



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:28 PM GMT

PDB ID : 3L6Y  
Title : Crystal structure of p120 catenin in complex with E-cadherin  
Authors : Ishiyama, N.; Lee, S.-H.; Liu, S.; Li, G.-Y.; Smith, M.J.; Reichardt, L.F.; Ikura, M.  
Deposited on : 2009-12-27  
Resolution : 3.00 Å(reported)

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

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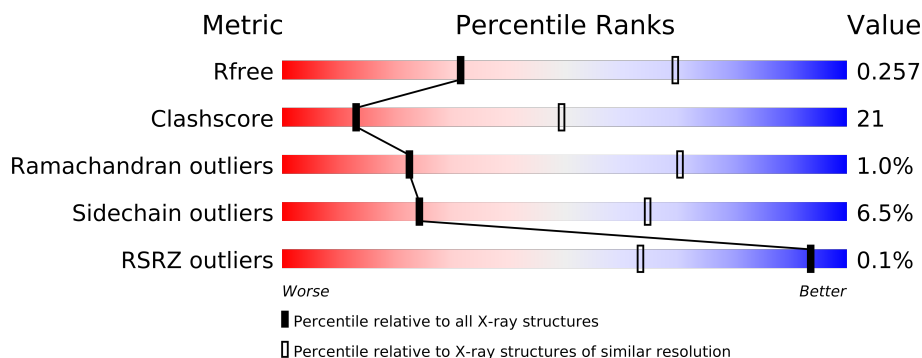
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	584	
1	C	584	
1	E	584	
2	B	18	
2	D	18	
2	F	18	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9099 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catenin delta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2725	1712	491	511	11			
1	C	376	Total	C	N	O	S	0	0	0
			2853	1788	514	540	11			
1	E	397	Total	C	N	O	S	0	0	0
			3045	1919	549	566	11			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	319	GLY	-	EXPRESSION TAG	UNP O60716
A	320	SER	-	EXPRESSION TAG	UNP O60716
A	321	PRO	-	EXPRESSION TAG	UNP O60716
A	322	GLU	-	EXPRESSION TAG	UNP O60716
A	323	PHE	-	EXPRESSION TAG	UNP O60716
A	?	-	PRO	DELETION	UNP O60716
A	?	-	HIS	DELETION	UNP O60716
A	?	-	ALA	DELETION	UNP O60716
A	?	-	ALA	DELETION	UNP O60716
A	?	-	SER	DELETION	UNP O60716
A	?	-	CYS	DELETION	UNP O60716
A	?	-	PHE	DELETION	UNP O60716
A	?	-	GLY	DELETION	UNP O60716
A	?	-	ALA	DELETION	UNP O60716
A	?	-	LYS	DELETION	UNP O60716
A	?	-	LYS	DELETION	UNP O60716
A	?	-	GLY	DELETION	UNP O60716
A	?	-	LYS	DELETION	UNP O60716
A	?	-	ASP	SEE REMARK 999	UNP O60716
A	?	-	GLU	SEE REMARK 999	UNP O60716
A	?	-	TRP	SEE REMARK 999	UNP O60716
A	?	-	PHE	SEE REMARK 999	UNP O60716
A	?	-	SER	SEE REMARK 999	UNP O60716

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	SEE REMARK 999	UNP O60716
A	?	-	GLY	DELETION	UNP O60716
A	?	-	LYS	DELETION	UNP O60716
A	?	-	LYS	DELETION	UNP O60716
A	?	-	PRO	DELETION	UNP O60716
A	?	-	ILE	DELETION	UNP O60716
A	?	-	GLU	DELETION	UNP O60716
A	?	-	ASP	DELETION	UNP O60716
A	?	-	PRO	DELETION	UNP O60716
A	?	-	ALA	DELETION	UNP O60716
A	?	-	ASN	DELETION	UNP O60716
A	?	-	ASP	DELETION	UNP O60716
A	?	-	THR	DELETION	UNP O60716
A	?	-	VAL	DELETION	UNP O60716
A	?	-	ASP	DELETION	UNP O60716
A	?	-	PHE	DELETION	UNP O60716
A	?	-	PRO	DELETION	UNP O60716
A	?	-	LYS	DELETION	UNP O60716
A	?	-	ARG	DELETION	UNP O60716
A	932	LYS	-	SEE REMARK 999	UNP O60716
A	933	ILE	-	SEE REMARK 999	UNP O60716
C	319	GLY	-	EXPRESSION TAG	UNP O60716
C	320	SER	-	EXPRESSION TAG	UNP O60716
C	321	PRO	-	EXPRESSION TAG	UNP O60716
C	322	GLU	-	EXPRESSION TAG	UNP O60716
C	323	PHE	-	EXPRESSION TAG	UNP O60716
C	?	-	PRO	DELETION	UNP O60716
C	?	-	HIS	DELETION	UNP O60716
C	?	-	ALA	DELETION	UNP O60716
C	?	-	ALA	DELETION	UNP O60716
C	?	-	SER	DELETION	UNP O60716
C	?	-	CYS	DELETION	UNP O60716
C	?	-	PHE	DELETION	UNP O60716
C	?	-	GLY	DELETION	UNP O60716
C	?	-	ALA	DELETION	UNP O60716
C	?	-	LYS	DELETION	UNP O60716
C	?	-	LYS	DELETION	UNP O60716
C	?	-	GLY	DELETION	UNP O60716
C	?	-	LYS	DELETION	UNP O60716
C	?	-	ASP	SEE REMARK 999	UNP O60716
C	?	-	GLU	SEE REMARK 999	UNP O60716
C	?	-	TRP	SEE REMARK 999	UNP O60716

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	SEE REMARK 999	UNP O60716
C	?	-	SER	SEE REMARK 999	UNP O60716
C	?	-	ARG	SEE REMARK 999	UNP O60716
C	?	-	GLY	DELETION	UNP O60716
C	?	-	LYS	DELETION	UNP O60716
C	?	-	LYS	DELETION	UNP O60716
C	?	-	PRO	DELETION	UNP O60716
C	?	-	ILE	DELETION	UNP O60716
C	?	-	GLU	DELETION	UNP O60716
C	?	-	ASP	DELETION	UNP O60716
C	?	-	PRO	DELETION	UNP O60716
C	?	-	ALA	DELETION	UNP O60716
C	?	-	ASN	DELETION	UNP O60716
C	?	-	ASP	DELETION	UNP O60716
C	?	-	THR	DELETION	UNP O60716
C	?	-	VAL	DELETION	UNP O60716
C	?	-	ASP	DELETION	UNP O60716
C	?	-	PHE	DELETION	UNP O60716
C	?	-	PRO	DELETION	UNP O60716
C	?	-	LYS	DELETION	UNP O60716
C	?	-	ARG	DELETION	UNP O60716
C	932	LYS	-	SEE REMARK 999	UNP O60716
C	933	ILE	-	SEE REMARK 999	UNP O60716
E	319	GLY	-	EXPRESSION TAG	UNP O60716
E	320	SER	-	EXPRESSION TAG	UNP O60716
E	321	PRO	-	EXPRESSION TAG	UNP O60716
E	322	GLU	-	EXPRESSION TAG	UNP O60716
E	323	PHE	-	EXPRESSION TAG	UNP O60716
E	?	-	PRO	DELETION	UNP O60716
E	?	-	HIS	DELETION	UNP O60716
E	?	-	ALA	DELETION	UNP O60716
E	?	-	ALA	DELETION	UNP O60716
E	?	-	SER	DELETION	UNP O60716
E	?	-	CYS	DELETION	UNP O60716
E	?	-	PHE	DELETION	UNP O60716
E	?	-	GLY	DELETION	UNP O60716
E	?	-	ALA	DELETION	UNP O60716
E	?	-	LYS	DELETION	UNP O60716
E	?	-	LYS	DELETION	UNP O60716
E	?	-	GLY	DELETION	UNP O60716
E	?	-	LYS	DELETION	UNP O60716
E	?	-	ASP	SEE REMARK 999	UNP O60716

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLU	SEE REMARK 999	UNP O60716
E	?	-	TRP	SEE REMARK 999	UNP O60716
E	?	-	PHE	SEE REMARK 999	UNP O60716
E	?	-	SER	SEE REMARK 999	UNP O60716
E	?	-	ARG	SEE REMARK 999	UNP O60716
E	?	-	GLY	DELETION	UNP O60716
E	?	-	LYS	DELETION	UNP O60716
E	?	-	LYS	DELETION	UNP O60716
E	?	-	PRO	DELETION	UNP O60716
E	?	-	ILE	DELETION	UNP O60716
E	?	-	GLU	DELETION	UNP O60716
E	?	-	ASP	DELETION	UNP O60716
E	?	-	PRO	DELETION	UNP O60716
E	?	-	ALA	DELETION	UNP O60716
E	?	-	ASN	DELETION	UNP O60716
E	?	-	ASP	DELETION	UNP O60716
E	?	-	THR	DELETION	UNP O60716
E	?	-	VAL	DELETION	UNP O60716
E	?	-	ASP	DELETION	UNP O60716
E	?	-	PHE	DELETION	UNP O60716
E	?	-	PRO	DELETION	UNP O60716
E	?	-	LYS	DELETION	UNP O60716
E	?	-	ARG	DELETION	UNP O60716
E	932	LYS	-	SEE REMARK 999	UNP O60716
E	933	ILE	-	SEE REMARK 999	UNP O60716

- Molecule 2 is a protein called E-cadherin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	18	Total C N O 141 82 22 37	0	0	0
2	D	18	Total C N O 141 82 22 37	0	0	0
2	F	18	Total C N O 141 82 22 37	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	C	17	Total O 17 17	0	0

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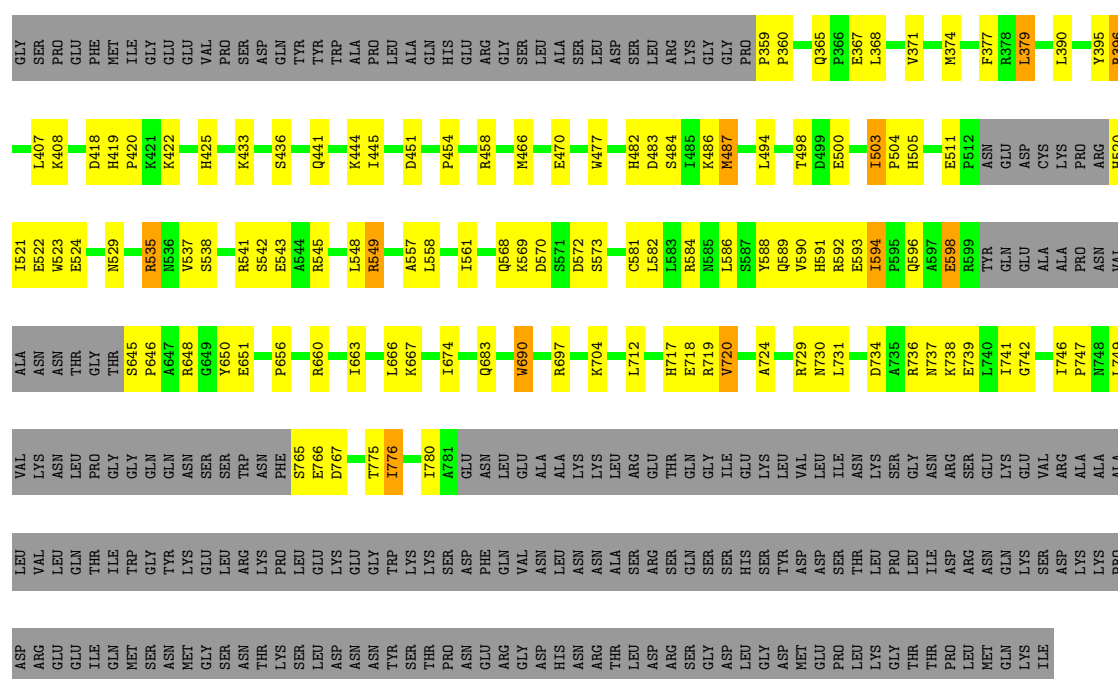
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total 3	O 3	0	0
3	E	23	Total 23	O 23	0	0
3	F	5	Total 5	O 5	0	0

### 3 Residue-property plots

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

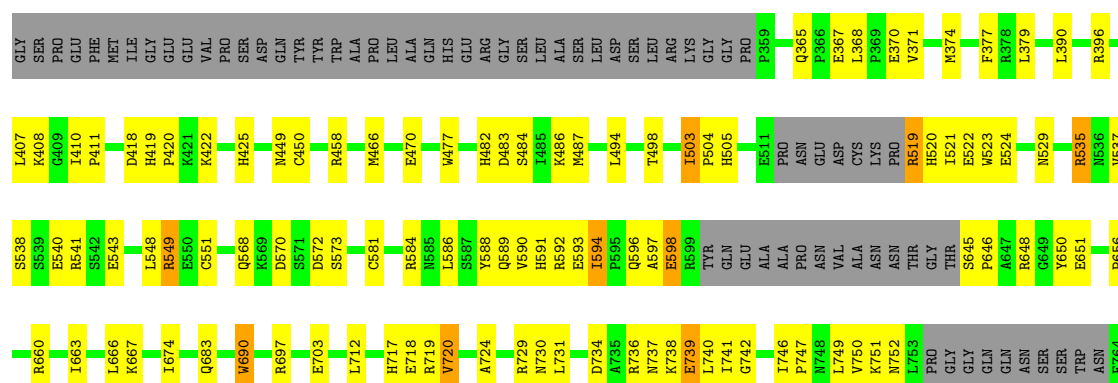
#### • Molecule 1: Catenin delta-1

Chain A:

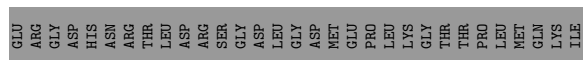


#### • Molecule 1: Catenin delta-1

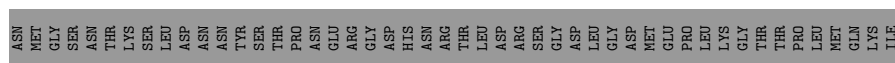
Chain C:







Chain E:



Chain B:



Chain D:



Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.18Å 106.18Å 173.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.00 – 3.00 34.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (35.00-3.00) 99.0 (34.75-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.81 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, $R_{free}$	0.232 , 0.264 0.227 , 0.257	Depositor DCC
$R_{free}$ test set	2178 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.014 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 43293 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9099	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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 23.32 % 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 4.7698e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/2768	0.62	0/3756
1	C	0.58	1/2894 (0.0%)	0.67	0/3931
1	E	0.62	1/3092 (0.0%)	0.71	0/4191
2	B	0.54	0/142	0.63	0/189
2	D	0.63	0/142	0.70	0/189
2	F	0.74	0/142	0.74	0/189
All	All	0.58	2/9180 (0.0%)	0.67	0/12445

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	551	CYS	CB-SG	-6.58	1.71	1.82
1	E	581	CYS	CB-SG	-5.59	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2725	0	2718	118	0
1	C	2853	0	2817	110	0
1	E	3045	0	3043	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	141	0	107	6	0
2	D	141	0	107	6	0
2	F	141	0	107	4	0
3	A	5	0	0	0	0
3	C	17	0	0	3	0
3	D	3	0	0	0	0
3	E	23	0	0	1	0
3	F	5	0	0	0	0
All	All	9099	0	8899	370	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (370) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:494:LEU:HD13	1:E:548:LEU:CD2	1.89	1.02
1:E:820:LEU:O	1:E:823:ILE:HG22	1.61	1.01
1:E:801:LEU:HD23	1:E:801:LEU:O	1.61	1.00
1:E:781:ALA:O	1:E:782:GLU:HG3	1.60	1.00
1:A:712:LEU:CD1	1:A:724:ALA:HB2	1.92	0.98
1:A:712:LEU:HD12	1:A:724:ALA:HB2	1.48	0.96
1:E:712:LEU:CD1	1:E:724:ALA:HB2	1.95	0.96
1:A:494:LEU:HD13	1:A:548:LEU:CD2	1.96	0.95
1:C:494:LEU:HD13	1:C:548:LEU:CD2	1.96	0.95
1:E:712:LEU:HD12	1:E:724:ALA:HB2	1.48	0.94
1:C:712:LEU:CD1	1:C:724:ALA:HB2	1.98	0.92
1:C:712:LEU:HD12	1:C:724:ALA:HB2	1.53	0.91
1:E:505:HIS:HD2	1:E:522:GLU:OE2	1.54	0.89
2:D:774:LEU:O	2:D:775:HIS:HB3	1.71	0.89
1:C:540:GLU:HB3	1:E:596:GLN:NE2	1.87	0.89
1:C:505:HIS:HD2	1:C:522:GLU:OE2	1.54	0.88
1:C:549:ARG:NH1	1:C:586:LEU:O	2.10	0.85
1:C:718:GLU:OE2	1:C:765:SER:HB3	1.75	0.84
1:C:549:ARG:NH2	1:C:593:GLU:OE1	2.11	0.84
2:B:774:LEU:O	2:B:775:HIS:HB3	1.78	0.84
1:C:540:GLU:HB3	1:E:596:GLN:HE21	1.40	0.83
2:F:774:LEU:O	2:F:775:HIS:HB3	1.78	0.82
1:A:718:GLU:OE2	1:A:765:SER:HB3	1.77	0.82
1:A:570:ASP:OD2	1:A:573:SER:HB3	1.79	0.82
1:E:508:TRP:HH2	1:E:648:ARG:HH21	1.24	0.82
1:A:549:ARG:NH2	1:A:593:GLU:OE1	2.12	0.82
1:A:549:ARG:NH1	1:A:586:LEU:O	2.13	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:718:GLU:OE2	1:E:765:SER:HB3	1.80	0.81
1:E:781:ALA:O	1:E:782:GLU:CG	2.30	0.79
1:A:505:HIS:HD2	1:A:522:GLU:OE2	1.65	0.79
1:E:494:LEU:HD13	1:E:548:LEU:HD23	1.63	0.77
1:A:422:LYS:HA	1:A:425:HIS:CE1	2.20	0.77
1:C:422:LYS:HA	1:C:425:HIS:CE1	2.20	0.76
1:E:549:ARG:NH2	1:E:593:GLU:OE1	2.17	0.76
2:D:771:LEU:HD12	2:D:774:LEU:HD12	1.69	0.74
1:E:570:ASP:OD2	1:E:573:SER:HB3	1.87	0.74
1:C:466:MET:HE2	1:C:523:TRP:CD2	2.21	0.74
1:E:820:LEU:O	1:E:823:ILE:CG2	2.36	0.73
1:C:739:GLU:HG3	1:C:740:LEU:N	2.04	0.72
1:E:549:ARG:NH1	1:E:586:LEU:O	2.22	0.72
1:A:535:ARG:HG3	1:A:581:CYS:HB2	1.71	0.70
1:E:520:HIS:HD2	1:E:521:ILE:N	1.89	0.70
2:B:771:LEU:HD12	2:B:774:LEU:HD12	1.74	0.70
1:E:801:LEU:O	1:E:801:LEU:CD2	2.38	0.69
1:C:535:ARG:HG3	1:C:581:CYS:HB2	1.74	0.69
1:E:422:LYS:HA	1:E:425:HIS:CE1	2.28	0.69
1:A:520:HIS:HD2	1:A:521:ILE:N	1.91	0.68
1:A:511:GLU:OE2	1:A:511:GLU:HA	1.92	0.68
1:C:466:MET:HE2	1:C:523:TRP:CE2	2.29	0.68
1:C:645:SER:N	1:C:646:PRO:CD	2.58	0.67
1:A:486:LYS:HD3	1:A:537:VAL:HA	1.76	0.67
1:E:796:ILE:HD11	1:E:823:ILE:CD1	2.25	0.67
1:E:773:LEU:HD11	1:E:816:ALA:HA	1.75	0.66
1:E:535:ARG:HG3	1:E:581:CYS:HB2	1.77	0.66
1:C:750:VAL:O	1:C:752:ASN:N	2.28	0.66
1:C:570:ASP:OD2	1:C:573:SER:HB3	1.96	0.65
1:A:667:LYS:HD3	1:A:704:LYS:HZ1	1.61	0.65
1:E:482:HIS:HD2	1:E:484:SER:H	1.43	0.65
1:A:766:GLU:HG2	1:A:767:ASP:N	2.12	0.65
1:E:749:LEU:HB3	1:E:776:ILE:HD11	1.79	0.65
1:E:378:ARG:HG2	1:E:378:ARG:HH11	1.61	0.64
1:A:494:LEU:HD13	1:A:548:LEU:HD23	1.78	0.64
1:C:541:ARG:HG2	3:C:38:HOH:O	1.97	0.64
1:C:449:ASN:HB3	1:E:499:ASP:OD2	1.98	0.63
1:C:503:ILE:HB	1:C:504:PRO:HD3	1.80	0.63
1:A:712:LEU:HD12	1:A:724:ALA:CB	2.27	0.63
1:E:773:LEU:HD11	1:E:816:ALA:CA	2.29	0.63
1:E:466:MET:HE2	1:E:523:TRP:CE2	2.34	0.63
1:A:645:SER:N	1:A:646:PRO:HD2	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:466:MET:HE2	1:A:523:TRP:CD2	2.34	0.62
1:C:645:SER:N	1:C:646:PRO:HD2	2.14	0.62
1:C:422:LYS:HA	1:C:425:HIS:NE2	2.14	0.62
1:A:645:SER:N	1:A:646:PRO:CD	2.63	0.62
1:E:663:ILE:HG22	1:E:667:LYS:HE3	1.81	0.61
1:E:781:ALA:O	1:E:782:GLU:CB	2.47	0.61
1:C:596:GLN:N	1:C:596:GLN:OE1	2.33	0.61
1:E:487:MET:HG2	1:E:541:ARG:HD3	1.81	0.61
2:F:771:LEU:HD12	2:F:774:LEU:HD12	1.82	0.61
1:C:486:LYS:HD3	1:C:537:VAL:HA	1.83	0.61
1:C:494:LEU:HD13	1:C:548:LEU:HD22	1.79	0.61
1:E:773:LEU:CD1	1:E:816:ALA:HA	2.30	0.61
1:C:494:LEU:HD13	1:C:548:LEU:HD23	1.80	0.61
1:C:765:SER:OG	1:C:766:GLU:N	2.34	0.61
1:E:520:HIS:CD2	1:E:521:ILE:N	2.68	0.61
1:C:741:ILE:HG23	1:C:742:GLY:N	2.15	0.61
1:A:749:LEU:HB3	1:A:776:ILE:HD11	1.81	0.60
1:A:741:ILE:HG23	1:A:742:GLY:N	2.13	0.60
1:E:494:LEU:HD13	1:E:548:LEU:HD22	1.79	0.60
1:A:477:TRP:CE2	2:B:761:GLY:HA3	2.35	0.60
1:E:482:HIS:CD2	1:E:484:SER:H	2.19	0.60
1:A:494:LEU:HD13	1:A:548:LEU:HD22	1.78	0.60
1:C:749:LEU:HB3	1:C:776:ILE:HD11	1.83	0.60
1:E:645:SER:N	1:E:646:PRO:HD2	2.17	0.60
1:E:697:ARG:HG2	1:E:731:LEU:HD23	1.84	0.60
1:A:569:LYS:HD2	1:A:569:LYS:N	2.15	0.60
1:A:477:TRP:CE3	1:A:529:ASN:HA	2.36	0.60
1:E:741:ILE:HG23	1:E:742:GLY:N	2.17	0.59
1:C:750:VAL:C	1:C:752:ASN:H	2.05	0.59
1:C:505:HIS:CD2	1:C:522:GLU:OE2	2.47	0.59
1:E:482:HIS:HD2	1:E:484:SER:N	2.00	0.59
1:E:645:SER:N	1:E:646:PRO:CD	2.65	0.59
1:E:419:HIS:ND1	1:E:420:PRO:HD2	2.17	0.59
1:A:648:ARG:O	1:A:651:GLU:HG2	2.03	0.58
1:E:466:MET:HE2	1:E:523:TRP:CD2	2.38	0.58
1:E:801:LEU:C	1:E:801:LEU:CD2	2.72	0.58
1:A:667:LYS:NZ	1:A:704:LYS:NZ	2.51	0.58
1:C:520:HIS:HD2	1:C:521:ILE:N	2.02	0.58
1:C:780:ILE:O	1:C:780:ILE:HG13	2.02	0.58
1:E:505:HIS:CD2	1:E:522:GLU:OE2	2.46	0.58
1:A:766:GLU:HG2	1:A:767:ASP:H	1.68	0.58
1:A:520:HIS:CD2	1:A:521:ILE:N	2.71	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:422:LYS:HA	1:E:425:HIS:NE2	2.19	0.57
1:C:419:HIS:ND1	1:C:420:PRO:HD2	2.19	0.57
1:E:801:LEU:HD23	1:E:801:LEU:C	2.25	0.57
1:A:780:ILE:O	1:A:780:ILE:HG13	2.03	0.57
1:A:418:ASP:OD2	1:A:458:ARG:NH1	2.38	0.56
1:A:592:ARG:HH22	1:C:596:GLN:HE22	1.51	0.56
1:E:782:GLU:HA	1:E:826:TYR:OH	2.05	0.56
1:C:477:TRP:CE3	1:C:529:ASN:HA	2.40	0.56
1:A:521:ILE:HG12	1:A:522:GLU:N	2.20	0.56
1:C:519:ARG:N	3:C:35:HOH:O	2.39	0.56
1:E:820:LEU:C	1:E:823:ILE:HG22	2.26	0.55
1:A:482:HIS:CD2	1:A:484:SER:H	2.25	0.55
1:E:648:ARG:O	1:E:651:GLU:HG2	2.07	0.55
1:A:445:ILE:HD11	1:A:482:HIS:NE2	2.21	0.55
2:D:774:LEU:O	2:D:775:HIS:CB	2.48	0.55
1:A:765:SER:OG	1:A:766:GLU:N	2.39	0.55
1:C:712:LEU:HD12	1:C:724:ALA:CB	2.34	0.55
1:E:712:LEU:HD12	1:E:724:ALA:CB	2.28	0.55
1:E:765:SER:OG	1:E:766:GLU:N	2.39	0.55
1:A:422:LYS:HA	1:A:425:HIS:NE2	2.21	0.55
1:E:494:LEU:CD1	1:E:548:LEU:CD2	2.76	0.55
1:A:520:HIS:HD2	1:A:521:ILE:H	1.54	0.54
1:A:596:GLN:N	1:A:596:GLN:OE1	2.40	0.54
1:A:697:ARG:HG2	1:A:731:LEU:HD23	1.89	0.54
1:A:477:TRP:CZ2	2:B:761:GLY:HA3	2.42	0.54
1:C:663:ILE:HG22	1:C:667:LYS:HE3	1.90	0.54
1:E:773:LEU:CD1	1:E:816:ALA:CA	2.86	0.54
1:C:650:TYR:CD1	1:C:650:TYR:C	2.81	0.54
1:A:487:MET:HG2	1:A:541:ARG:HD3	1.90	0.53
1:E:588:TYR:CE2	1:E:589:GLN:HG3	2.43	0.53
1:E:746:ILE:O	1:E:747:PRO:C	2.44	0.53
2:F:774:LEU:O	2:F:775:HIS:CB	2.53	0.53
1:A:663:ILE:HG22	1:A:667:LYS:HE3	1.90	0.53
1:C:487:MET:HG2	1:C:541:ARG:HD3	1.90	0.53
1:A:650:TYR:CD1	1:A:650:TYR:C	2.82	0.53
1:A:483:ASP:HA	1:A:486:LYS:HG3	1.90	0.53
1:A:592:ARG:NH2	1:C:596:GLN:HE22	2.06	0.53
1:E:781:ALA:C	1:E:782:GLU:HG3	2.27	0.53
1:C:591:HIS:HB3	1:C:690:TRP:CE2	2.44	0.53
1:C:541:ARG:NH1	3:C:1:HOH:O	2.42	0.53
1:C:524:GLU:N	1:C:524:GLU:OE1	2.38	0.53
1:E:666:LEU:HD22	1:E:712:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:466:MET:HE2	1:A:523:TRP:CG	2.44	0.52
1:E:570:ASP:OD2	1:E:573:SER:CB	2.55	0.52
2:B:774:LEU:O	2:B:775:HIS:CB	2.54	0.52
1:E:796:ILE:HD11	1:E:823:ILE:HD12	1.91	0.52
1:E:823:ILE:HG23	1:E:824:TRP:N	2.24	0.52
1:A:741:ILE:CG2	1:A:742:GLY:N	2.73	0.52
1:A:667:LYS:HZ3	1:A:704:LYS:CE	2.23	0.52
1:E:780:ILE:HG13	1:E:780:ILE:O	2.09	0.52
1:E:596:GLN:OE1	1:E:596:GLN:N	2.43	0.52
1:C:596:GLN:HB3	1:C:598:GLU:OE1	2.09	0.52
1:E:699:ALA:O	1:E:702:GLN:HG3	2.10	0.52
1:E:650:TYR:CD1	1:E:650:TYR:C	2.83	0.51
1:C:588:TYR:CE2	1:C:589:GLN:HG3	2.44	0.51
1:E:737:ASN:O	1:E:739:GLU:N	2.43	0.51
1:A:451:ASP:O	1:A:454:PRO:HD2	2.10	0.51
1:C:746:ILE:O	1:C:747:PRO:C	2.47	0.51
1:E:750:VAL:HG12	1:E:751:LYS:N	2.25	0.51
1:C:749:LEU:HD11	1:C:775:THR:HG22	1.93	0.51
1:A:482:HIS:HD2	1:A:484:SER:N	2.08	0.51
1:C:494:LEU:CD1	1:C:548:LEU:CD2	2.80	0.51
1:E:773:LEU:CD1	1:E:816:ALA:N	2.74	0.51
1:C:648:ARG:O	1:C:651:GLU:CG	2.59	0.51
1:A:374:MET:HA	1:A:377:PHE:CD1	2.45	0.51
1:E:374:MET:HA	1:E:377:PHE:CD1	2.46	0.50
1:A:588:TYR:CE2	1:A:589:GLN:HG3	2.46	0.50
1:A:648:ARG:O	1:A:651:GLU:CG	2.58	0.50
1:E:648:ARG:O	1:E:651:GLU:CG	2.60	0.50
1:C:741:ILE:CG2	1:C:742:GLY:N	2.74	0.50
1:C:450:CYS:HA	1:E:461:ARG:NH2	2.27	0.50
1:A:666:LEU:HD22	1:A:712:LEU:HD21	1.93	0.50
1:C:450:CYS:HA	1:E:461:ARG:HH22	1.76	0.50
1:E:494:LEU:CD1	1:E:548:LEU:HD23	2.40	0.50
1:E:796:ILE:O	1:E:796:ILE:CG2	2.60	0.50
1:A:482:HIS:HD2	1:A:484:SER:H	1.60	0.50
1:A:466:MET:HE2	1:A:523:TRP:CE2	2.46	0.50
1:E:418:ASP:OD1	1:E:458:ARG:NH1	2.42	0.50
1:E:591:HIS:HB3	1:E:690:TRP:CE2	2.47	0.50
1:E:366:PRO:HG2	1:E:374:MET:HE1	1.94	0.49
1:E:599:ARG:O	1:E:600:TYR:C	2.50	0.49
1:A:591:HIS:HB3	1:A:690:TRP:CE2	2.47	0.49
1:C:482:HIS:CD2	1:C:484:SER:H	2.30	0.49
1:C:418:ASP:OD2	1:C:458:ARG:NH1	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:477:TRP:CE3	1:E:529:ASN:HA	2.48	0.49
1:C:374:MET:HA	1:C:377:PHE:CD1	2.47	0.49
1:C:663:ILE:O	1:C:667:LYS:HG3	2.13	0.49
1:C:697:ARG:HG2	1:C:731:LEU:HD23	1.93	0.49
1:C:697:ARG:NH1	1:C:734:ASP:OD2	2.46	0.49
1:E:503:ILE:HB	1:E:504:PRO:HD3	1.93	0.49
1:C:520:HIS:CD2	1:C:521:ILE:N	2.80	0.49
1:E:749:LEU:HB3	1:E:776:ILE:CD1	2.41	0.49
1:E:524:GLU:OE1	1:E:524:GLU:N	2.44	0.49
1:A:746:ILE:O	1:A:747:PRO:C	2.47	0.49
1:C:521:ILE:HG12	1:C:522:GLU:N	2.28	0.49
1:C:418:ASP:OD1	1:C:458:ARG:NH1	2.45	0.48
1:E:520:HIS:HD2	1:E:521:ILE:H	1.58	0.48
1:C:734:ASP:O	1:C:736:ARG:HG3	2.14	0.48
1:A:494:LEU:CD1	1:A:548:LEU:CD2	2.81	0.48
1:C:466:MET:CE	1:C:523:TRP:CE2	2.95	0.48
1:E:445:ILE:HD11	1:E:482:HIS:NE2	2.28	0.48
1:E:752:ASN:CB	1:E:772:ILE:CD1	2.92	0.48
1:A:494:LEU:CD1	1:A:548:LEU:HD22	2.44	0.48
1:E:752:ASN:CB	1:E:772:ILE:HD13	2.44	0.48
1:A:557:ALA:O	1:A:561:ILE:HG13	2.14	0.48
1:C:823:ILE:HD12	1:C:823:ILE:H	1.79	0.48
1:A:524:GLU:OE1	1:A:524:GLU:N	2.43	0.48
1:A:683:GLN:HG3	1:A:730:ASN:ND2	2.28	0.48
1:A:667:LYS:HZ3	1:A:704:LYS:HE2	1.78	0.48
1:A:500:GLU:O	1:A:504:PRO:HG2	2.14	0.48
1:A:737:ASN:O	1:A:739:GLU:N	2.47	0.48
1:A:596:GLN:HB3	1:A:598:GLU:OE1	2.14	0.48
1:C:717:HIS:O	1:C:720:VAL:HG13	2.14	0.48
1:C:570:ASP:OD2	1:C:573:SER:CB	2.61	0.47
1:E:737:ASN:C	1:E:739:GLU:N	2.67	0.47
1:A:520:HIS:CD2	1:A:521:ILE:H	2.31	0.47
1:C:750:VAL:C	1:C:752:ASN:N	2.65	0.47
1:E:486:LYS:HD3	1:E:537:VAL:HA	1.96	0.47
1:C:466:MET:HE2	1:C:523:TRP:CG	2.49	0.47
1:E:746:ILE:HB	1:E:747:PRO:HD3	1.96	0.47
1:C:390:LEU:HD12	1:C:390:LEU:HA	1.40	0.47
1:C:483:ASP:HA	1:C:486:LYS:HG3	1.97	0.47
1:E:418:ASP:OD2	1:E:458:ARG:NH1	2.46	0.47
1:A:486:LYS:HA	1:A:537:VAL:HG12	1.95	0.47
1:E:775:THR:O	1:E:779:VAL:HG23	2.14	0.47
1:A:749:LEU:HB3	1:A:776:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:734:ASP:O	1:E:736:ARG:HG3	2.14	0.47
1:E:741:ILE:CG2	1:E:742:GLY:N	2.77	0.47
1:C:477:TRP:CZ2	2:D:761:GLY:HA3	2.50	0.47
1:C:666:LEU:HD22	1:C:712:LEU:HD21	1.96	0.47
1:A:667:LYS:HZ3	1:A:704:LYS:NZ	2.11	0.47
1:A:418:ASP:OD1	1:A:458:ARG:NH1	2.48	0.47
1:E:500:GLU:O	1:E:504:PRO:HG2	2.14	0.47
1:E:749:LEU:HD11	1:E:775:THR:HG22	1.96	0.46
1:E:483:ASP:HA	1:E:486:LYS:HG3	1.97	0.46
1:C:648:ARG:O	1:C:651:GLU:HG2	2.15	0.46
1:A:570:ASP:OD2	1:A:573:SER:CB	2.57	0.46
1:A:589:GLN:O	1:A:593:GLU:HG3	2.16	0.46
1:C:819:VAL:O	1:C:823:ILE:HD12	2.15	0.46
1:C:683:GLN:HG3	1:C:730:ASN:ND2	2.31	0.46
1:A:558:LEU:CD1	1:A:582:LEU:HD23	2.46	0.46
1:C:540:GLU:CB	1:E:596:GLN:NE2	2.69	0.46
1:C:449:ASN:O	1:E:495:HIS:HB3	2.16	0.46
1:C:494:LEU:CD1	1:C:548:LEU:HD22	2.44	0.46
1:A:749:LEU:HD11	1:A:775:THR:HG22	1.98	0.46
1:C:749:LEU:HB3	1:C:776:ILE:CD1	2.45	0.46
1:A:572:ASP:HA	1:A:674:ILE:HD12	1.98	0.46
1:C:697:ARG:NH1	1:C:734:ASP:CG	2.69	0.46
1:C:482:HIS:HD2	1:C:484:SER:N	2.14	0.46
1:A:734:ASP:O	1:A:736:ARG:HG3	2.16	0.46
1:A:498:THR:O	1:A:503:ILE:HG13	2.16	0.46
1:E:679:ALA:HB3	1:E:723:ALA:HB1	1.98	0.46
1:C:739:GLU:CG	1:C:740:LEU:N	2.78	0.45
1:E:697:ARG:NH1	1:E:734:ASP:OD2	2.48	0.45
1:C:466:MET:CE	1:C:523:TRP:CD1	2.99	0.45
1:E:584:ARG:HD2	3:E:21:HOH:O	2.16	0.45
1:E:820:LEU:HA	1:E:823:ILE:CG2	2.46	0.45
1:C:746:ILE:HB	1:C:747:PRO:HD3	1.98	0.45
1:C:410:ILE:N	1:C:411:PRO:CD	2.79	0.45
1:C:697:ARG:NH1	1:C:734:ASP:OD1	2.49	0.45
1:A:503:ILE:HB	1:A:504:PRO:HD3	1.99	0.45
1:E:508:TRP:HH2	1:E:648:ARG:NH2	2.01	0.45
1:A:505:HIS:CE1	1:A:523:TRP:CE3	3.05	0.45
1:E:697:ARG:NH1	1:E:734:ASP:CG	2.70	0.45
1:E:520:HIS:CD2	1:E:521:ILE:H	2.33	0.45
1:C:650:TYR:CD1	1:C:651:GLU:N	2.84	0.45
1:C:370:GLU:O	1:C:374:MET:HG3	2.17	0.45
1:E:572:ASP:HA	1:E:674:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:648:ARG:O	1:C:651:GLU:HG3	2.17	0.44
1:A:590:VAL:C	1:A:592:ARG:H	2.21	0.44
1:C:367:GLU:O	1:C:371:VAL:HG23	2.18	0.44
1:C:522:GLU:O	1:C:523:TRP:HB2	2.18	0.44
1:C:749:LEU:CD1	1:C:775:THR:HG22	2.48	0.44
1:A:746:ILE:HB	1:A:747:PRO:HD3	2.00	0.44
1:C:572:ASP:HA	1:C:674:ILE:HD12	2.00	0.44
1:A:436:SER:O	1:A:444:LYS:HE3	2.17	0.44
1:A:590:VAL:O	1:A:594:ILE:HG22	2.18	0.44
1:C:594:ILE:HD11	1:C:650:TYR:HE1	1.82	0.44
1:A:737:ASN:C	1:A:739:GLU:N	2.70	0.44
1:A:407:LEU:O	1:A:408:LYS:HB2	2.18	0.44
1:A:667:LYS:NZ	1:A:704:LYS:HZ1	2.15	0.44
1:A:650:TYR:CD1	1:A:651:GLU:N	2.85	0.44
1:E:820:LEU:HA	1:E:823:ILE:HG22	2.00	0.44
1:E:494:LEU:CD1	1:E:548:LEU:HD22	2.46	0.43
1:A:538:SER:HB3	1:A:548:LEU:HD12	2.00	0.43
1:A:482:HIS:CD2	1:A:484:SER:HB2	2.53	0.43
1:C:729:ARG:HB2	1:C:775:THR:OG1	2.18	0.43
1:C:594:ILE:CG1	1:C:650:TYR:CE1	3.01	0.43
1:E:656:PRO:O	1:E:660:ARG:HG3	2.19	0.43
1:E:395:TYR:CE2	1:E:396:ARG:HG3	2.54	0.43
1:E:777:ASN:HB2	1:E:819:VAL:HG22	2.00	0.43
1:A:729:ARG:HB2	1:A:775:THR:OG1	2.19	0.43
1:A:367:GLU:O	1:A:371:VAL:HG23	2.19	0.43
1:E:419:HIS:HA	1:E:420:PRO:HD3	1.88	0.43
1:C:477:TRP:CE2	2:D:761:GLY:HA3	2.54	0.43
1:E:737:ASN:O	1:E:738:LYS:C	2.57	0.43
1:E:803:ASN:O	1:E:803:ASN:OD1	2.37	0.43
1:E:521:ILE:HG12	1:E:522:GLU:N	2.33	0.42
1:C:505:HIS:CE1	1:C:523:TRP:CE3	3.07	0.42
1:C:503:ILE:HB	1:C:504:PRO:CD	2.47	0.42
1:A:558:LEU:HD11	1:A:582:LEU:CD2	2.48	0.42
1:E:435:ILE:O	1:E:435:ILE:HG22	2.19	0.42
1:A:718:GLU:OE2	1:A:765:SER:CB	2.59	0.42
1:A:395:TYR:CE2	1:A:396:ARG:HG3	2.54	0.42
1:C:538:SER:HB3	1:C:548:LEU:HD12	2.00	0.42
2:D:771:LEU:HA	2:D:771:LEU:HD12	1.72	0.42
1:C:737:ASN:O	1:C:739:GLU:N	2.53	0.42
1:E:740:LEU:HA	1:E:740:LEU:HD23	1.86	0.42
1:C:498:THR:O	1:C:503:ILE:HG13	2.18	0.42
1:A:390:LEU:HA	1:A:390:LEU:HD12	1.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:522:GLU:O	1:A:523:TRP:HB2	2.20	0.42
1:E:700:LEU:HD23	1:E:700:LEU:HA	1.88	0.42
1:C:740:LEU:HD23	1:C:740:LEU:HA	1.87	0.42
1:A:749:LEU:CD1	1:A:775:THR:HG22	2.50	0.42
1:E:746:ILE:HB	1:E:747:PRO:CD	2.50	0.42
1:A:433:LYS:NZ	2:B:765:GLU:HG3	2.34	0.42
1:A:505:HIS:CD2	1:A:522:GLU:OE2	2.57	0.42
1:A:466:MET:CE	1:A:523:TRP:CD1	3.03	0.42
1:C:407:LEU:O	1:C:408:LYS:HB2	2.20	0.42
1:A:717:HIS:O	1:A:720:VAL:HG13	2.20	0.42
1:E:766:GLU:HG2	1:E:812:GLU:OE1	2.19	0.42
1:A:418:ASP:CG	1:A:458:ARG:NH1	2.74	0.42
1:A:656:PRO:O	1:A:660:ARG:HG3	2.20	0.42
1:E:470:GLU:OE2	1:E:525:SER:OG	2.33	0.42
1:A:697:ARG:NH1	1:A:734:ASP:OD2	2.53	0.41
1:E:370:GLU:O	1:E:374:MET:HG3	2.20	0.41
1:C:737:ASN:C	1:C:739:GLU:N	2.71	0.41
1:A:542:SER:HA	1:A:545:ARG:NH2	2.35	0.41
1:E:407:LEU:O	1:E:408:LYS:HB2	2.19	0.41
1:E:683:GLN:HG3	1:E:730:ASN:ND2	2.35	0.41
1:E:796:ILE:O	1:E:796:ILE:HG22	2.20	0.41
1:C:656:PRO:O	1:C:660:ARG:HG3	2.21	0.41
1:E:781:ALA:O	1:E:782:GLU:HB2	2.19	0.41
1:E:746:ILE:H	1:E:746:ILE:HG12	1.72	0.41
1:A:717:HIS:HB2	1:A:720:VAL:HG13	2.02	0.41
1:E:476:LEU:HA	1:E:476:LEU:HD23	1.87	0.41
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.89	0.41
1:E:505:HIS:CE1	1:E:523:TRP:CE3	3.09	0.41
1:A:594:ILE:HG13	1:A:650:TYR:CE1	2.55	0.41
1:C:418:ASP:CG	1:C:458:ARG:NH1	2.74	0.41
1:C:590:VAL:C	1:C:592:ARG:H	2.23	0.41
1:E:820:LEU:CA	1:E:823:ILE:HG22	2.50	0.41
1:E:487:MET:HE2	1:E:541:ARG:HB3	2.02	0.41
1:E:697:ARG:NH1	1:E:734:ASP:OD1	2.54	0.41
1:E:666:LEU:HD21	1:E:678:SER:HB2	2.03	0.41
1:A:667:LYS:HZ2	1:A:704:LYS:NZ	2.18	0.41
1:E:717:HIS:HB2	1:E:720:VAL:HG13	2.02	0.41
1:E:796:ILE:O	1:E:800:VAL:HG23	2.21	0.40
1:E:796:ILE:HD11	1:E:823:ILE:HD13	2.00	0.40
1:E:650:TYR:CD1	1:E:651:GLU:N	2.90	0.40
1:A:486:LYS:CD	1:A:537:VAL:HA	2.47	0.40
1:A:441:GLN:OE1	1:A:444:LYS:HD2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:359:PRO:HA	1:A:360:PRO:HD2	1.96	0.40
2:F:771:LEU:HA	2:F:771:LEU:HD12	1.70	0.40
1:E:749:LEU:CD1	1:E:775:THR:HG22	2.50	0.40
1:E:777:ASN:HB2	1:E:819:VAL:CG2	2.52	0.40
1:A:663:ILE:O	1:A:667:LYS:HG3	2.21	0.40
1:A:419:HIS:ND1	1:A:420:PRO:HD2	2.36	0.40
1:E:594:ILE:HG12	1:E:595:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

## 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	348/584 (60%)	327 (94%)	20 (6%)	1 (0%)	50 90
1	C	366/584 (63%)	340 (93%)	20 (6%)	6 (2%)	14 56
1	E	385/584 (66%)	360 (94%)	21 (6%)	4 (1%)	22 70
2	B	16/18 (89%)	15 (94%)	1 (6%)	0	100 100
2	D	16/18 (89%)	16 (100%)	0	0	100 100
2	F	16/18 (89%)	16 (100%)	0	0	100 100
All	All	1147/1806 (64%)	1074 (94%)	62 (5%)	11 (1%)	22 70

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	751	LYS
1	A	738	LYS
1	E	738	LYS
1	E	809	SER
1	C	738	LYS
1	C	810	GLU
1	E	739	GLU
1	C	597	ALA

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Mol	Chain	Res	Type
1	C	703	GLU
1	C	739	GLU
1	E	599	ARG

### 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	288/503 (57%)	270 (94%)	18 (6%)	25	66
1	C	298/503 (59%)	280 (94%)	18 (6%)	27	69
1	E	320/503 (64%)	297 (93%)	23 (7%)	21	59
2	B	15/15 (100%)	14 (93%)	1 (7%)	23	64
2	D	15/15 (100%)	14 (93%)	1 (7%)	23	64
2	F	15/15 (100%)	14 (93%)	1 (7%)	23	64
All	All	951/1554 (61%)	889 (94%)	62 (6%)	24	65

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	GLN
1	A	368	LEU
1	A	379	LEU
1	A	396	ARG
1	A	470	GLU
1	A	487	MET
1	A	503	ILE
1	A	535	ARG
1	A	543	GLU
1	A	549	ARG
1	A	568	GLN
1	A	584	ARG
1	A	594	ILE
1	A	598	GLU
1	A	690	TRP
1	A	719	ARG

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Mol	Chain	Res	Type
1	A	720	VAL
1	A	776	ILE
2	B	771	LEU
1	C	365	GLN
1	C	368	LEU
1	C	379	LEU
1	C	396	ARG
1	C	470	GLU
1	C	503	ILE
1	C	519	ARG
1	C	535	ARG
1	C	543	GLU
1	C	549	ARG
1	C	568	GLN
1	C	584	ARG
1	C	594	ILE
1	C	598	GLU
1	C	690	TRP
1	C	719	ARG
1	C	720	VAL
1	C	776	ILE
2	D	771	LEU
1	E	365	GLN
1	E	368	LEU
1	E	378	ARG
1	E	379	LEU
1	E	396	ARG
1	E	399	LYS
1	E	470	GLU
1	E	503	ILE
1	E	535	ARG
1	E	543	GLU
1	E	549	ARG
1	E	552	ASP
1	E	568	GLN
1	E	584	ARG
1	E	594	ILE
1	E	598	GLU
1	E	690	TRP
1	E	712	LEU
1	E	719	ARG
1	E	720	VAL

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Mol	Chain	Res	Type
1	E	773	LEU
1	E	776	ILE
1	E	801	LEU
2	F	771	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	GLN
1	A	482	HIS
1	A	505	HIS
1	A	520	HIS
1	A	585	ASN
1	C	365	GLN
1	C	482	HIS
1	C	505	HIS
1	C	520	HIS
1	C	585	ASN
1	E	365	GLN
1	E	482	HIS
1	E	495	HIS
1	E	505	HIS
1	E	520	HIS
1	E	585	ASN
1	E	803	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	356/584 (60%)	-0.24	0	100	100	43, 51, 72, 87	0
1	C	376/584 (64%)	-0.26	0	100	100	43, 51, 86, 116	0
1	E	397/584 (67%)	-0.26	1 (0%)	91	48	43, 52, 114, 120	0
2	B	18/18 (100%)	-0.28	0	100	100	48, 55, 67, 68	0
2	D	18/18 (100%)	-0.39	0	100	100	48, 55, 67, 68	0
2	F	18/18 (100%)	-0.28	0	100	100	48, 55, 67, 68	0
All	All	1183/1806 (65%)	-0.26	1 (0%)	93	63	43, 51, 85, 120	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	824	TRP	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.