



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:05 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

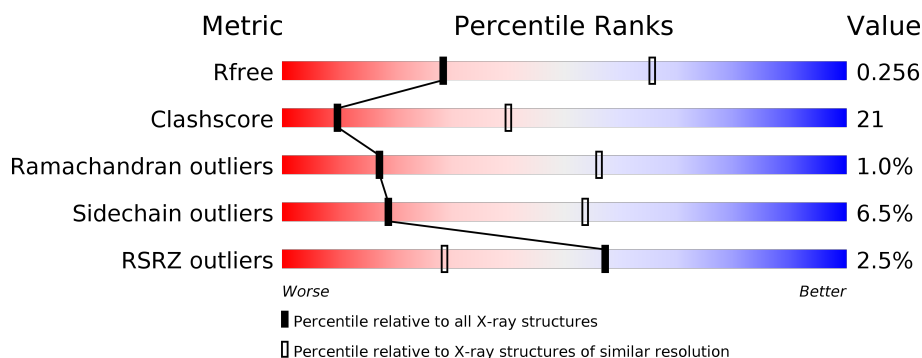
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (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 ≥ 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	584	<div> <div>2%</div> <div> <div>41%</div> <div>18%</div> <div>•</div> <div>39%</div> </div> </div>
1	C	584	<div> <div>%</div> <div> <div>45%</div> <div>18%</div> <div>•</div> <div>36%</div> </div> </div>
1	E	584	<div> <div>2%</div> <div> <div>45%</div> <div>20%</div> <div>•</div> <div>32%</div> </div> </div>
2	B	18	<div> <div>72%</div> <div>22%</div> <div>6%</div> </div>
2	D	18	<div> <div>78%</div> <div>17%</div> <div>6%</div> </div>
2	F	18	<div> <div>6%</div> <div> <div>83%</div> <div>11%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9099 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 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	0	0	0
			141	82	22	37			
2	D	18	Total	C	N	O	0	0	0
			141	82	22	37			
2	F	18	Total	C	N	O	0	0	0
			141	82	22	37			

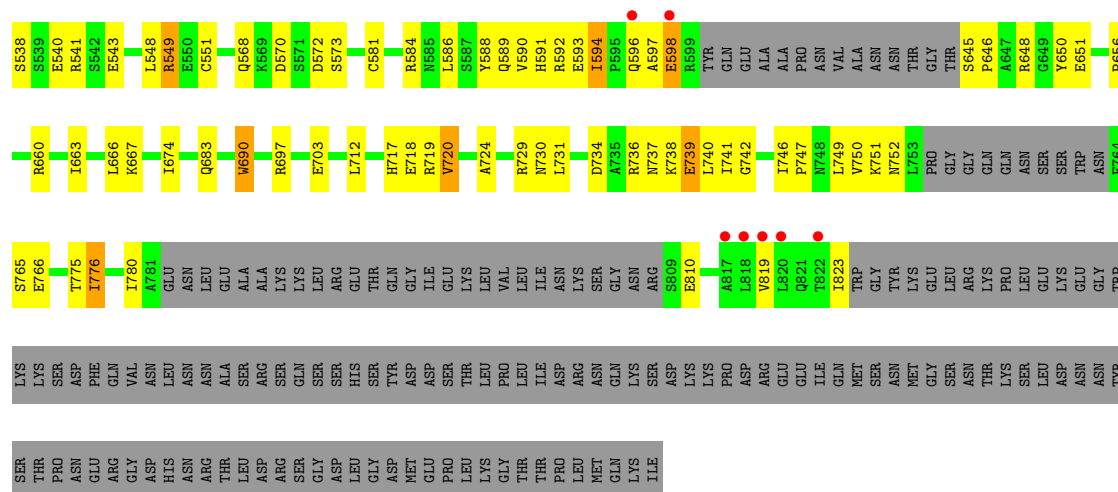
- Molecule 3 is water.

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

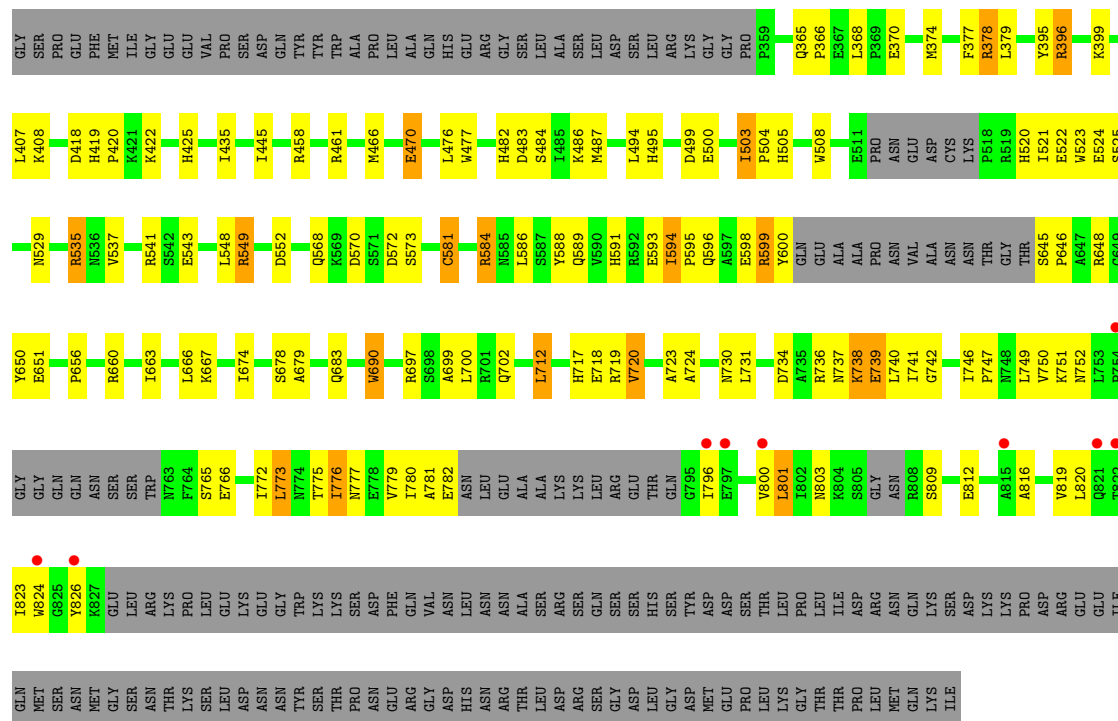
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total 3	O 3	0	0
3	E	23	Total 23	O 23	0	0
3	F	5	Total 5	O 5	0	0



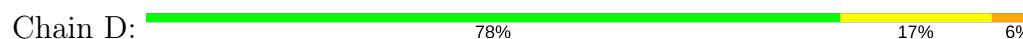
• Molecule 1: Catenin delta-1



• Molecule 2: E-cadherin

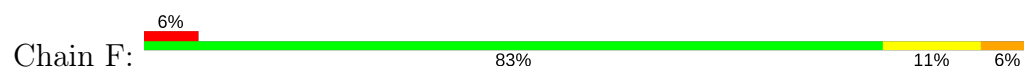


• Molecule 2: E-cadherin





● Molecule 2: E-cadherin



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.81 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.264 0.225 , 0.256	Depositor DCC
R_{free} test set	2178 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.014 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9099	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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	2725	0	2718	118	0
1	C	2853	0	2817	110	0
1	E	3045	0	3043	140	0
2	B	141	0	107	6	0
2	D	141	0	107	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 21.

All (370) 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: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
2:B:774:LEU:O	2:B:775:HIS:HB3	1.78	0.84
1:C:549:ARG:NH2	1:C:593:GLU:OE1	2.11	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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:SER:N	1:A:646:PRO:HD2	2.14	0.62
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:A:645:SER:N	1:A:646:PRO:CD	2.63	0.62
1:C:422:LYS:HA	1:C:425:HIS:NE2	2.14	0.62
1:E:663:ILE:HG22	1:E:667:LYS:HE3	1.81	0.61
1:C:596:GLN:N	1:C:596:GLN:OE1	2.33	0.61
1:E:781:ALA:O	1:E:782:GLU:CB	2.47	0.61
1:E:487:MET:HG2	1:E:541:ARG:HD3	1.81	0.61
1:C:486:LYS:HD3	1:C:537:VAL:HA	1.83	0.61
2:F:771:LEU:HD12	2:F:774:LEU:HD12	1.82	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:C:741:ILE:HG23	1:C:742:GLY:N	2.15	0.61
1:E:520:HIS:CD2	1:E:521:ILE:N	2.68	0.61
1:A:741:ILE:HG23	1:A:742:GLY:N	2.13	0.60
1:A:749:LEU:HB3	1:A:776:ILE:HD11	1.81	0.60
1:A:477:TRP:CE2	2:B:761:GLY:HA3	2.35	0.60
1:E:494:LEU:HD13	1:E:548:LEU:HD22	1.79	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:A:667:LYS:NZ	1:A:704:LYS:NZ	2.51	0.58
1:E:801:LEU:C	1:E:801:LEU:CD2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:780:ILE:O	1:A:780:ILE:HG13	2.03	0.57
1:E:801:LEU:HD23	1:E:801:LEU:C	2.25	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:C:477:TRP:CE3	1:C:529:ASN:HA	2.40	0.56
1:E:782:GLU:HA	1:E:826:TYR:OH	2.05	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:A:482:HIS:CD2	1:A:484:SER:H	2.25	0.55
1:E:820:LEU:C	1:E:823:ILE:HG22	2.26	0.55
1:A:445:ILE:HD11	1:A:482:HIS:NE2	2.21	0.55
1:E:648:ARG:O	1:E:651:GLU:HG2	2.07	0.55
1:A:765:SER:OG	1:A:766:GLU:N	2.39	0.55
2:D:774:LEU:O	2:D:775:HIS:CB	2.48	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:C	1:C:650:TYR:CD1	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
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
2:F:774:LEU:O	2:F:775:HIS:CB	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:GLU:OE1	1:C:524:GLU:N	2.38	0.53
1:C:541:ARG:NH1	3:C:1:HOH:O	2.42	0.53
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
1:E:666:LEU:HD22	1:E:712:LEU:HD21	1.90	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:A:741:ILE:CG2	1:A:742:GLY:N	2.73	0.52
1:E:823:ILE:HG23	1:E:824:TRP:N	2.24	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:A:451:ASP:O	1:A:454:PRO:HD2	2.10	0.51
1:C:588:TYR:CE2	1:C:589:GLN:HG3	2.44	0.51
1:E:650:TYR:CD1	1:E:650:TYR:C	2.83	0.51
1:E:737:ASN:O	1:E:739:GLU:N	2.43	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:A:374:MET:HA	1:A:377:PHE:CD1	2.45	0.51
1:C:494:LEU:CD1	1:C:548:LEU:CD2	2.80	0.51
1:C:648:ARG:O	1:C:651:GLU:CG	2.59	0.51
1:E:773:LEU:CD1	1:E:816:ALA:N	2.74	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:A:482:HIS:HD2	1:A:484:SER:H	1.60	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: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:A:591:HIS:HB3	1:A:690:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:418:ASP:OD2	1:C:458:ARG:NH1	2.43	0.49
1:C:482:HIS:CD2	1:C:484:SER:H	2.30	0.49
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:524:GLU:OE1	1:E:524:GLU:N	2.44	0.49
1:E:749:LEU:HB3	1:E:776:ILE:CD1	2.41	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:A:524:GLU:OE1	1:A:524:GLU:N	2.43	0.48
1:A:557:ALA:O	1:A:561:ILE:HG13	2.14	0.48
1:A:683:GLN:HG3	1:A:730:ASN:ND2	2.28	0.48
1:C:823:ILE:HD12	1:C:823:ILE:H	1.79	0.48
1:E:752:ASN:CB	1:E:772:ILE:HD13	2.44	0.48
1:A:500:GLU:O	1:A:504:PRO:HG2	2.14	0.48
1:A:667:LYS:HZ3	1:A:704:LYS:HE2	1.78	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:390:LEU:HD12	1:C:390:LEU:HA	1.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:749:LEU:HB3	1:A:776:ILE:CD1	2.44	0.47
1:E:734:ASP:O	1:E:736:ARG:HG3	2.14	0.47
1:E:775:THR:O	1:E:779:VAL:HG23	2.14	0.47
1:C:477:TRP:CZ2	2:D:761:GLY:HA3	2.50	0.47
1:E:741:ILE:CG2	1:E:742:GLY:N	2.77	0.47
1:A:667:LYS:HZ3	1:A:704:LYS:NZ	2.11	0.47
1:C:666:LEU:HD22	1:C:712:LEU:HD21	1.96	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:483:ASP:HA	1:E:486:LYS:HG3	1.97	0.46
1:E:749:LEU:HD11	1:E:775:THR:HG22	1.96	0.46
1:C:648:ARG:O	1:C:651:GLU:HG2	2.15	0.46
1:A:558:LEU:CD1	1:A:582:LEU:HD23	2.46	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:683:GLN:HG3	1:C:730:ASN:ND2	2.31	0.46
1:C:819:VAL:O	1:C:823:ILE:HD12	2.15	0.46
1:C:449:ASN:O	1:E:495:HIS:HB3	2.16	0.46
1:C:540:GLU:CB	1:E:596:GLN:NE2	2.69	0.46
1:A:572:ASP:HA	1:A:674:ILE:HD12	1.98	0.46
1:A:749:LEU:HD11	1:A:775:THR:HG22	1.98	0.46
1:C:494:LEU:CD1	1:C:548:LEU:HD22	2.44	0.46
1:C:749:LEU:HB3	1:C:776:ILE:CD1	2.45	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:498:THR:O	1:A:503:ILE:HG13	2.16	0.46
1:A:734:ASP:O	1:A:736:ARG:HG3	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:410:ILE:N	1:C:411:PRO:CD	2.79	0.45
1:C:746:ILE:HB	1:C:747:PRO:HD3	1.98	0.45
1:A:503:ILE:HB	1:A:504:PRO:HD3	1.99	0.45
1:C:697:ARG:NH1	1:C:734:ASP:OD1	2.49	0.45
1:A:505:HIS:CE1	1:A:523:TRP:CE3	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:TRP:HH2	1:E:648:ARG:NH2	2.01	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:370:GLU:O	1:C:374:MET:HG3	2.17	0.45
1:C:650:TYR:CD1	1:C:651:GLU:N	2.84	0.45
1:E:572:ASP:HA	1:E:674:ILE:HD12	1.99	0.45
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:436:SER:O	1:A:444:LYS:HE3	2.17	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: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:407:LEU:O	1:A:408:LYS:HB2	2.18	0.44
1:A:737:ASN:C	1:A:739:GLU:N	2.70	0.44
1:A:650:TYR:CD1	1:A:651:GLU:N	2.85	0.44
1:A:667:LYS:NZ	1:A:704:LYS:HZ1	2.15	0.44
1:E:820:LEU:HA	1:E:823:ILE:HG22	2.00	0.44
1:A:482:HIS:CD2	1:A:484:SER:HB2	2.53	0.43
1:A:538:SER:HB3	1:A:548:LEU:HD12	2.00	0.43
1:E:494:LEU:CD1	1:E:548:LEU:HD22	2.46	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:395:TYR:CE2	1:E:396:ARG:HG3	2.54	0.43
1:E:656:PRO:O	1:E:660:ARG:HG3	2.19	0.43
1:E:777:ASN:HB2	1:E:819:VAL:HG22	2.00	0.43
1:A:367:GLU:O	1:A:371:VAL:HG23	2.19	0.43
1:A:729:ARG:HB2	1:A:775:THR:OG1	2.19	0.43
1:C:477:TRP:CE2	2:D:761:GLY:HA3	2.54	0.43
1:E:419:HIS:HA	1:E:420:PRO:HD3	1.88	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:C:505:HIS:CE1	1:C:523:TRP:CE3	3.07	0.42
1:E:521:ILE:HG12	1:E:522:GLU:N	2.33	0.42
1:A:558:LEU:HD11	1:A:582:LEU:CD2	2.48	0.42
1:C:503:ILE:HB	1:C:504:PRO:CD	2.47	0.42
1:E:435:ILE:O	1:E:435:ILE:HG22	2.19	0.42
1:A:395:TYR:CE2	1:A:396:ARG:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:GLU:OE2	1:A:765:SER:CB	2.59	0.42
1:C:538:SER:HB3	1:C:548:LEU:HD12	2.00	0.42
1:C:737:ASN:O	1:C:739:GLU:N	2.53	0.42
2:D:771:LEU:HA	2:D:771:LEU:HD12	1.72	0.42
1:E:740:LEU:HA	1:E:740:LEU:HD23	1.86	0.42
1:A:390:LEU:HA	1:A:390:LEU:HD12	1.48	0.42
1:C:498:THR:O	1:C:503:ILE:HG13	2.18	0.42
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:A:749:LEU:CD1	1:A:775:THR:HG22	2.50	0.42
1:A:433:LYS:NZ	2:B:765:GLU:HG3	2.34	0.42
1:C:740:LEU:HD23	1:C:740:LEU:HA	1.87	0.42
1:E:746:ILE:HB	1:E:747:PRO:CD	2.50	0.42
1:A:466:MET:CE	1:A:523:TRP:CD1	3.03	0.42
1:A:505:HIS:CD2	1:A:522:GLU:OE2	2.57	0.42
1:A:717:HIS:O	1:A:720:VAL:HG13	2.20	0.42
1:C:407:LEU:O	1:C:408:LYS:HB2	2.20	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:E:766:GLU:HG2	1:E:812:GLU:OE1	2.19	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:A:542:SER:HA	1:A:545:ARG:NH2	2.35	0.41
1:C:737:ASN:C	1:C:739:GLU:N	2.71	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:C:656:PRO:O	1:C:660:ARG:HG3	2.21	0.41
1:E:796:ILE:O	1:E:796:ILE:HG22	2.20	0.41
1:E:781:ALA:O	1:E:782:GLU:HB2	2.19	0.41
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.89	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:E:746:ILE:H	1:E:746:ILE:HG12	1.72	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:505:HIS:CE1	1:E:523:TRP:CE3	3.09	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:820:LEU:CA	1:E:823:ILE:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:LYS:HZ2	1:A:704:LYS:NZ	2.18	0.41
1:E:666:LEU:HD21	1:E:678:SER:HB2	2.03	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:A:441:GLN:OE1	1:A:444:LYS:HD2	2.21	0.40
1:A:486:LYS:CD	1:A:537:VAL:HA	2.47	0.40
1:E:650:TYR:CD1	1:E:651:GLU:N	2.90	0.40
1:E:796:ILE:HD11	1:E:823:ILE:HD13	2.00	0.40
1:A:359:PRO:HA	1:A:360:PRO:HD2	1.96	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
2:F:771:LEU:HA	2:F:771:LEU:HD12	1.70	0.40
1:A:419:HIS:ND1	1:A:420:PRO:HD2	2.36	0.40
1:A:663:ILE:O	1:A:667:LYS:HG3	2.21	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%)	43	80
1	C	366/584 (63%)	340 (93%)	20 (6%)	6 (2%)	11	43
1	E	385/584 (66%)	360 (94%)	21 (6%)	4 (1%)	17	56
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%)	17	56

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
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%)	20	55
1	C	298/503 (59%)	280 (94%)	18 (6%)	21	57
1	E	320/503 (64%)	297 (93%)	23 (7%)	16	49
2	B	15/15 (100%)	14 (93%)	1 (7%)	18	52
2	D	15/15 (100%)	14 (93%)	1 (7%)	18	52
2	F	15/15 (100%)	14 (93%)	1 (7%)	18	52
All	All	951/1554 (61%)	889 (94%)	62 (6%)	19	54

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	356/584 (60%)	-0.19	12 (3%) 45 19	43, 51, 72, 87	0
1	C	376/584 (64%)	-0.18	7 (1%) 66 37	43, 51, 86, 116	0
1	E	397/584 (67%)	-0.17	9 (2%) 60 31	43, 52, 114, 120	0
2	B	18/18 (100%)	-0.20	0 100 100	48, 55, 67, 68	0
2	D	18/18 (100%)	-0.35	0 100 100	48, 55, 67, 68	0
2	F	18/18 (100%)	-0.19	1 (5%) 24 8	48, 55, 67, 68	0
All	All	1183/1806 (65%)	-0.18	29 (2%) 57 29	43, 51, 85, 120	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	824	TRP	5.2
1	A	512	PRO	3.9
1	A	774	ASN	3.7
1	E	796	ILE	3.6
1	E	754	PRO	3.6
1	A	780	ILE	3.5
1	E	797	GLU	3.3
1	C	817	ALA	3.0
1	E	815	ALA	2.9
1	E	800	VAL	2.8
1	E	826	TYR	2.8
1	A	773	LEU	2.7
2	F	775	HIS	2.7
1	E	822	THR	2.6
1	C	819	VAL	2.5
1	C	596	GLN	2.5
1	A	359	PRO	2.5
1	E	821	GLN	2.5
1	A	746	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	775	THR	2.3
1	A	781	ALA	2.3
1	C	818	LEU	2.2
1	C	598	GLU	2.2
1	A	777	ASN	2.2
1	A	771	SER	2.2
1	C	822	THR	2.1
1	A	770	ILE	2.1
1	C	820	LEU	2.1
1	A	596	GLN	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.