A:156:LEU:HB2	2.00	0.44
1:B:70:LEU:HA	1:B:107:LEU:HD13	1.99	0.44
1:C:572:GLN:OE1	1:C:815:CYS:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:514:LEU:HD12	1:H:518:ILE:HG13	1.98	0.44
1:B:416:LEU:HD23	1:B:506:HIS:CD2	2.53	0.44
1:C:153:TYR:HA	1:C:156:LEU:HB2	2.00	0.44
1:E:270:ASN:O	1:E:274:GLN:HG3	2.17	0.44
1:E:441:THR:O	1:E:445:ILE:HG12	2.17	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:G:365:ILE:HG23	1:G:394:PHE:HE1	1.83	0.44
1:H:619:GLY:HA3	1:H:624:GLN:OE1	2.18	0.44
1:B:123:HIS:O	1:B:127:ILE:HG13	2.17	0.43
1:B:566:LEU:HD12	1:B:566:LEU:O	2.19	0.43
1:B:628:TYR:O	1:B:631:GLN:HG2	2.18	0.43
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:D:798:LEU:O	1:D:801:ILE:HG22	2.18	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:E:698:ASP:HB3	1:E:701:ASN:HB2	2.00	0.43
1:F:165:GLN:HE22	1:F:198:LEU:HA	1.83	0.43
1:G:148:VAL:HG21	1:G:187:LEU:HD11	1.99	0.43
1:H:153:TYR:O	1:H:157:VAL:HG23	2.17	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:C:604:TYR:HE2	1:C:630:LEU:HB2	1.84	0.43
1:D:708:PHE:O	1:D:712:ILE:HG12	2.18	0.43
1:F:678:SER:O	1:F:684:PRO:HD2	2.17	0.43
1:A:371:ILE:O	1:A:375:SER:OG	2.20	0.43
1:C:28:LEU:HD23	1:C:186:LEU:HD12	2.00	0.43
1:C:41:LEU:HA	1:C:44:VAL:HG12	2.00	0.43
1:C:792:GLU:HA	1:C:795:ASN:ND2	2.34	0.43
1:E:71:LYS:HE3	1:E:71:LYS:HB3	1.82	0.43
1:G:94:LYS:O	1:G:98:LYS:HG3	2.17	0.43
1:H:89:TYR:O	1:H:93:THR:HG23	2.18	0.43
1:D:48:GLN:NE2	1:D:99:ILE:HG23	2.32	0.43
1:D:89:TYR:HA	1:D:90:PRO:HD3	1.62	0.43
1:H:418:TRP:O	1:H:422:SER:HB3	2.18	0.43
1:B:61:PRO:HD2	1:B:110:HIS:CE1	2.54	0.43
1:C:463:CYS:O	1:C:467:MSE:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LEU:O	1:D:128:HIS:HB3	2.18	0.43
1:E:684:PRO:HB2	1:E:685:GLY:H	1.70	0.43
1:G:52:HIS:HA	1:G:55:VAL:HG22	2.01	0.43
1:G:536:ARG:HD3	1:G:544:MSE:SE	2.69	0.43
1:H:625:THR:HG21	1:H:665:PHE:CE2	2.54	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:A:655:ILE:HD12	1:A:677:LEU:HD22	1.99	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:E:25:ARG:NH2	1:E:357:SER:HB2	2.33	0.43
1:F:173:LEU:HA	1:F:173:LEU:HD23	1.49	0.43
1:H:123:HIS:O	1:H:127:ILE:HG13	2.18	0.43
1:H:575:HIS:O	1:H:810:ARG:NH1	2.51	0.43
1:A:173:LEU:HA	1:A:173:LEU:HD23	1.76	0.43
1:B:419:LEU:HG	1:B:513:THR:HG22	2.01	0.43
1:E:125:LEU:O	1:E:129:ASN:ND2	2.46	0.43
1:F:59:ASN:O	1:F:110:HIS:NE2	2.52	0.43
1:F:398:LEU:HD11	1:F:438:ALA:HB1	2.01	0.43
1:F:453:LEU:HD22	1:F:769:ILE:HD13	2.01	0.43
1:H:89:TYR:CD1	1:H:90:PRO:HD2	2.54	0.43
1:H:578:LEU:HD22	1:H:636:PHE:CD2	2.53	0.43
1:H:594:LEU:HD23	1:H:640:MSE:HE3	2.01	0.43
1:A:508:GLU:O	1:A:512:LYS:HG3	2.18	0.43
1:B:161:ILE:O	1:B:165:GLN:HG3	2.18	0.43
1:C:371:ILE:HD12	1:C:371:ILE:HA	1.91	0.43
1:D:255:PHE:HA	1:D:256:PRO:HD3	1.88	0.43
1:E:708:PHE:CE1	1:E:712:ILE:HD11	2.54	0.43
1:F:102:ASN:O	1:F:106:ILE:HG13	2.18	0.43
1:F:514:LEU:HD22	1:F:528:ALA:HB1	2.00	0.43
1:F:578:LEU:HA	1:F:581:LEU:HD12	2.01	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:H:216:ASN:HA	1:H:217:PRO:HD3	1.90	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:A:793:TYR:CZ	1:A:797:LEU:HD11	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:D:361:ILE:HD12	1:D:361:ILE:H	1.84	0.43
1:F:194:ILE:O	1:F:198:LEU:HG	2.18	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: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
1:F:419:LEU:HD11	1:F:513:THR:HA	2.00	0.43
1:A:292:TYR:O	1:A:295:ILE:HG22	2.19	0.43
1:B:618:MSE:HE1	1:B:817:TYR:CD1	2.51	0.43
1:E:27:ARG:NH1	1:E:52:HIS:HD2	2.12	0.43
1:E:337:ILE:HD11	1:E:379:ASP:HB3	2.01	0.43
1:B:402:TYR:CE1	1:B:435:LEU:HD12	2.54	0.42
1:F:76:LEU:O	1:F:80:MSE:HG2	2.18	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:C:350:TYR:CE1	1:C:359:ARG:HB2	2.54	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:A:288:ASN:HA	1:A:289:PRO:HD3	1.87	0.42
1:B:41:LEU:HD13	1:B:96:VAL:HG22	2.00	0.42
1:D:446:ARG:NH1	1:D:461:TYR:OH	2.53	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:A:180:PRO:HG2	1:A:188:PHE:CE2	2.55	0.42
1:A:494:GLN:HB3	1:A:518:ILE:HG12	2.01	0.42
1:D:77:GLU:HB2	1:D:100:LEU:HD21	2.02	0.42
1:D:604:TYR:CZ	1:D:630:LEU:HB2	2.55	0.42
1:D:743:THR:OG1	1:D:744:PHE:N	2.52	0.42
1:E:291:TRP:O	1:E:294:PHE:HB3	2.19	0.42
1:E:313:MSE:HE3	1:E:371:ILE:HD13	2.01	0.42
1:F:92:ILE:HD12	1:F:92:ILE:H	1.84	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:C:765:ILE:HD11	1:C:781:LEU:HD22	2.01	0.42
1:F:293:ASN:O	1:F:296:ILE:HG22	2.19	0.42
1:F:325:ASP:O	1:F:329:LYS:HG3	2.19	0.42
1:F:809:ILE:HG22	1:F:810:ARG:HG3	2.01	0.42
1:G:14:SER:OG	1:G:15:LYS:N	2.52	0.42
1:G:163:ILE:O	1:G:167:VAL:HG12	2.20	0.42
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.66	0.42
1:E:590:THR:O	1:E:594:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:802:LYS:O	1:E:806:LEU:HG	2.19	0.42
1:F:135:LYS:NZ	1:F:143:ASP:OD2	2.45	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:G:690:GLU:O	1:G:693:THR:OG1	2.32	0.42
1:H:542:LYS:HE2	1:H:809:ILE:HD11	2.00	0.42
1:A:340:PHE:O	1:A:343:PHE:HB3	2.20	0.42
1:C:153:TYR:O	1:C:157:VAL:HG23	2.19	0.42
1:D:94:LYS:O	1:D:98:LYS:HG3	2.20	0.42
1:D:111:ARG:NH1	1:D:113:GLN:OE1	2.51	0.42
1:D:143:ASP:O	1:D:147:ILE:HG12	2.18	0.42
1:G:48:GLN:NE2	1:G:99:ILE:HG23	2.34	0.42
1:H:519:LEU:HD23	1:H:529:TRP:CE2	2.55	0.42
1:A:161:ILE:HD13	1:A:199:ARG:HH12	1.84	0.42
1:F:781:LEU:HG	1:F:785:TYR:CE2	2.53	0.42
1:G:291:TRP:O	1:G:294:PHE:HB3	2.20	0.42
1:H:136:THR:OG1	1:H:139:MSE:HB3	2.20	0.42
1:H:224:MSE:HE2	1:H:276:TYR:HA	2.02	0.42
1:C:513:THR:HG23	1:C:517:LEU:HD12	2.01	0.42
1:D:250:LEU:HD23	1:D:250:LEU:HA	1.87	0.42
1:G:795:ASN:O	1:G:799:LYS:HD2	2.20	0.42
1:A:468:LEU:O	1:A:469:SER:HB2	2.20	0.42
1:A:631:GLN:O	1:A:635:ILE:HG12	2.20	0.42
1:B:450:LEU:HD21	1:B:772:TYR:CD2	2.55	0.42
1:C:310:LYS:NZ	1:C:363:SER:OG	2.40	0.42
1:E:546:TYR:O	1:E:549:VAL:HG22	2.18	0.42
1:F:292:TYR:O	1:F:295:ILE:HG22	2.20	0.42
1:G:543:GLU:HB3	1:G:547:LYS:NZ	2.35	0.42
1:C:221:PHE:CZ	1:C:225:ILE:HD11	2.54	0.41
1:C:270:ASN:OD1	1:C:308:VAL:HG22	2.20	0.41
1:C:361:ILE:H	1:C:361:ILE:HD12	1.84	0.41
1:C:410:MSE:HE2	1:C:410:MSE:HB2	1.78	0.41
1:D:793:TYR:CZ	1:D:797:LEU:HD11	2.55	0.41
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:H:405:TYR:HB2	1:H:407:LEU:HG	2.01	0.41
1:H:746:ASN:O	1:H:750:ARG:HG3	2.20	0.41
1:A:571:TRP:CE3	1:A:629:LEU:HG	2.55	0.41
1:A:712:ILE:HD12	1:A:757:LEU:HG	2.02	0.41
1:B:490:LEU:HD23	1:B:490:LEU:HA	1.84	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:D:153:TYR:O	1:D:157:VAL:HG23	2.20	0.41
1:D:255:PHE:CD1	1:D:256:PRO:HD2	2.55	0.41
1:E:708:PHE:O	1:E:712:ILE:HD12	2.21	0.41
1:F:638:ALA:O	1:F:642:MSE:HG3	2.20	0.41
1:A:495:PHE:CE2	1:A:527:LYS:HE2	2.55	0.41
1:B:712:ILE:O	1:B:750:ARG:NH1	2.53	0.41
1:D:291:TRP:O	1:D:294:PHE:HB3	2.20	0.41
1:E:313:MSE:HE1	1:E:371:ILE:HB	2.03	0.41
1:F:659:SER:HA	1:F:670:CYS:SG	2.60	0.41
1:G:90:PRO:O	1:G:94:LYS:HG3	2.20	0.41
1:A:203:ILE:HG22	1:A:214:VAL:HG23	2.01	0.41
1:A:371:ILE:HD12	1:A:371:ILE:HA	1.91	0.41
1:B:398:LEU:HD11	1:B:438:ALA:HB1	2.02	0.41
1:C:160:ASP:OD1	1:C:161:ILE:N	2.53	0.41
1:C:510:ALA:O	1:C:514:LEU:HB2	2.21	0.41
1:C:639:ASN:O	1:C:643:ARG:HG3	2.20	0.41
1:E:143:ASP:O	1:E:147:ILE:HG13	2.21	0.41
1:E:278:LYS:O	1:E:282:ILE:HG13	2.20	0.41
1:E:280:THR:HG22	1:E:285:ILE:O	2.20	0.41
1:F:340:PHE:O	1:F:344:VAL:HG23	2.20	0.41
1:H:106:ILE:HG23	1:H:153:TYR:CE2	2.56	0.41
1:A:163:ILE:O	1:A:167:VAL:HG12	2.20	0.41
1:B:441:THR:O	1:B:445:ILE:HG13	2.20	0.41
1:C:549:VAL:O	1:C:553:LEU:HB2	2.21	0.41
1:D:107:LEU:O	1:D:111:ARG:HG3	2.20	0.41
1:D:620:PRO:HD2	1:D:624:GLN:NE2	2.36	0.41
1:E:463:CYS:O	1:E:467:MSE:HG3	2.21	0.41
1:E:507:ILE:HD13	1:E:538:VAL:HG11	2.02	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:A:152:TYR:HA	1:A:168:PHE:CE1	2.56	0.41
1:A:350:TYR:CD1	1:A:359:ARG:HG2	2.56	0.41
1:A:571:TRP:CZ3	1:A:629:LEU:HG	2.55	0.41
1:B:161:ILE:HD13	1:B:199:ARG:HH12	1.86	0.41
1:B:371:ILE:O	1:B:375:SER:OG	2.29	0.41
1:B:412:GLN:HG2	1:B:455:SER:O	2.20	0.41
1:B:505:ARG:NE	1:B:773:TYR:HB3	2.35	0.41
1:C:28:LEU:HD22	1:C:184:ASN:OD1	2.21	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:A:398:LEU:HD23	1:A:398:LEU:HA	1.95	0.41
1:C:544:MSE:HE3	1:C:548:ILE:HD11	2.02	0.41
1:C:582:ALA:O	1:C:585:GLU:HB3	2.21	0.41
1:C:760:LEU:HD23	1:C:760:LEU:HA	1.94	0.41
1:D:505:ARG:HB3	1:D:806:LEU:HD13	2.03	0.41
1:D:581:LEU:HD11	1:D:600:VAL:CG2	2.45	0.41
1:E:101:PHE:HA	1:E:104:LEU:HD12	2.02	0.41
1:E:256:PRO:HG2	1:E:262:ASN:OD1	2.20	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:A:341:VAL:HG21	1:A:384:VAL:HG12	2.02	0.41
1:C:372:LEU:HD23	1:C:372:LEU:HA	1.92	0.41
1:E:255:PHE:HA	1:E:256:PRO:HD3	1.84	0.41
1:E:630:LEU:HD23	1:E:630:LEU:HA	1.95	0.41
1:E:702:LEU:O	1:E:706:VAL:HG23	2.20	0.41
1:F:350:TYR:CE1	1:F:359:ARG:HB3	2.56	0.41
1:F:377:LYS:HE2	1:F:388:ASP:OD1	2.21	0.41
1:F:634:TRP:CB	1:F:658:ALA:HB2	2.51	0.41
1:F:695:LEU:CD1	1:F:704:ALA:HB1	2.50	0.41
1:G:51:LEU:O	1:G:55:VAL:HG22	2.20	0.41
1:G:678:SER:CB	1:G:687:ALA:HB2	2.50	0.41
1:H:163:ILE:O	1:H:167:VAL:HG12	2.21	0.41
1:H:179:ILE:HA	1:H:180:PRO:HD3	1.83	0.41
1:H:542:LYS:CE	1:H:809:ILE:HD11	2.51	0.41
1:A:27:ARG:HD3	1:A:48:GLN:NE2	2.30	0.41
1:A:228:PHE:CE1	1:A:279:PHE:HD1	2.39	0.41
1:A:503:GLN:OE1	1:A:769:ILE:HG21	2.20	0.41
1:B:48:GLN:OE1	1:B:145:TYR:OH	2.18	0.41
1:C:216:ASN:HA	1:C:217:PRO:HD3	1.81	0.41
1:C:225:ILE:HG22	1:C:229:GLN:HE21	1.86	0.41
1:D:570:ARG:HB3	1:D:607:LEU:HD22	2.03	0.41
1:E:256:PRO:HG3	1:E:262:ASN:HA	2.03	0.41
1:E:656:LYS:HE3	1:E:656:LYS:HB2	1.87	0.41
1:F:44:VAL:HG21	1:F:96:VAL:CG1	2.49	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: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:B:38:PHE:HD1	1:B:85:GLU:CD	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:GLN:HE22	1:E:333:LYS:HE2	1.86	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
1:F:559:SER:HA	1:F:563:ASN:HB2	2.03	0.40
1:G:425:CYS:HB2	1:G:468:LEU:HD23	2.03	0.40
1:A:700:ASN:HB3	1:A:768:SER:OG	2.21	0.40
1:B:47:LEU:HD21	1:B:73:SER:HB3	2.03	0.40
1:B:514:LEU:HD11	1:B:528:ALA:HB1	2.02	0.40
1:C:345:LYS:HE3	1:C:345:LYS:HB2	1.90	0.40
1:C:652:LYS:HG2	1:C:677:LEU:HD21	2.02	0.40
1:H:25:ARG:HH11	1:H:25:ARG:HD3	1.78	0.40
1:H:48:GLN:NE2	1:H:99:ILE:HG23	2.36	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:20:VAL:O	1:H:24:LEU:HG	2.20	0.40
1:H:80:MSE:HE2	1:H:80:MSE:HB2	1.98	0.40
1:A:107:LEU:O	1:A:111:ARG:HG3	2.21	0.40
1:A:277:PHE:CE2	1:A:315:LEU:HB2	2.57	0.40
1:A:410:MSE:HE3	1:A:463:CYS:SG	2.61	0.40
1:E:63:LYS:HA	1:E:66:CYS:HB2	2.03	0.40
1:E:348:ASP:O	1:E:352:GLN:HG3	2.21	0.40
1:F:288:ASN:HA	1:F:289:PRO:HD3	1.81	0.40
1:F:412:GLN:NE2	1:F:457:ASN:OD1	2.32	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:H:798:LEU:HD23	1:H:798:LEU:HA	1.91	0.40
1:A:341:VAL:HG12	1:A:345:LYS:HE3	2.03	0.40
1:A:505:ARG:HB3	1:A:806:LEU:HD13	2.03	0.40
1:C:507:ILE:HD13	1:C:538:VAL:HG21	2.03	0.40
1:E:412:GLN:O	1:E:415:SER:OG	2.33	0.40
1:G:418:TRP:HE3	1:G:517:LEU:HD11	1.87	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

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%)	48	77
1	E	709/802 (88%)	691 (98%)	18 (2%)	0	100	100
1	F	709/802 (88%)	688 (97%)	20 (3%)	1 (0%)	48	77
1	G	719/802 (90%)	699 (97%)	19 (3%)	1 (0%)	48	77
1	H	718/802 (90%)	700 (98%)	18 (2%)	0	100	100
All	All	5779/6416 (90%)	5624 (97%)	152 (3%)	3 (0%)	48	77

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%)	81	87
1	B	685/724 (95%)	682 (100%)	3 (0%)	89	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	681/724 (94%)	677 (99%)	4 (1%)	84	89
1	D	701/724 (97%)	695 (99%)	6 (1%)	75	84
1	E	671/724 (93%)	664 (99%)	7 (1%)	73	82
1	F	671/724 (93%)	667 (99%)	4 (1%)	84	89
1	G	678/724 (94%)	672 (99%)	6 (1%)	75	84
1	H	678/724 (94%)	670 (99%)	8 (1%)	67	79
All	All	5453/5792 (94%)	5410 (99%)	43 (1%)	79	86

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

Sometimes 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 oligosaccharides 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%)	-0.30	1 (0%) 92 91	26, 69, 112, 156	0
1	B	724/802 (90%)	-0.25	1 (0%) 92 91	35, 67, 107, 142	0
1	C	720/802 (89%)	-0.28	2 (0%) 90 85	30, 68, 106, 140	0
1	D	740/802 (92%)	-0.32	3 (0%) 89 82	27, 61, 102, 144	0
1	E	712/802 (88%)	-0.27	2 (0%) 90 85	30, 62, 101, 131	0
1	F	712/802 (88%)	-0.23	7 (0%) 79 68	25, 69, 117, 155	0
1	G	720/802 (89%)	-0.22	5 (0%) 84 75	27, 75, 116, 144	0
1	H	718/802 (89%)	-0.12	7 (0%) 79 68	34, 77, 126, 152	0
All	All	5774/6416 (89%)	-0.25	28 (0%) 87 80	25, 68, 112, 156	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	669	ASN	4.7
1	H	666	LYS	3.1
1	E	92	ILE	3.0
1	C	667	ASN	2.9
1	H	650	ASP	2.6
1	C	786	GLU	2.5
1	G	607	LEU	2.5
1	F	160	ASP	2.5
1	D	561	GLN	2.4
1	D	560	LEU	2.3
1	G	86	LEU	2.3
1	E	679	ILE	2.3
1	H	673	ALA	2.3
1	G	535	CYS	2.2
1	H	607	LEU	2.2
1	F	469	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	744	PHE	2.2
1	A	667	ASN	2.1
1	H	709	ALA	2.1
1	F	607	LEU	2.1
1	H	257	THR	2.1
1	F	358	HIS	2.1
1	G	358	HIS	2.1
1	H	92	ILE	2.0
1	F	57	GLY	2.0
1	D	86	LEU	2.0
1	F	90	PRO	2.0
1	F	815	CYS	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 monosaccharides 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.