



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2017 – 12:47 PM EST

PDB ID : 5U9O  
Title : Cocystal structure of the intermembrane space region of the plastid division proteins PARC6 and PDV1  
Authors : Delmar, J.A.; Chou, T.H.  
Deposited on : unknown  
Resolution : 3.37 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

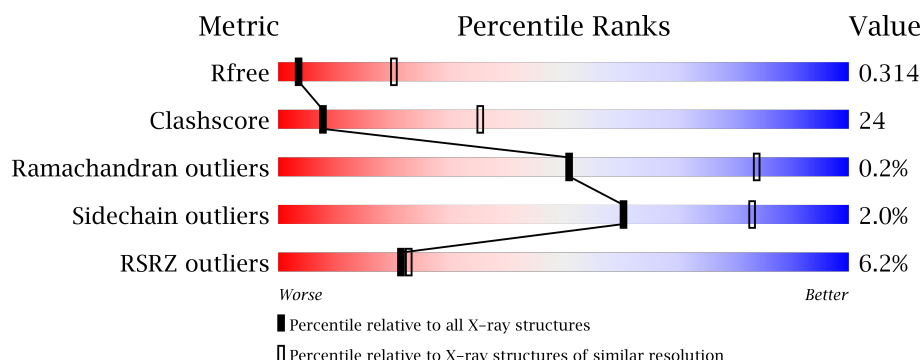
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.37 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))
$R_{free}$	100719	1241 (3.46-3.30)
Clashscore	112137	1319 (3.46-3.30)
Ramachandran outliers	110173	1298 (3.46-3.30)
Sidechain outliers	110143	1297 (3.46-3.30)
RSRZ outliers	101464	1251 (3.46-3.30)

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	187	<div> <div>6%</div> <div>34%</div> <div>41%</div> <div>•</div> <div>22%</div> </div>
1	B	187	<div> <div>3%</div> <div>38%</div> <div>38%</div> <div>•</div> <div>23%</div> </div>
1	C	187	<div> <div>2%</div> <div>39%</div> <div>37%</div> <div>•</div> <div>22%</div> </div>
1	D	187	<div> <div>5%</div> <div>40%</div> <div>37%</div> <div>•</div> <div>22%</div> </div>
1	E	187	<div> <div>5%</div> <div>44%</div> <div>32%</div> <div>•</div> <div>23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	187	<div><div></div><div>6%</div><div>45%</div><div>30%</div><div>•</div><div>24%</div></div>
1	G	187	<div><div></div><div>8%</div><div>37%</div><div>36%</div><div>•</div><div>26%</div></div>
1	H	187	<div><div></div><div>3%</div><div>37%</div><div>37%</div><div>•</div><div>25%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9299 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 Plastid division protein CDP1, chloroplastic, Plastid division protein PDV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1174	745	195	228	6			
1	B	144	Total	C	N	O	S	0	0	0
			1173	745	195	227	6			
1	C	145	Total	C	N	O	S	0	0	0
			1178	747	195	230	6			
1	D	146	Total	C	N	O	S	0	0	0
			1188	755	196	231	6			
1	E	144	Total	C	N	O	S	0	0	0
			1170	744	192	228	6			
1	F	142	Total	C	N	O	S	0	0	0
			1156	734	192	224	6			
1	G	139	Total	C	N	O	S	0	0	0
			1127	716	184	221	6			
1	H	140	Total	C	N	O	S	0	0	0
			1133	721	183	223	6			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	MET	-	initiating methionine	UNP Q8VY16
A	671	GLY	-	expression tag	UNP Q8VY16
A	672	HIS	-	expression tag	UNP Q8VY16
A	673	HIS	-	expression tag	UNP Q8VY16
A	674	HIS	-	expression tag	UNP Q8VY16
A	675	HIS	-	expression tag	UNP Q8VY16
A	676	HIS	-	expression tag	UNP Q8VY16
A	677	HIS	-	expression tag	UNP Q8VY16
A	678	LEU	-	expression tag	UNP Q8VY16
A	679	VAL	-	expression tag	UNP Q8VY16
A	680	PRO	-	expression tag	UNP Q8VY16
A	681	ARG	-	expression tag	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	-	expression tag	UNP Q8VY16
A	683	SER	-	expression tag	UNP Q8VY16
A	820	GLY	-	linker	UNP Q8VY16
A	821	SER	-	linker	UNP Q8VY16
A	822	GLY	-	linker	UNP Q8VY16
A	823	SER	-	linker	UNP Q8VY16
A	824	GLY	-	linker	UNP Q8VY16
A	825	SER	-	linker	UNP Q8VY16
A	826	GLY	-	linker	UNP Q8VY16
A	827	SER	-	linker	UNP Q8VY16
A	828	GLY	-	linker	UNP Q8VY16
A	829	SER	-	linker	UNP Q8VY16
A	830	GLY	-	linker	UNP Q8VY16
A	831	SER	-	linker	UNP Q8VY16
B	670	MET	-	initiating methionine	UNP Q8VY16
B	671	GLY	-	expression tag	UNP Q8VY16
B	672	HIS	-	expression tag	UNP Q8VY16
B	673	HIS	-	expression tag	UNP Q8VY16
B	674	HIS	-	expression tag	UNP Q8VY16
B	675	HIS	-	expression tag	UNP Q8VY16
B	676	HIS	-	expression tag	UNP Q8VY16
B	677	HIS	-	expression tag	UNP Q8VY16
B	678	LEU	-	expression tag	UNP Q8VY16
B	679	VAL	-	expression tag	UNP Q8VY16
B	680	PRO	-	expression tag	UNP Q8VY16
B	681	ARG	-	expression tag	UNP Q8VY16
B	682	GLY	-	expression tag	UNP Q8VY16
B	683	SER	-	expression tag	UNP Q8VY16
B	820	GLY	-	linker	UNP Q8VY16
B	821	SER	-	linker	UNP Q8VY16
B	822	GLY	-	linker	UNP Q8VY16
B	823	SER	-	linker	UNP Q8VY16
B	824	GLY	-	linker	UNP Q8VY16
B	825	SER	-	linker	UNP Q8VY16
B	826	GLY	-	linker	UNP Q8VY16
B	827	SER	-	linker	UNP Q8VY16
B	828	GLY	-	linker	UNP Q8VY16
B	829	SER	-	linker	UNP Q8VY16
B	830	GLY	-	linker	UNP Q8VY16
B	831	SER	-	linker	UNP Q8VY16
C	670	MET	-	initiating methionine	UNP Q8VY16
C	671	GLY	-	expression tag	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
C	672	HIS	-	expression tag	UNP Q8VY16
C	673	HIS	-	expression tag	UNP Q8VY16
C	674	HIS	-	expression tag	UNP Q8VY16
C	675	HIS	-	expression tag	UNP Q8VY16
C	676	HIS	-	expression tag	UNP Q8VY16
C	677	HIS	-	expression tag	UNP Q8VY16
C	678	LEU	-	expression tag	UNP Q8VY16
C	679	VAL	-	expression tag	UNP Q8VY16
C	680	PRO	-	expression tag	UNP Q8VY16
C	681	ARG	-	expression tag	UNP Q8VY16
C	682	GLY	-	expression tag	UNP Q8VY16
C	683	SER	-	expression tag	UNP Q8VY16
C	820	GLY	-	linker	UNP Q8VY16
C	821	SER	-	linker	UNP Q8VY16
C	822	GLY	-	linker	UNP Q8VY16
C	823	SER	-	linker	UNP Q8VY16
C	824	GLY	-	linker	UNP Q8VY16
C	825	SER	-	linker	UNP Q8VY16
C	826	GLY	-	linker	UNP Q8VY16
C	827	SER	-	linker	UNP Q8VY16
C	828	GLY	-	linker	UNP Q8VY16
C	829	SER	-	linker	UNP Q8VY16
C	830	GLY	-	linker	UNP Q8VY16
C	831	SER	-	linker	UNP Q8VY16
D	670	MET	-	initiating methionine	UNP Q8VY16
D	671	GLY	-	expression tag	UNP Q8VY16
D	672	HIS	-	expression tag	UNP Q8VY16
D	673	HIS	-	expression tag	UNP Q8VY16
D	674	HIS	-	expression tag	UNP Q8VY16
D	675	HIS	-	expression tag	UNP Q8VY16
D	676	HIS	-	expression tag	UNP Q8VY16
D	677	HIS	-	expression tag	UNP Q8VY16
D	678	LEU	-	expression tag	UNP Q8VY16
D	679	VAL	-	expression tag	UNP Q8VY16
D	680	PRO	-	expression tag	UNP Q8VY16
D	681	ARG	-	expression tag	UNP Q8VY16
D	682	GLY	-	expression tag	UNP Q8VY16
D	683	SER	-	expression tag	UNP Q8VY16
D	820	GLY	-	linker	UNP Q8VY16
D	821	SER	-	linker	UNP Q8VY16
D	822	GLY	-	linker	UNP Q8VY16
D	823	SER	-	linker	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
D	824	GLY	-	linker	UNP Q8VY16
D	825	SER	-	linker	UNP Q8VY16
D	826	GLY	-	linker	UNP Q8VY16
D	827	SER	-	linker	UNP Q8VY16
D	828	GLY	-	linker	UNP Q8VY16
D	829	SER	-	linker	UNP Q8VY16
D	830	GLY	-	linker	UNP Q8VY16
D	831	SER	-	linker	UNP Q8VY16
E	670	MET	-	initiating methionine	UNP Q8VY16
E	671	GLY	-	expression tag	UNP Q8VY16
E	672	HIS	-	expression tag	UNP Q8VY16
E	673	HIS	-	expression tag	UNP Q8VY16
E	674	HIS	-	expression tag	UNP Q8VY16
E	675	HIS	-	expression tag	UNP Q8VY16
E	676	HIS	-	expression tag	UNP Q8VY16
E	677	HIS	-	expression tag	UNP Q8VY16
E	678	LEU	-	expression tag	UNP Q8VY16
E	679	VAL	-	expression tag	UNP Q8VY16
E	680	PRO	-	expression tag	UNP Q8VY16
E	681	ARG	-	expression tag	UNP Q8VY16
E	682	GLY	-	expression tag	UNP Q8VY16
E	683	SER	-	expression tag	UNP Q8VY16
E	820	GLY	-	linker	UNP Q8VY16
E	821	SER	-	linker	UNP Q8VY16
E	822	GLY	-	linker	UNP Q8VY16
E	823	SER	-	linker	UNP Q8VY16
E	824	GLY	-	linker	UNP Q8VY16
E	825	SER	-	linker	UNP Q8VY16
E	826	GLY	-	linker	UNP Q8VY16
E	827	SER	-	linker	UNP Q8VY16
E	828	GLY	-	linker	UNP Q8VY16
E	829	SER	-	linker	UNP Q8VY16
E	830	GLY	-	linker	UNP Q8VY16
E	831	SER	-	linker	UNP Q8VY16
F	670	MET	-	initiating methionine	UNP Q8VY16
F	671	GLY	-	expression tag	UNP Q8VY16
F	672	HIS	-	expression tag	UNP Q8VY16
F	673	HIS	-	expression tag	UNP Q8VY16
F	674	HIS	-	expression tag	UNP Q8VY16
F	675	HIS	-	expression tag	UNP Q8VY16
F	676	HIS	-	expression tag	UNP Q8VY16
F	677	HIS	-	expression tag	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
F	678	LEU	-	expression tag	UNP Q8VY16
F	679	VAL	-	expression tag	UNP Q8VY16
F	680	PRO	-	expression tag	UNP Q8VY16
F	681	ARG	-	expression tag	UNP Q8VY16
F	682	GLY	-	expression tag	UNP Q8VY16
F	683	SER	-	expression tag	UNP Q8VY16
F	820	GLY	-	linker	UNP Q8VY16
F	821	SER	-	linker	UNP Q8VY16
F	822	GLY	-	linker	UNP Q8VY16
F	823	SER	-	linker	UNP Q8VY16
F	824	GLY	-	linker	UNP Q8VY16
F	825	SER	-	linker	UNP Q8VY16
F	826	GLY	-	linker	UNP Q8VY16
F	827	SER	-	linker	UNP Q8VY16
F	828	GLY	-	linker	UNP Q8VY16
F	829	SER	-	linker	UNP Q8VY16
F	830	GLY	-	linker	UNP Q8VY16
F	831	SER	-	linker	UNP Q8VY16
G	670	MET	-	initiating methionine	UNP Q8VY16
G	671	GLY	-	expression tag	UNP Q8VY16
G	672	HIS	-	expression tag	UNP Q8VY16
G	673	HIS	-	expression tag	UNP Q8VY16
G	674	HIS	-	expression tag	UNP Q8VY16
G	675	HIS	-	expression tag	UNP Q8VY16
G	676	HIS	-	expression tag	UNP Q8VY16
G	677	HIS	-	expression tag	UNP Q8VY16
G	678	LEU	-	expression tag	UNP Q8VY16
G	679	VAL	-	expression tag	UNP Q8VY16
G	680	PRO	-	expression tag	UNP Q8VY16
G	681	ARG	-	expression tag	UNP Q8VY16
G	682	GLY	-	expression tag	UNP Q8VY16
G	683	SER	-	expression tag	UNP Q8VY16
G	820	GLY	-	linker	UNP Q8VY16
G	821	SER	-	linker	UNP Q8VY16
G	822	GLY	-	linker	UNP Q8VY16
G	823	SER	-	linker	UNP Q8VY16
G	824	GLY	-	linker	UNP Q8VY16
G	825	SER	-	linker	UNP Q8VY16
G	826	GLY	-	linker	UNP Q8VY16
G	827	SER	-	linker	UNP Q8VY16
G	828	GLY	-	linker	UNP Q8VY16
G	829	SER	-	linker	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
G	830	GLY	-	linker	UNP Q8VY16
G	831	SER	-	linker	UNP Q8VY16
H	670	MET	-	initiating methionine	UNP Q8VY16
H	671	GLY	-	expression tag	UNP Q8VY16
H	672	HIS	-	expression tag	UNP Q8VY16
H	673	HIS	-	expression tag	UNP Q8VY16
H	674	HIS	-	expression tag	UNP Q8VY16
H	675	HIS	-	expression tag	UNP Q8VY16
H	676	HIS	-	expression tag	UNP Q8VY16
H	677	HIS	-	expression tag	UNP Q8VY16
H	678	LEU	-	expression tag	UNP Q8VY16
H	679	VAL	-	expression tag	UNP Q8VY16
H	680	PRO	-	expression tag	UNP Q8VY16
H	681	ARG	-	expression tag	UNP Q8VY16
H	682	GLY	-	expression tag	UNP Q8VY16
H	683	SER	-	expression tag	UNP Q8VY16
H	820	GLY	-	linker	UNP Q8VY16
H	821	SER	-	linker	UNP Q8VY16
H	822	GLY	-	linker	UNP Q8VY16
H	823	SER	-	linker	UNP Q8VY16
H	824	GLY	-	linker	UNP Q8VY16
H	825	SER	-	linker	UNP Q8VY16
H	826	GLY	-	linker	UNP Q8VY16
H	827	SER	-	linker	UNP Q8VY16
H	828	GLY	-	linker	UNP Q8VY16
H	829	SER	-	linker	UNP Q8VY16
H	830	GLY	-	linker	UNP Q8VY16
H	831	SER	-	linker	UNP Q8VY16







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.23Å 80.19Å 84.07Å 88.36° 80.99° 83.49°	Depositor
Resolution (Å)	38.23 – 3.37 38.23 – 3.37	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.23-3.37) 97.5 (38.23-3.37)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155, Coot	Depositor
R, $R_{free}$	0.250 , 0.318 0.248 , 0.314	Depositor DCC
$R_{free}$ test set	1028 reflections (4.76%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.1	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.40	0/1197	0.64	1/1617 (0.1%)
1	B	0.35	0/1196	0.59	0/1616
1	C	0.44	0/1201	0.57	0/1623
1	D	0.37	0/1210	0.58	0/1634
1	E	0.38	1/1192 (0.1%)	0.55	0/1611
1	F	0.31	0/1179	0.52	0/1593
1	G	0.33	0/1148	0.58	0/1552
1	H	0.34	0/1154	0.53	0/1560
All	All	0.37	1/9477 (0.0%)	0.57	1/12806 (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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	759	GLU	CG-CD	-5.10	1.44	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	759	GLU	OE1-CD-OE2	-5.52	116.67	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	759	GLU	Peptide
1	D	761	GLY	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	1174	0	1139	79	0
1	B	1173	0	1139	66	0
1	C	1178	0	1140	73	0
1	D	1188	0	1160	55	0
1	E	1170	0	1139	45	1
1	F	1156	0	1120	39	1
1	G	1127	0	1093	57	0
1	H	1133	0	1100	70	0
All	All	9299	0	9030	442	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 24.

All (442) 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:684:HIS:HB3	1:A:686:ARG:HH12	1.26	1.00
1:G:796:ILE:HG13	1:G:815:ILE:HG12	1.47	0.96
1:A:684:HIS:HB3	1:A:686:ARG:NH1	1.88	0.87
1:A:789:LYS:HG3	1:G:748:LEU:HA	1.59	0.85
1:E:745:PHE:HB3	1:E:777:ALA:HB2	1.59	0.83
1:C:765:GLU:HG2	1:C:802:LYS:HE2	1.61	0.82
1:B:701:GLU:HG2	1:B:747:LEU:HD22	1.64	0.79
1:B:745:PHE:HZ	1:B:854:ALA:HB1	1.46	0.79
1:A:706:GLU:HB3	1:A:713:GLN:HG3	1.65	0.78
1:A:691:GLU:O	1:A:695:GLU:HG2	1.84	0.77
1:H:815:ILE:HD12	1:H:855:ARG:NH1	1.98	0.77
1:A:692:GLU:O	1:A:696:LEU:HB2	1.85	0.77
1:C:725:MET:SD	1:C:813:SER:OG	2.42	0.77
1:E:701:GLU:HG2	1:E:747:LEU:HD22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:SER:OG	1:B:855:ARG:NH1	2.19	0.76
1:A:700:TRP:NE1	1:A:856:GLY:O	2.19	0.75
1:B:779:LEU:HB2	1:B:851:VAL:HG13	1.69	0.75
1:F:850:ASP:HB3	1:F:853:MET:HG3	1.68	0.75
1:B:787:ASN:ND2	1:C:702:ASN:OD1	2.18	0.74
1:C:769:ILE:HD13	1:C:800:LEU:HD13	1.70	0.73
1:B:710:PRO:HB2	1:C:711:THR:HG23	1.70	0.73
1:A:689:ASP:HB3	1:A:692:GLU:HB2	1.71	0.73
1:A:802:LYS:NZ	1:H:719:GLU:OE1	2.17	0.73
1:C:702:ASN:ND2	1:C:706:GLU:OE1	2.21	0.72
1:D:759:GLU:HB3	1:D:765:GLU:HA	1.71	0.72
1:D:717:LEU:HB3	1:D:721:LEU:HD12	1.70	0.72
1:H:744:ARG:HH12	1:H:780:VAL:HG21	1.54	0.72
1:C:725:MET:HA	1:C:728:GLN:HG3	1.72	0.72
1:H:815:ILE:HD12	1:H:855:ARG:HH11	1.54	0.72
1:C:725:MET:HA	1:C:728:GLN:CG	2.20	0.71
1:G:700:TRP:NE1	1:G:856:GLY:O	2.17	0.71
1:B:763:ALA:HA	1:G:710:PRO:HG2	1.73	0.71
1:C:775:GLU:OE2	1:C:794:TYR:OH	2.06	0.71
1:G:760:ASP:OD1	1:G:761:GLY:N	2.24	0.70
1:D:773:LEU:HD22	1:D:856:GLY:HA2	1.74	0.70
1:E:802:LYS:HZ2	1:E:808:TRP:HE1	1.39	0.70
1:A:713:GLN:OE1	1:A:715:TYR:OH	2.03	0.69
1:A:808:TRP:HB2	1:H:805:ASP:OD2	1.93	0.69
1:B:754:GLN:H	1:B:770:GLU:HB3	1.57	0.69
1:F:714:VAL:HG11	1:F:734:GLN:HG3	1.74	0.69
1:H:701:GLU:OE2	1:H:704:LYS:NZ	2.22	0.68
1:H:700:TRP:CZ3	1:H:721:LEU:HD21	2.29	0.68
1:A:765:GLU:HB3	1:A:802:LYS:HB2	1.76	0.68
1:F:757:ILE:HG22	1:F:759:GLU:OE2	1.94	0.68
1:G:796:ILE:HG23	1:G:798:TYR:CE1	2.29	0.68
1:A:796:ILE:HD11	1:A:813:SER:HB2	1.75	0.67
1:D:725:MET:HE1	1:D:810:PHE:HB3	1.77	0.67
1:E:794:TYR:OH	1:E:856:GLY:N	2.27	0.67
1:H:691:GLU:HA	1:H:694:GLU:HG2	1.76	0.67
1:D:796:ILE:HD11	1:D:813:SER:HB2	1.75	0.67
1:E:711:THR:HG23	1:H:710:PRO:HB2	1.78	0.66
1:A:762:ILE:HG22	1:A:763:ALA:H	1.61	0.66
1:D:817:ILE:HD13	1:D:819:LYS:HD2	1.77	0.66
1:C:800:LEU:HD11	1:C:810:PHE:CD2	2.31	0.65
1:B:697:VAL:O	1:B:700:TRP:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:773:LEU:HD22	1:G:856:GLY:HA2	1.78	0.65
1:A:745:PHE:O	1:G:744:ARG:NH2	2.29	0.65
1:F:754:GLN:NE2	1:F:768:GLU:OE2	2.28	0.65
1:D:688:MET:HB2	1:D:757:ILE:HG13	1.79	0.65
1:D:701:GLU:HG2	1:D:747:LEU:HD22	1.78	0.65
1:A:802:LYS:HA	1:A:807:LEU:O	1.97	0.65
1:B:748:LEU:O	1:C:789:LYS:HD3	1.98	0.64
1:B:781:ASP:OD1	1:B:782:GLU:N	2.30	0.64
1:A:712:HIS:CD2	1:A:737:GLU:HA	2.33	0.64
1:F:698:ARG:HG2	1:F:750:LEU:HD23	1.79	0.63
1:H:744:ARG:NH1	1:H:780:VAL:HG21	2.13	0.63
1:E:689:ASP:HB3	1:E:692:GLU:HB3	1.80	0.63
1:G:686:ARG:NH1	1:G:758:PHE:HD1	1.96	0.63
1:H:717:LEU:HA	1:H:721:LEU:HD23	1.80	0.63
1:D:725:MET:CE	1:D:810:PHE:HB3	2.28	0.62
1:D:698:ARG:HH22	1:F:786:LYS:NZ	1.97	0.62
1:B:779:LEU:HD12	1:B:851:VAL:HA	1.81	0.62
1:H:800:LEU:HB3	1:H:810:PHE:HA	1.82	0.62
1:B:778:GLU:HA	1:B:789:LYS:HA	1.82	0.62
1:G:766:ALA:HA	1:G:801:LYS:HA	1.82	0.62
1:B:694:GLU:HG3	1:B:750:LEU:HD11	1.81	0.61
1:C:698:ARG:HH11	1:C:749:HIS:CE1	2.18	0.61
1:F:765:GLU:OE2	1:F:802:LYS:HB2	2.00	0.61
1:A:807:LEU:HD23	1:A:808:TRP:H	1.65	0.61
1:A:850:ASP:OD1	1:A:851:VAL:N	2.34	0.61
1:H:714:VAL:HG11	1:H:734:GLN:HG3	1.80	0.61
1:H:788:ALA:HB1	1:H:851:VAL:HG11	1.81	0.61
1:C:721:LEU:HD23	1:C:810:PHE:HB2	1.82	0.61
1:E:777:ALA:HB3	1:E:790:TYR:CE2	2.36	0.61
1:G:749:HIS:NE2	1:G:751:GLU:HB2	2.15	0.61
1:C:770:GLU:HG3	1:C:797:ARG:HG2	1.82	0.61
1:D:794:TYR:OH	1:D:856:GLY:N	2.33	0.61
1:A:791:TYR:HB2	1:G:748:LEU:HD21	1.82	0.61
1:A:709:GLY:O	1:A:712:HIS:ND1	2.34	0.60
1:F:699:GLN:O	1:F:703:VAL:N	2.34	0.60
1:D:708:LEU:HB3	1:D:743:TRP:HB2	1.84	0.60
1:A:712:HIS:HD2	1:A:737:GLU:HA	1.67	0.59
1:C:768:GLU:OE2	1:C:797:ARG:HD3	2.03	0.59
1:C:852:MET:SD	1:C:855:ARG:HD2	2.42	0.59
1:C:717:LEU:HB3	1:C:721:LEU:HD12	1.84	0.58
1:C:745:PHE:CZ	1:C:854:ALA:HB1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:786:LYS:HA	1:H:698:ARG:HD2	1.85	0.58
1:D:805:ASP:OD1	1:D:806:GLY:N	2.36	0.58
1:B:710:PRO:HG2	1:C:710:PRO:HG2	1.86	0.58
1:A:800:LEU:O	1:A:801:LYS:HD3	2.02	0.58
1:B:711:THR:HB	1:B:713:GLN:HG3	1.85	0.58
1:C:707:ALA:HA	1:C:713:GLN:O	2.03	0.58
1:G:688:MET:HB2	1:G:757:ILE:HD11	1.85	0.58
1:A:699:GLN:HG3	1:H:806:GLY:HA3	1.86	0.58
1:A:744:ARG:HH21	1:B:762:ILE:HG22	1.69	0.58
1:D:774:GLU:OE2	1:D:791:TYR:OH	2.22	0.57
1:B:701:GLU:OE1	1:B:701:GLU:N	2.37	0.57
1:G:777:ALA:HB3	1:G:790:TYR:CE2	2.40	0.57
1:B:739:LYS:HB3	1:B:741:CYS:SG	2.45	0.57
1:B:770:GLU:OE2	1:B:797:ARG:HG2	2.05	0.57
1:H:794:TYR:OH	1:H:855:ARG:O	2.18	0.57
1:A:799:ILE:O	1:A:811:CYS:N	2.29	0.57
1:G:803:GLN:N	1:G:807:LEU:O	2.38	0.57
1:B:728:GLN:HG2	1:H:759:GLU:HB2	1.85	0.57
1:D:803:GLN:HG3	1:D:804:GLU:N	2.20	0.57
1:A:794:TYR:OH	1:A:856:GLY:N	2.26	0.56
1:C:701:GLU:OE2	1:C:704:LYS:NZ	2.24	0.56
1:A:748:LEU:HD23	1:G:789:LYS:HB3	1.88	0.56
1:G:752:VAL:HG12	1:G:753:LEU:O	2.06	0.56
1:C:725:MET:HG3	1:C:728:GLN:HG3	1.87	0.56
1:H:696:LEU:HD11	1:H:808:TRP:HB3	1.88	0.56
1:B:697:VAL:O	1:B:701:GLU:OE1	2.24	0.55
1:C:686:ARG:HB3	1:C:687:PRO:HD2	1.87	0.55
1:F:694:GLU:HB3	1:F:752:VAL:HG21	1.87	0.55
1:H:770:GLU:HG2	1:H:797:ARG:HG2	1.89	0.55
1:F:721:LEU:HB2	1:F:726:LEU:HD13	1.88	0.55
1:B:729:TRP:CZ2	1:H:762:ILE:HB	2.42	0.55
1:E:708:LEU:HB3	1:E:743:TRP:HB2	1.87	0.55
1:E:697:VAL:HB	1:E:750:LEU:HD11	1.89	0.55
1:B:702:ASN:O	1:B:706:GLU:HG3	2.07	0.55
1:B:728:GLN:HB3	1:H:761:GLY:O	2.06	0.55
1:B:815:ILE:HD11	1:H:762:ILE:HD13	1.89	0.55
1:D:698:ARG:HH22	1:F:786:LYS:HZ1	1.54	0.55
1:A:712:HIS:HE1	1:A:742:TYR:HB3	1.71	0.55
1:D:748:LEU:HD23	1:F:791:TYR:HB2	1.89	0.55
1:G:712:HIS:HB3	1:G:737:GLU:HG3	1.89	0.55
1:H:805:ASP:HB3	1:H:807:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:GLU:HB2	1:C:811:CYS:HB2	1.89	0.55
1:G:756:HIS:C	1:G:757:ILE:HD12	2.27	0.55
1:B:792:SER:HG	1:B:855:ARG:NH1	2.04	0.54
1:E:792:SER:HG	1:E:855:ARG:HH21	1.49	0.54
1:A:722:ASP:OD1	1:A:723:GLU:N	2.36	0.54
1:G:796:ILE:HD11	1:G:813:SER:OG	2.06	0.54
1:C:770:GLU:OE2	1:C:797:ARG:NH1	2.40	0.54
1:C:721:LEU:HB3	1:C:726:LEU:HA	1.90	0.54
1:G:781:ASP:HB3	1:G:783:SER:O	2.08	0.54
1:A:687:PRO:HD2	1:E:782:GLU:HB2	1.88	0.54
1:G:721:LEU:HD22	1:G:725:MET:HB3	1.89	0.54
1:F:779:LEU:HB3	1:F:851:VAL:HG22	1.90	0.54
1:A:713:GLN:HB2	1:A:716:SER:HB3	1.89	0.53
1:F:767:ALA:HB3	1:F:800:LEU:HB2	1.89	0.53
1:G:747:LEU:HD13	1:G:775:GLU:HB3	1.91	0.53
1:A:710:PRO:HD3	1:A:742:TYR:CD1	2.44	0.53
1:B:776:ALA:O	1:C:746:VAL:HG21	2.09	0.53
1:G:686:ARG:HB2	1:G:757:ILE:O	2.09	0.53
1:A:799:ILE:HB	1:A:812:GLN:HG2	1.89	0.53
1:C:725:MET:HA	1:C:728:GLN:HG2	1.91	0.53
1:F:805:ASP:OD1	1:F:806:GLY:N	2.36	0.53
1:A:688:MET:HG3	1:A:757:ILE:HD11	1.90	0.53
1:B:803:GLN:HB3	1:B:805:ASP:OD1	2.08	0.53
1:E:704:LYS:HD2	1:E:854:ALA:HB1	1.89	0.53
1:G:760:ASP:H	1:G:765:GLU:HA	1.73	0.53
1:A:801:LYS:O	1:A:808:TRP:HA	2.09	0.53
1:G:853:MET:HA	1:G:855:ARG:NH1	2.23	0.53
1:C:849:LEU:HD22	1:C:853:MET:HG3	1.92	0.52
1:A:799:ILE:HG22	1:A:811:CYS:HB3	1.91	0.52
1:F:736:ALA:HB1	1:F:741:CYS:O	2.10	0.52
1:F:701:GLU:OE2	1:F:773:LEU:HD22	2.09	0.52
1:H:720:VAL:HG22	1:H:810:PHE:HD1	1.75	0.52
1:D:790:TYR:HD2	1:D:851:VAL:HB	1.74	0.52
1:E:805:ASP:OD1	1:E:805:ASP:N	2.41	0.52
1:G:703:VAL:HG21	1:G:720:VAL:HG11	1.90	0.52
1:G:801:LYS:HG2	1:G:811:CYS:SG	2.49	0.52
1:C:762:ILE:HG23	1:C:763:ALA:H	1.73	0.52
1:C:784:GLN:NE2	1:C:786:LYS:O	2.43	0.52
1:E:850:ASP:O	1:E:853:MET:HG2	2.10	0.52
1:C:758:PHE:HE2	1:C:768:GLU:HB2	1.75	0.51
1:D:710:PRO:HD3	1:D:742:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:710:PRO:HG2	1:H:710:PRO:HG2	1.91	0.51
1:H:741:CYS:HB3	1:H:779:LEU:HD11	1.91	0.51
1:G:699:GLN:O	1:G:703:VAL:HG23	2.11	0.51
1:H:812:GLN:HG2	1:H:813:SER:N	2.24	0.51
1:F:689:ASP:HB3	1:F:692:GLU:HB3	1.93	0.51
1:C:700:TRP:NE1	1:C:856:GLY:O	2.44	0.51
1:D:713:GLN:O	1:D:716:SER:OG	2.27	0.51
1:A:744:ARG:NH2	1:B:762:ILE:HG22	2.25	0.51
1:C:790:TYR:OH	1:C:855:ARG:HG3	2.11	0.51
1:D:793:THR:HG22	1:D:818:GLN:OE1	2.10	0.50
1:A:708:LEU:HD23	1:A:854:ALA:HB2	1.93	0.50
1:D:807:LEU:H	1:D:807:LEU:HD23	1.75	0.50
1:D:777:ALA:HB3	1:D:790:TYR:CE2	2.45	0.50
1:D:797:ARG:NH1	1:D:812:GLN:OE1	2.44	0.50
1:F:797:ARG:CZ	1:F:799:ILE:HD11	2.41	0.50
1:A:717:LEU:HD13	1:A:730:GLN:HA	1.92	0.50
1:A:778:GLU:HA	1:A:789:LYS:HA	1.92	0.50
1:G:742:TYR:CZ	1:G:780:VAL:HG11	2.46	0.50
1:B:722:ASP:O	1:B:811:CYS:HA	2.10	0.50
1:F:803:GLN:HG2	1:F:804:GLU:OE1	2.11	0.50
1:B:777:ALA:HB3	1:B:790:TYR:CE2	2.46	0.50
1:G:703:VAL:HG13	1:G:716:SER:HB3	1.93	0.50
1:B:779:LEU:HD11	1:B:849:LEU:CD1	2.42	0.50
1:D:691:GLU:N	1:D:691:GLU:OE2	2.44	0.50
1:D:796:ILE:HD13	1:D:856:GLY:HA3	1.94	0.50
1:G:853:MET:HA	1:G:855:ARG:HH12	1.76	0.50
1:F:739:LYS:NZ	1:F:848:HIS:HB2	2.27	0.49
1:B:751:GLU:HG2	1:B:753:LEU:HD23	1.94	0.49
1:B:796:ILE:HD13	1:B:798:TYR:CZ	2.47	0.49
1:D:803:GLN:HG3	1:D:804:GLU:H	1.77	0.49
1:F:704:LYS:HZ3	1:F:856:GLY:N	2.09	0.49
1:A:697:VAL:O	1:A:700:TRP:N	2.45	0.49
1:E:686:ARG:HB3	1:E:757:ILE:O	2.13	0.49
1:H:802:LYS:HB2	1:H:808:TRP:CZ3	2.47	0.49
1:A:755:ALA:HA	1:A:769:ILE:HG22	1.94	0.49
1:H:688:MET:HE1	1:H:767:ALA:HB1	1.93	0.49
1:D:776:ALA:HB2	1:D:791:TYR:HD1	1.77	0.49
1:G:762:ILE:HG22	1:G:763:ALA:N	2.27	0.49
1:A:702:ASN:O	1:A:706:GLU:HG3	2.12	0.49
1:C:739:LYS:HZ1	1:C:847:ASP:HB2	1.78	0.49
1:C:743:TRP:NE1	1:C:854:ALA:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:742:TYR:O	1:G:780:VAL:HG12	2.13	0.49
1:C:698:ARG:NH1	1:C:749:HIS:CE1	2.81	0.49
1:C:790:TYR:CZ	1:C:855:ARG:HG3	2.48	0.49
1:H:726:LEU:O	1:H:730:GLN:HB2	2.12	0.49
1:B:695:GLU:O	1:B:699:GLN:HB2	2.12	0.49
1:C:739:LYS:NZ	1:C:847:ASP:HB2	2.28	0.49
1:B:728:GLN:HA	1:H:759:GLU:O	2.13	0.49
1:H:725:MET:CE	1:H:813:SER:HB3	2.42	0.49
1:G:704:LYS:NZ	1:G:745:PHE:CZ	2.81	0.49
1:C:736:ALA:HB1	1:C:741:CYS:O	2.13	0.48
1:G:790:TYR:OH	1:G:854:ALA:O	2.25	0.48
1:H:774:GLU:HG3	1:H:793:THR:HB	1.95	0.48
1:C:772:LEU:HD21	1:C:793:THR:HG22	1.94	0.48
1:H:775:GLU:OE2	1:H:794:TYR:OH	2.32	0.48
1:H:798:TYR:HA	1:H:813:SER:HB2	1.96	0.48
1:D:699:GLN:O	1:D:703:VAL:HG13	2.13	0.48
1:C:799:ILE:C	1:C:800:LEU:HD12	2.34	0.48
1:D:748:LEU:CD2	1:F:791:TYR:HB2	2.44	0.48
1:E:691:GLU:O	1:E:695:GLU:HG2	2.13	0.48
1:G:700:TRP:CZ3	1:G:721:LEU:HD11	2.49	0.48
1:A:748:LEU:HB2	1:A:774:GLU:HG2	1.95	0.48
1:D:690:THR:OG1	1:D:691:GLU:OE2	2.32	0.48
1:B:688:MET:HB3	1:B:755:ALA:HB1	1.95	0.48
1:E:743:TRP:CZ2	1:E:853:MET:HB2	2.48	0.48
1:E:767:ALA:O	1:E:799:ILE:HA	2.13	0.48
1:C:709:GLY:O	1:C:712:HIS:N	2.31	0.48
1:B:745:PHE:CZ	1:B:854:ALA:HB1	2.37	0.47
1:E:799:ILE:HD11	1:E:812:GLN:HB3	1.96	0.47
1:G:692:GLU:O	1:G:696:LEU:HG	2.14	0.47
1:H:707:ALA:HA	1:H:713:GLN:O	2.14	0.47
1:E:719:GLU:O	1:E:809:LYS:HE2	2.14	0.47
1:G:757:ILE:HG13	1:G:767:ALA:CB	2.44	0.47
1:D:710:PRO:HA	1:D:712:HIS:CE1	2.49	0.47
1:F:803:GLN:OE1	1:F:805:ASP:HB3	2.13	0.47
1:A:747:LEU:HD13	1:A:775:GLU:HB3	1.97	0.47
1:C:688:MET:HB3	1:C:755:ALA:HB1	1.96	0.47
1:D:704:LYS:HE3	1:D:745:PHE:CZ	2.48	0.47
1:D:720:VAL:HG12	1:D:810:PHE:CD1	2.50	0.47
1:D:748:LEU:HD22	1:D:791:TYR:HE1	1.80	0.47
1:A:804:GLU:OE1	1:A:804:GLU:N	2.47	0.47
1:D:787:ASN:OD1	1:D:789:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:688:MET:HB3	1:E:755:ALA:C	2.34	0.47
1:B:800:LEU:HG	1:B:810:PHE:HA	1.97	0.47
1:F:694:GLU:HB3	1:F:752:VAL:CG2	2.45	0.47
1:B:724:SER:OG	1:B:811:CYS:O	2.32	0.47
1:D:742:TYR:OH	1:D:744:ARG:NH2	2.47	0.47
1:A:717:LEU:O	1:A:721:LEU:HB2	2.14	0.47
1:B:699:GLN:O	1:B:703:VAL:HG23	2.15	0.47
1:E:802:LYS:HD2	1:E:808:TRP:CZ2	2.49	0.47
1:H:731:THR:O	1:H:735:THR:N	2.47	0.47
1:H:746:VAL:HG12	1:H:748:LEU:HD12	1.97	0.47
1:E:724:SER:O	1:E:728:GLN:HG3	2.15	0.47
1:B:792:SER:HG	1:B:794:TYR:HD1	1.61	0.46
1:A:711:THR:HB	1:A:713:GLN:NE2	2.31	0.46
1:C:763:ALA:HB1	1:C:801:LYS:HE3	1.98	0.46
1:D:748:LEU:N	1:D:774:GLU:O	2.43	0.46
1:D:817:ILE:O	1:D:817:ILE:HD12	2.15	0.46
1:C:767:ALA:O	1:C:799:ILE:HA	2.15	0.46
1:A:854:ALA:O	1:A:855:ARG:HG3	2.15	0.46
1:E:694:GLU:OE1	1:E:698:ARG:HG3	2.16	0.46
1:H:781:ASP:OD1	1:H:783:SER:OG	2.30	0.46
1:D:723:GLU:HB2	1:D:811:CYS:HB3	1.97	0.46
1:C:773:LEU:HD12	1:C:796:ILE:HG21	1.98	0.46
1:D:698:ARG:HG3	1:D:750:LEU:HD23	1.96	0.46
1:G:722:ASP:O	1:G:811:CYS:HA	2.16	0.46
1:H:802:LYS:NZ	1:H:808:TRP:NE1	2.64	0.46
1:B:724:SER:O	1:B:728:GLN:HG3	2.16	0.46
1:E:725:MET:O	1:E:729:TRP:HD1	1.99	0.46
1:H:700:TRP:CH2	1:H:704:LYS:HB2	2.51	0.46
1:B:709:GLY:HA2	1:B:742:TYR:HB2	1.98	0.46
1:F:790:TYR:HD2	1:F:851:VAL:HG12	1.81	0.46
1:G:712:HIS:CE1	1:G:742:TYR:HB3	2.51	0.46
1:H:792:SER:HB3	1:H:794:TYR:CD1	2.51	0.46
1:C:702:ASN:O	1:C:706:GLU:HG3	2.15	0.46
1:D:720:VAL:HG12	1:D:810:PHE:HD1	1.81	0.46
1:D:704:LYS:HD2	1:D:729:TRP:CZ3	2.51	0.46
1:G:706:GLU:HB3	1:G:713:GLN:OE1	2.15	0.46
1:F:750:LEU:HD13	1:F:773:LEU:HD23	1.98	0.45
1:F:723:GLU:OE2	1:F:801:LYS:HE3	2.17	0.45
1:G:708:LEU:HB3	1:G:743:TRP:HB2	1.98	0.45
1:A:720:VAL:HG23	1:A:721:LEU:HD13	1.98	0.45
1:E:748:LEU:HD12	1:E:791:TYR:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:795:LYS:HE2	1:F:816:GLN:HG3	1.99	0.45
1:A:779:LEU:HB3	1:A:851:VAL:HG22	1.98	0.45
1:H:802:LYS:HB2	1:H:808:TRP:CH2	2.52	0.45
1:C:850:ASP:OD1	1:C:851:VAL:N	2.47	0.45
1:E:721:LEU:HD23	1:E:810:PHE:HB2	1.97	0.45
1:C:725:MET:N	1:C:811:CYS:O	2.49	0.45
1:F:756:HIS:HB2	1:F:758:PHE:HE1	1.81	0.45
1:H:850:ASP:OD1	1:H:851:VAL:N	2.50	0.45
1:H:852:MET:O	1:H:855:ARG:HG3	2.16	0.45
1:B:849:LEU:HD13	1:B:850:ASP:N	2.32	0.45
1:C:686:ARG:HB3	1:C:687:PRO:CD	2.46	0.45
1:C:755:ALA:HA	1:C:768:GLU:O	2.16	0.45
1:A:789:LYS:HG3	1:G:748:LEU:CA	2.38	0.45
1:C:758:PHE:CE2	1:C:768:GLU:HB2	2.52	0.45
1:A:715:TYR:CE2	1:B:797:ARG:HD2	2.52	0.45
1:C:812:GLN:HG2	1:C:813:SER:N	2.32	0.45
1:D:722:ASP:O	1:D:811:CYS:HA	2.17	0.45
1:A:740:SER:O	1:A:740:SER:OG	2.35	0.44
1:D:805:ASP:CG	1:D:806:GLY:H	2.20	0.44
1:E:703:VAL:HG11	1:E:720:VAL:HG22	1.99	0.44
1:E:698:ARG:HG2	1:E:750:LEU:HD13	1.98	0.44
1:A:720:VAL:O	1:A:810:PHE:N	2.44	0.44
1:D:770:GLU:HA	1:D:797:ARG:HA	1.99	0.44
1:B:721:LEU:HD22	1:B:725:MET:HG2	1.99	0.44
1:F:722:ASP:OD1	1:F:723:GLU:N	2.50	0.44
1:F:750:LEU:HD12	1:F:751:GLU:N	2.32	0.44
1:A:710:PRO:HG3	1:B:761:GLY:N	2.33	0.44
1:B:686:ARG:HB3	1:B:687:PRO:HD3	2.00	0.44
1:B:686:ARG:O	1:B:756:HIS:HA	2.18	0.44
1:H:721:LEU:HD13	1:H:810:PHE:HB2	1.98	0.44
1:B:801:LYS:HG3	1:B:811:CYS:SG	2.58	0.44
1:H:777:ALA:HB3	1:H:790:TYR:CE2	2.52	0.44
1:A:777:ALA:HB3	1:A:790:TYR:CE2	2.52	0.44
1:B:853:MET:HG2	1:B:853:MET:H	1.56	0.44
1:E:723:GLU:OE2	1:E:801:LYS:HD2	2.18	0.44
1:H:688:MET:HB3	1:H:755:ALA:HB1	2.00	0.44
1:A:736:ALA:HB1	1:A:741:CYS:O	2.18	0.43
1:F:712:HIS:CE1	1:F:742:TYR:HB3	2.53	0.43
1:A:788:ALA:HB3	1:A:851:VAL:HG21	1.99	0.43
1:G:739:LYS:HB3	1:G:741:CYS:SG	2.58	0.43
1:G:756:HIS:N	1:G:768:GLU:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LEU:HD12	1:B:770:GLU:HG3	1.99	0.43
1:F:759:GLU:OE1	1:F:765:GLU:HG2	2.18	0.43
1:F:701:GLU:OE1	1:F:747:LEU:HB2	2.18	0.43
1:A:744:ARG:NH1	1:B:761:GLY:HA3	2.33	0.43
1:C:698:ARG:HH12	1:C:749:HIS:CD2	2.36	0.43
1:D:812:GLN:HG2	1:D:813:SER:N	2.33	0.43
1:G:757:ILE:HG13	1:G:767:ALA:HB2	1.99	0.43
1:G:774:GLU:HB2	1:G:793:THR:HG23	2.00	0.43
1:H:725:MET:HE3	1:H:813:SER:HB3	1.99	0.43
1:H:767:ALA:HB3	1:H:800:LEU:HD11	1.99	0.43
1:A:699:GLN:CG	1:H:806:GLY:HA3	2.49	0.43
1:E:745:PHE:HB3	1:E:777:ALA:CB	2.38	0.43
1:E:803:GLN:HE22	1:E:809:LYS:HZ3	1.66	0.43
1:C:748:LEU:HD23	1:C:748:LEU:HA	1.71	0.43
1:C:758:PHE:N	1:C:766:ALA:O	2.33	0.43
1:H:694:GLU:HG3	1:H:695:GLU:N	2.34	0.43
1:B:709:GLY:CA	1:B:742:TYR:HB2	2.49	0.43
1:C:783:SER:HA	1:D:687:PRO:HG2	2.01	0.43
1:E:799:ILE:HG13	1:E:811:CYS:SG	2.58	0.43
1:G:851:VAL:HG12	1:G:852:MET:N	2.34	0.43
1:H:725:MET:HG3	1:H:729:TRP:CD1	2.54	0.43
1:B:707:ALA:HA	1:B:713:GLN:O	2.19	0.43
1:H:697:VAL:HG22	1:H:810:PHE:HZ	1.82	0.43
1:A:725:MET:HB2	1:A:812:GLN:HA	2.01	0.43
1:B:700:TRP:HA	1:B:720:VAL:HG21	2.00	0.43
1:E:751:GLU:HB3	1:E:772:LEU:HB3	2.01	0.43
1:F:750:LEU:HD13	1:F:773:LEU:CD2	2.49	0.43
1:B:731:THR:HG21	1:H:758:PHE:HB2	2.01	0.42
1:B:732:LEU:HB2	1:H:761:GLY:N	2.33	0.42
1:C:767:ALA:HB3	1:C:800:LEU:HB2	2.00	0.42
1:E:773:LEU:HD13	1:E:856:GLY:HA2	2.00	0.42
1:F:803:GLN:OE1	1:F:807:LEU:HD23	2.18	0.42
1:A:808:TRP:CB	1:H:805:ASP:OD2	2.63	0.42
1:H:717:LEU:HB3	1:H:726:LEU:HD13	2.02	0.42
1:H:743:TRP:HD1	1:H:777:ALA:HB1	1.84	0.42
1:H:796:ILE:HD12	1:H:815:ILE:HG22	2.02	0.42
1:H:769:ILE:HD11	1:H:800:LEU:HD21	2.01	0.42
1:A:786:LYS:HD2	1:A:786:LYS:HA	1.89	0.42
1:C:705:ALA:O	1:C:709:GLY:N	2.52	0.42
1:A:701:GLU:OE2	1:A:856:GLY:O	2.37	0.42
1:A:741:CYS:SG	1:A:849:LEU:HD12	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:GLN:OE1	1:B:784:GLN:N	2.38	0.42
1:A:774:GLU:HG3	1:A:793:THR:HG22	2.02	0.42
1:C:698:ARG:NH1	1:C:749:HIS:NE2	2.67	0.42
1:C:745:PHE:CE1	1:C:854:ALA:HB1	2.54	0.42
1:D:753:LEU:HD21	1:D:772:LEU:HB2	2.01	0.42
1:C:772:LEU:HD23	1:C:795:LYS:HG3	2.00	0.42
1:D:726:LEU:O	1:D:730:GLN:N	2.50	0.42
1:F:748:LEU:HA	1:F:748:LEU:HD23	1.82	0.42
1:A:708:LEU:HD12	1:A:733:ALA:HB2	2.02	0.42
1:C:721:LEU:HD22	1:C:725:MET:HG2	2.01	0.42
1:C:800:LEU:HD11	1:C:810:PHE:CE2	2.54	0.42
1:D:694:GLU:OE2	1:D:698:ARG:NE	2.53	0.42
1:E:722:ASP:OD1	1:E:723:GLU:N	2.52	0.42
1:F:694:GLU:O	1:F:698:ARG:N	2.34	0.42
1:H:721:LEU:HD12	1:H:725:MET:HG2	2.00	0.42
1:B:791:TYR:HB2	1:C:748:LEU:HD21	2.02	0.41
1:E:739:LYS:HB3	1:E:739:LYS:HE2	1.79	0.41
1:G:757:ILE:N	1:G:757:ILE:HD12	2.35	0.41
1:B:729:TRP:HZ2	1:H:762:ILE:HB	1.82	0.41
1:H:800:LEU:HD13	1:H:808:TRP:CE3	2.55	0.41
1:B:746:VAL:HG21	1:C:777:ALA:HA	2.01	0.41
1:E:722:ASP:O	1:E:811:CYS:HA	2.20	0.41
1:A:800:LEU:C	1:A:801:LYS:HD3	2.40	0.41
1:G:688:MET:HB2	1:G:757:ILE:CD1	2.50	0.41
1:A:807:LEU:HD23	1:A:808:TRP:N	2.32	0.41
1:D:739:LYS:HG2	1:D:849:LEU:HD23	2.03	0.41
1:G:753:LEU:HB2	1:G:770:GLU:HB3	2.03	0.41
1:A:759:GLU:OE2	1:A:762:ILE:O	2.37	0.41
1:C:790:TYR:OH	1:C:855:ARG:CG	2.68	0.41
1:D:729:TRP:HH2	1:D:855:ARG:H	1.68	0.41
1:E:803:GLN:HE22	1:E:809:LYS:NZ	2.18	0.41
1:G:698:ARG:HG2	1:G:750:LEU:HD13	2.03	0.41
1:G:721:LEU:HD13	1:G:725:MET:O	2.21	0.41
1:C:713:GLN:OE1	1:C:715:TYR:OH	2.31	0.41
1:A:732:LEU:HD11	1:A:743:TRP:CH2	2.56	0.41
1:E:686:ARG:HA	1:E:686:ARG:HD3	1.66	0.41
1:A:777:ALA:O	1:A:790:TYR:N	2.54	0.41
1:E:792:SER:HG	1:E:794:TYR:HD1	1.69	0.41
1:G:790:TYR:CD2	1:G:852:MET:HB3	2.56	0.41
1:B:746:VAL:HG23	1:C:746:VAL:HG23	2.02	0.41
1:C:743:TRP:CD1	1:C:854:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:802:LYS:HB2	1:E:808:TRP:CH2	2.56	0.41
1:C:796:ILE:HD12	1:C:856:GLY:HA2	2.02	0.40
1:A:712:HIS:HD2	1:A:737:GLU:CA	2.33	0.40
1:A:725:MET:O	1:A:729:TRP:HD1	2.04	0.40
1:B:754:GLN:N	1:B:770:GLU:HB3	2.30	0.40
1:E:802:LYS:HG2	1:E:806:GLY:HA2	2.02	0.40
1:A:688:MET:HG2	1:A:692:GLU:OE1	2.21	0.40
1:A:696:LEU:O	1:A:699:GLN:HB2	2.22	0.40
1:D:700:TRP:NE1	1:D:856:GLY:O	2.46	0.40
1:H:718:SER:O	1:H:809:LYS:NZ	2.54	0.40
1:A:791:TYR:HB2	1:G:748:LEU:CD2	2.50	0.40
1:C:745:PHE:HZ	1:C:854:ALA:HB1	1.86	0.40
1:G:686:ARG:NH1	1:G:686:ARG:HB3	2.37	0.40
1:H:696:LEU:HD22	1:H:810:PHE:CE1	2.56	0.40
1:H:800:LEU:HD23	1:H:810:PHE:CE2	2.57	0.40
1:H:788:ALA:CB	1:H:851:VAL:HG21	2.51	0.40
1:D:769:ILE:O	1:D:798:TYR:N	2.45	0.40
1:H:813:SER:OG	1:H:814:ASP:N	2.54	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:E:719:GLU:OE2	1:F:686:ARG:NH1[1_664]	2.11	0.09

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	141/187 (75%)	133 (94%)	7 (5%)	1 (1%)	25 64
1	B	140/187 (75%)	138 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	141/187 (75%)	136 (96%)	5 (4%)	0	100	100
1	D	142/187 (76%)	136 (96%)	6 (4%)	0	100	100
1	E	140/187 (75%)	137 (98%)	3 (2%)	0	100	100
1	F	138/187 (74%)	134 (97%)	4 (3%)	0	100	100
1	G	135/187 (72%)	129 (96%)	5 (4%)	1 (1%)	25	64
1	H	136/187 (73%)	131 (96%)	5 (4%)	0	100	100
All	All	1113/1496 (74%)	1074 (96%)	37 (3%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	762	ILE
1	G	762	ILE

### 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	124/157 (79%)	120 (97%)	4 (3%)	44	76
1	B	124/157 (79%)	121 (98%)	3 (2%)	54	80
1	C	125/157 (80%)	122 (98%)	3 (2%)	54	80
1	D	126/157 (80%)	123 (98%)	3 (2%)	54	80
1	E	124/157 (79%)	122 (98%)	2 (2%)	68	85
1	F	122/157 (78%)	119 (98%)	3 (2%)	53	80
1	G	119/157 (76%)	118 (99%)	1 (1%)	85	93
1	H	120/157 (76%)	119 (99%)	1 (1%)	85	93
All	All	984/1256 (78%)	964 (98%)	20 (2%)	60	83

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	686	ARG
1	A	726	LEU
1	A	789	LYS
1	A	808	TRP
1	B	789	LYS
1	B	790	TYR
1	B	848	HIS
1	C	728	GLN
1	C	765	GLU
1	C	790	TYR
1	D	689	ASP
1	D	743	TRP
1	D	786	LYS
1	E	745	PHE
1	E	789	LYS
1	F	743	TRP
1	F	790	TYR
1	F	808	TRP
1	G	743	TRP
1	H	743	TRP

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

Mol	Chain	Res	Type
1	A	699	GLN
1	F	754	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	145/187 (77%)	0.35	11 (7%) 15 16	28, 48, 99, 134	0
1	B	144/187 (77%)	0.24	5 (3%) 44 45	30, 45, 77, 99	0
1	C	145/187 (77%)	0.18	4 (2%) 53 55	34, 48, 66, 88	0
1	D	146/187 (78%)	0.40	9 (6%) 21 23	30, 52, 86, 106	0
1	E	144/187 (77%)	0.38	9 (6%) 21 22	44, 58, 82, 97	0
1	F	142/187 (75%)	0.54	12 (8%) 11 13	32, 58, 86, 115	0
1	G	139/187 (74%)	0.73	15 (10%) 6 7	39, 64, 91, 122	0
1	H	140/187 (74%)	0.38	6 (4%) 36 37	39, 55, 84, 103	0
All	All	1145/1496 (76%)	0.40	71 (6%) 21 23	28, 54, 86, 134	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	760	ASP	5.6
1	A	764	GLY	4.9
1	A	763	ALA	4.8
1	D	760	ASP	4.8
1	G	763	ALA	4.8
1	D	818	GLN	4.1
1	F	763	ALA	4.0
1	F	848	HIS	3.9
1	A	765	GLU	3.9
1	G	765	GLU	3.7
1	G	762	ILE	3.4
1	G	759	GLU	3.4
1	F	762	ILE	3.4
1	H	787	ASN	3.4
1	E	846	LEU	3.3
1	A	761	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	795	LYS	3.2
1	C	738	ALA	3.2
1	F	783	SER	3.2
1	C	785	PRO	3.2
1	G	804	GLU	3.1
1	F	738	ALA	3.0
1	G	769	ILE	3.0
1	B	686	ARG	3.0
1	F	849	LEU	2.9
1	D	761	GLY	2.8
1	G	764	GLY	2.8
1	F	723	GLU	2.8
1	H	818	GLN	2.7
1	F	801	LYS	2.7
1	D	817	ILE	2.7
1	A	795	LYS	2.6
1	D	847	ASP	2.6
1	B	785	PRO	2.6
1	D	739	LYS	2.6
1	E	685	LYS	2.5
1	G	856	GLY	2.5
1	E	686	ARG	2.5
1	D	685	LYS	2.5
1	G	811	CYS	2.5
1	H	751	GLU	2.5
1	E	688	MET	2.4
1	A	762	ILE	2.4
1	G	760	ASP	2.4
1	H	795	LYS	2.4
1	C	816	GLN	2.4
1	E	789	LYS	2.4
1	H	783	SER	2.4
1	A	759	GLU	2.3
1	E	817	ILE	2.3
1	G	727	VAL	2.3
1	F	724	SER	2.3
1	F	754	GLN	2.3
1	A	805	ASP	2.3
1	E	756	HIS	2.3
1	A	758	PHE	2.2
1	B	753	LEU	2.2
1	B	782	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	758	PHE	2.2
1	G	772	LEU	2.2
1	E	816	GLN	2.2
1	A	766	ALA	2.2
1	H	788	ALA	2.2
1	D	738	ALA	2.1
1	C	786	LYS	2.1
1	D	782	GLU	2.1
1	E	785	PRO	2.1
1	B	816	GLN	2.1
1	F	751	GLU	2.1
1	F	764	GLY	2.0
1	G	688	MET	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.