



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2022 – 06:14 pm GMT

PDB ID : 8BEN  
Title : LRR domain Structure of the LRRC8C protein  
Authors : Sawicka, M.; Dutzler, R.  
Deposited on : 2022-10-21  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

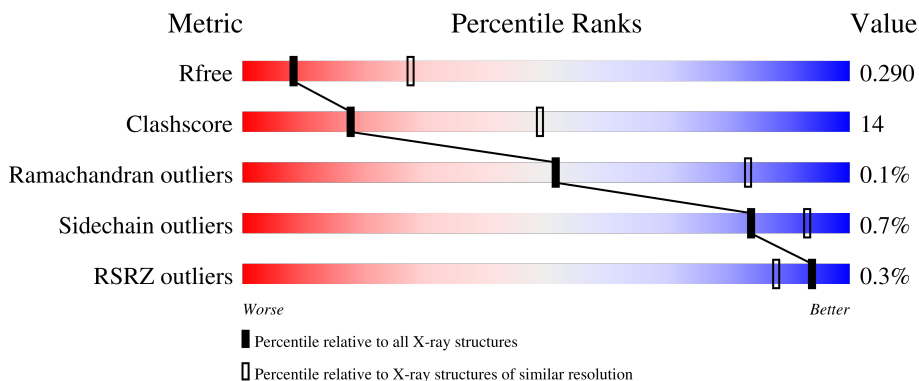
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	412	
1	B	412	
1	C	412	
1	D	412	

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 13038 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 Volume-regulated anion channel subunit LRRC8C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	3249	2094	546	593	16	0	0	0
1	B	406	3266	2104	549	597	16	0	0	0
1	C	408	3287	2116	553	602	16	0	0	0
1	D	401	3236	2086	544	590	16	0	0	0

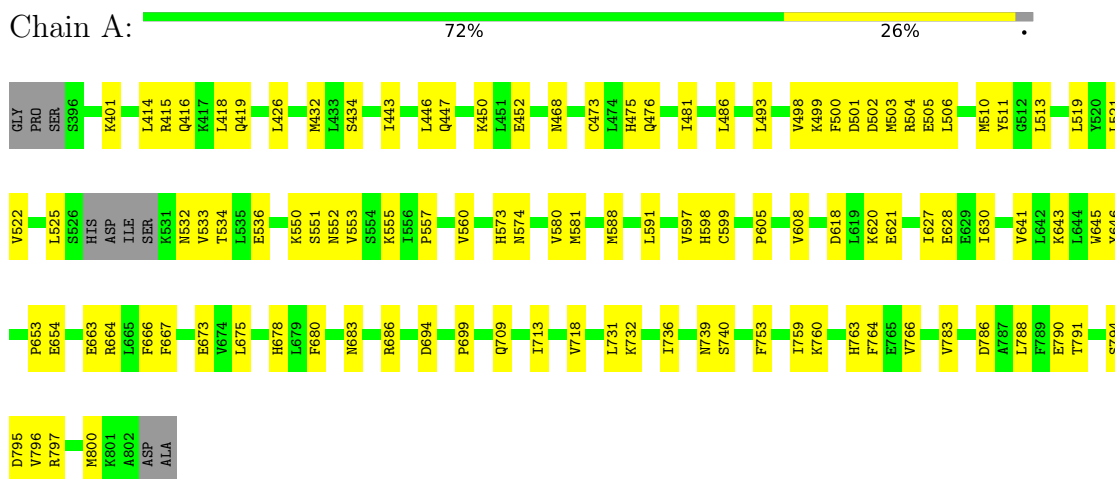
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	GLY	-	expression tag	UNP Q8R502
A	394	PRO	-	expression tag	UNP Q8R502
A	395	SER	-	expression tag	UNP Q8R502
A	804	ALA	-	expression tag	UNP Q8R502
B	393	GLY	-	expression tag	UNP Q8R502
B	394	PRO	-	expression tag	UNP Q8R502
B	395	SER	-	expression tag	UNP Q8R502
B	804	ALA	-	expression tag	UNP Q8R502
C	393	GLY	-	expression tag	UNP Q8R502
C	394	PRO	-	expression tag	UNP Q8R502
C	395	SER	-	expression tag	UNP Q8R502
C	804	ALA	-	expression tag	UNP Q8R502
D	393	GLY	-	expression tag	UNP Q8R502
D	394	PRO	-	expression tag	UNP Q8R502
D	395	SER	-	expression tag	UNP Q8R502
D	804	ALA	-	expression tag	UNP Q8R502

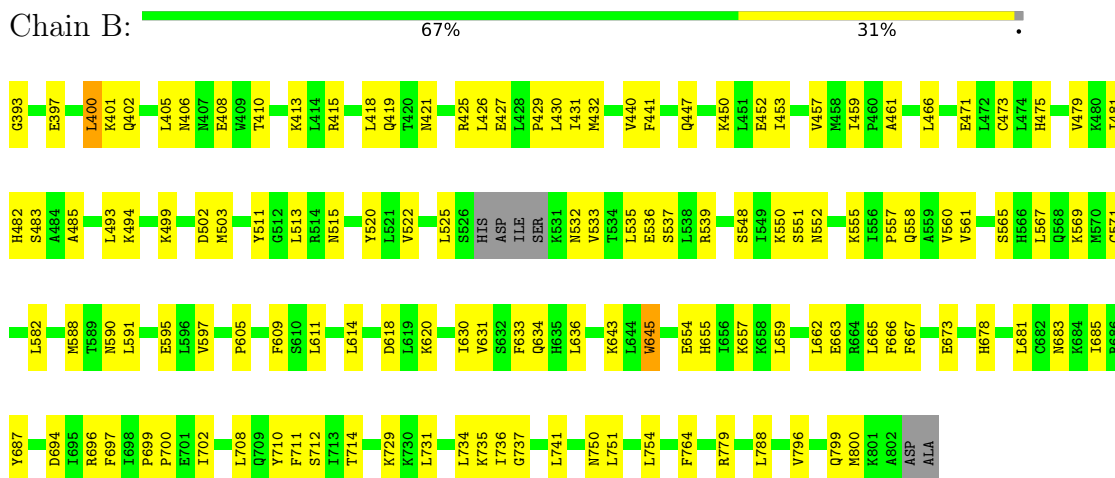
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Volume-regulated anion channel subunit LRRC8C

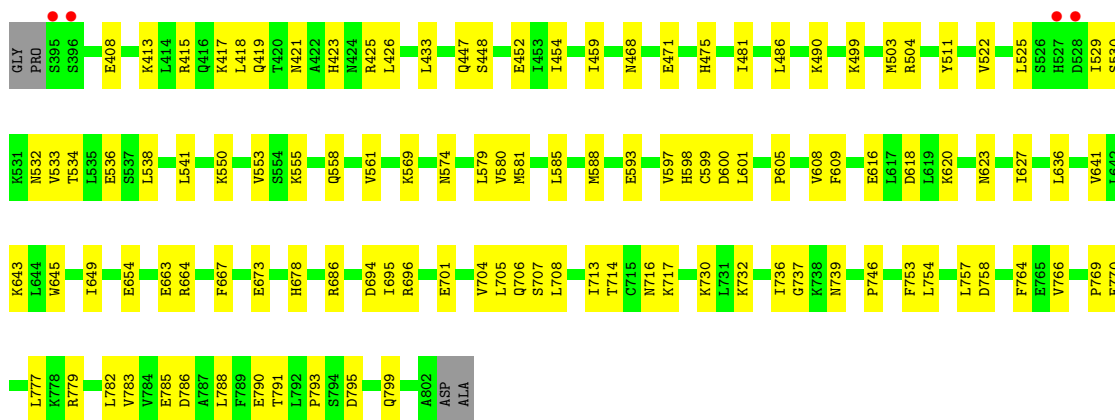


- Molecule 1: Volume-regulated anion channel subunit LRRC8C

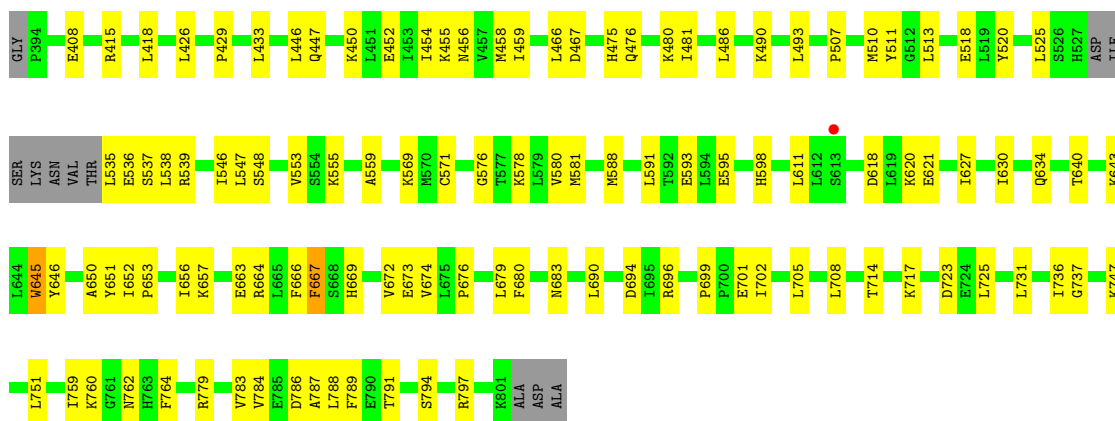


- Molecule 1: Volume-regulated anion channel subunit LRRC8C





● Molecule 1: Volume-regulated anion channel subunit LRRC8C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.38Å 104.73Å 111.83Å 90.00° 94.71° 90.00°	Depositor
Resolution (Å)	49.19 – 3.10 49.19 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.19-3.10) 98.9 (49.19-3.10)	Depositor EDS
$R_{merge}$	0.35	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.241 , 0.290 0.241 , 0.290	Depositor DCC
$R_{free}$ test set	2006 reflections (6.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.238	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	13038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.48% 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 [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	0.39	1/3305 (0.0%)	0.56	0/4465
1	B	0.42	0/3323	0.59	1/4490 (0.0%)
1	C	0.35	0/3345	0.54	0/4521
1	D	0.33	0/3294	0.56	2/4450 (0.0%)
All	All	0.37	1/13267 (0.0%)	0.56	3/17926 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	599	CYS	CB-SG	-5.58	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	LEU	CB-CG-CD1	-7.00	99.10	111.00
1	D	537	SER	N-CA-CB	-5.58	102.13	110.50
1	D	786	ASP	CB-CG-OD2	5.17	122.95	118.30

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	3249	0	3403	111	0
1	B	3266	0	3418	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3287	0	3436	74	0
1	D	3236	0	3383	85	0
All	All	13038	0	13640	363	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 14.

All (363) 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:620:LYS:HE3	1:A:645:TRP:CZ3	1.28	1.66
1:A:620:LYS:CE	1:A:645:TRP:CZ3	1.99	1.45
1:A:645:TRP:HE3	1:A:646:TYR:CD1	1.47	1.32
1:A:620:LYS:CE	1:A:645:TRP:CH2	2.12	1.32
1:A:620:LYS:NZ	1:A:645:TRP:CH2	1.99	1.29
1:A:645:TRP:CE3	1:A:646:TYR:CD1	2.25	1.23
1:A:481:ILE:HD12	1:A:486:LEU:CB	1.75	1.17
1:A:481:ILE:CD1	1:A:486:LEU:HB2	1.76	1.14
1:A:645:TRP:HE3	1:A:646:TYR:CE1	1.66	1.12
1:A:588:MET:HB3	1:A:591:LEU:HD13	1.27	1.12
1:A:481:ILE:HD13	1:A:486:LEU:HD13	1.34	1.08
1:B:561:VAL:HA	1:B:588:MET:HE1	1.28	1.08
1:A:645:TRP:CE3	1:A:646:TYR:CE1	2.42	1.07
1:A:620:LYS:NZ	1:A:645:TRP:HH2	1.42	1.02
1:A:620:LYS:CD	1:A:645:TRP:CH2	2.43	1.01
1:A:481:ILE:CD1	1:A:486:LEU:HD13	1.90	1.01
1:A:620:LYS:HD2	1:A:645:TRP:CH2	1.95	1.01
1:A:502:ASP:HB3	1:A:504:ARG:HG2	1.42	1.00
1:D:535:LEU:HD12	1:D:536:GLU:H	1.26	1.00
1:A:620:LYS:HD2	1:A:645:TRP:CZ2	1.98	0.98
1:C:701:GLU:O	1:C:704:VAL:HG22	1.65	0.97
1:D:588:MET:HB3	1:D:591:LEU:HD13	1.45	0.96
1:D:535:LEU:HD12	1:D:536:GLU:HG2	1.46	0.94
1:A:620:LYS:NZ	1:A:645:TRP:CZ3	2.29	0.93
1:A:432:MET:SD	1:B:400:LEU:HD11	2.10	0.92
1:A:481:ILE:HD11	1:A:486:LEU:HD22	1.56	0.88
1:B:558:GLN:O	1:B:561:VAL:HG22	1.75	0.86
1:A:620:LYS:HE3	1:A:645:TRP:CE3	2.07	0.85
1:B:631:VAL:HG12	1:B:655:HIS:CG	2.12	0.85
1:A:620:LYS:HE3	1:A:645:TRP:HZ3	1.33	0.84
1:B:631:VAL:CG1	1:B:655:HIS:ND1	2.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:VAL:HG23	1:B:479:VAL:HA	1.61	0.82
1:D:535:LEU:CD1	1:D:536:GLU:HG2	2.09	0.81
1:D:667:PHE:HE2	1:D:672:VAL:HG11	1.45	0.81
1:B:734:LEU:HG	1:B:736:ILE:HD13	1.64	0.79
1:B:457:VAL:HG21	1:B:479:VAL:HG22	1.63	0.78
1:A:481:ILE:CD1	1:A:486:LEU:CD1	2.64	0.75
1:D:664:ARG:HH21	1:D:666:PHE:HZ	1.34	0.75
1:A:645:TRP:CE3	1:A:646:TYR:HD1	1.99	0.75
1:A:481:ILE:HD12	1:A:486:LEU:HB2	0.84	0.74
1:A:620:LYS:CE	1:A:645:TRP:HZ3	1.93	0.74
1:A:551:SER:HB3	1:A:553:VAL:HG23	1.70	0.72
1:A:502:ASP:OD1	1:A:503:MET:N	2.22	0.71
1:D:588:MET:HB3	1:D:591:LEU:CD1	2.20	0.71
1:A:504:ARG:HG3	1:A:505:GLU:HG3	1.73	0.71
1:B:502:ASP:OD1	1:B:503:MET:N	2.24	0.70
1:B:532:ASN:HA	1:B:555:LYS:HE3	1.73	0.70
1:A:645:TRP:HE3	1:A:646:TYR:HD1	1.28	0.69
1:B:631:VAL:CG1	1:B:655:HIS:CG	2.75	0.69
1:C:448:SER:HB3	1:C:471:GLU:HB3	1.73	0.69
1:B:419:GLN:NE2	1:B:427:GLU:OE1	2.24	0.69
1:D:535:LEU:CD1	1:D:536:GLU:H	2.04	0.69
1:D:656:ILE:HD13	1:D:679:LEU:HA	1.75	0.69
1:D:535:LEU:HD12	1:D:536:GLU:CG	2.23	0.69
1:C:758:ASP:OD1	1:C:783:VAL:HG13	1.93	0.68
1:A:481:ILE:HD13	1:A:486:LEU:CD1	2.20	0.68
1:A:643:LYS:HB3	1:A:645:TRP:CD1	2.29	0.68
1:B:590:ASN:OD1	1:B:590:ASN:C	2.32	0.67
1:D:535:LEU:HD12	1:D:536:GLU:N	2.05	0.67
1:B:393:GLY:CA	1:C:408:GLU:OE1	2.42	0.67
1:D:664:ARG:NH2	1:D:666:PHE:HZ	1.92	0.67
1:A:795:ASP:OD2	1:D:664:ARG:NH2	2.27	0.67
1:B:533:VAL:HG12	1:B:535:LEU:H	1.59	0.67
1:A:597:VAL:HG13	1:A:620:LYS:HB3	1.77	0.66
1:B:657:LYS:HB2	1:B:681:LEU:HD23	1.77	0.66
1:A:645:TRP:CZ3	1:A:646:TYR:CE1	2.83	0.66
1:A:416:GLN:O	1:D:456:ASN:ND2	2.29	0.65
1:D:667:PHE:CE2	1:D:672:VAL:HG11	2.27	0.65
1:D:525:LEU:HB3	1:D:535:LEU:HD13	1.77	0.65
1:D:620:LYS:HE3	1:D:646:TYR:CD2	2.32	0.65
1:B:421:ASN:ND2	1:B:471:GLU:OE1	2.31	0.64
1:A:401:LYS:HE2	1:A:434:SER:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ARG:HH11	1:B:471:GLU:HB2	1.62	0.64
1:B:525:LEU:HB3	1:B:533:VAL:HG13	1.78	0.64
1:C:785:GLU:OE1	1:C:785:GLU:N	2.24	0.64
1:D:696:ARG:HE	1:D:717:LYS:HD2	1.63	0.64
1:A:764:PHE:HB2	1:A:788:LEU:HD21	1.79	0.64
1:A:620:LYS:HG2	1:A:621:GLU:HG3	1.80	0.63
1:A:506:LEU:HD11	1:A:521:LEU:HD11	1.81	0.63
1:B:631:VAL:HG12	1:B:655:HIS:HB3	1.81	0.63
1:A:555:LYS:NZ	1:A:557:PRO:HA	2.13	0.63
1:A:550:LYS:HD2	1:A:573:HIS:HB2	1.79	0.63
1:C:786:ASP:O	1:C:790:GLU:HG2	1.98	0.63
1:B:631:VAL:HG11	1:B:655:HIS:ND1	2.13	0.63
1:A:732:LYS:HE3	1:A:753:PHE:HB3	1.80	0.62
1:C:764:PHE:HB2	1:C:788:LEU:HD21	1.80	0.62
1:D:760:LYS:HD2	1:D:783:VAL:HG12	1.81	0.62
1:D:764:PHE:HB2	1:D:788:LEU:HD11	1.79	0.62
1:B:537:SER:OG	1:B:539:ARG:HG2	1.99	0.62
1:B:618:ASP:HA	1:B:643:LYS:HB2	1.81	0.62
1:A:481:ILE:CD1	1:A:486:LEU:CG	2.77	0.62
1:B:588:MET:HB3	1:B:591:LEU:HD13	1.80	0.62
1:B:634:GLN:O	1:B:634:GLN:HG3	1.99	0.62
1:B:673:GLU:HG3	1:B:694:ASP:HB3	1.81	0.62
1:D:493:LEU:HD23	1:D:513:LEU:HD13	1.82	0.62
1:C:499:LYS:HG2	1:C:522:VAL:HB	1.82	0.61
1:B:645:TRP:HH2	1:C:799:GLN:OE1	1.82	0.61
1:A:510:MET:HE2	1:A:519:LEU:HD11	1.81	0.61
1:C:529:ILE:HG13	1:C:530:SER:H	1.66	0.61
1:B:631:VAL:HG12	1:B:655:HIS:CB	2.31	0.61
1:C:673:GLU:HG2	1:C:694:ASP:HB3	1.82	0.61
1:B:565:SER:O	1:B:590:ASN:ND2	2.34	0.60
1:A:796:VAL:HG12	1:A:800:MET:HE3	1.82	0.60
1:B:657:LYS:HB3	1:B:678:HIS:HB3	1.84	0.60
1:C:585:LEU:HD12	1:C:588:MET:HG3	1.82	0.60
1:A:481:ILE:CD1	1:A:486:LEU:CB	2.54	0.59
1:B:734:LEU:HG	1:B:736:ILE:CD1	2.31	0.59
1:A:588:MET:HB3	1:A:591:LEU:CD1	2.18	0.59
1:B:533:VAL:HG21	1:B:557:PRO:HG3	1.83	0.59
1:A:443:ILE:HB	1:A:446:LEU:HD23	1.85	0.59
1:C:538:LEU:HB3	1:C:541:LEU:HD23	1.85	0.59
1:D:620:LYS:HE3	1:D:646:TYR:HD2	1.67	0.58
1:B:393:GLY:HA2	1:C:408:GLU:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LYS:O	1:B:405:LEU:HG	2.02	0.58
1:A:740:SER:HA	1:A:763:HIS:CE1	2.39	0.58
1:C:618:ASP:HA	1:C:643:LYS:HB2	1.86	0.57
1:D:630:ILE:HD11	1:D:653:PRO:HG2	1.84	0.57
1:B:494:LYS:HD3	1:B:515:ASN:O	2.03	0.57
1:A:643:LYS:HA	1:A:666:PHE:HB2	1.86	0.57
1:C:736:ILE:O	1:C:739:ASN:ND2	2.38	0.57
1:D:723:ASP:HB3	1:D:747:LYS:HD2	1.86	0.57
1:C:701:GLU:O	1:C:704:VAL:CG2	2.49	0.56
1:D:459:ILE:HB	1:D:481:ILE:HG13	1.87	0.56
1:A:499:LYS:HG2	1:A:522:VAL:HB	1.87	0.56
1:A:500:PHE:HE1	1:A:521:LEU:HD12	1.71	0.56
1:B:764:PHE:HB2	1:B:788:LEU:HD21	1.87	0.56
1:D:415:ARG:HA	1:D:418:LEU:HG	1.88	0.56
1:A:452:GLU:HG2	1:A:475:HIS:HB2	1.88	0.55
1:A:766:VAL:HG23	1:A:791:THR:HB	1.88	0.55
1:B:457:VAL:CG2	1:B:479:VAL:HA	2.34	0.55
1:B:662:LEU:HD21	1:B:665:LEU:HD13	1.89	0.55
1:D:576:GLY:N	1:D:598:HIS:CD2	2.75	0.55
1:D:539:ARG:HH12	1:D:547:LEU:HD22	1.72	0.55
1:C:558:GLN:O	1:C:561:VAL:HG22	2.06	0.55
1:D:656:ILE:CD1	1:D:679:LEU:HA	2.36	0.55
1:C:553:VAL:O	1:C:574:ASN:ND2	2.35	0.55
1:D:620:LYS:HB2	1:D:645:TRP:HE1	1.72	0.55
1:B:558:GLN:OE1	1:B:561:VAL:HG21	2.08	0.54
1:A:654:GLU:HA	1:A:678:HIS:CD2	2.42	0.54
1:B:522:VAL:HA	1:B:550:LYS:HB3	1.89	0.54
1:C:707:SER:HA	1:C:730:LYS:HD2	1.89	0.54
1:D:664:ARG:NH2	1:D:666:PHE:CZ	2.74	0.54
1:A:522:VAL:HA	1:A:550:LYS:HB2	1.89	0.54
1:A:760:LYS:HB2	1:A:783:VAL:HG12	1.89	0.54
1:C:732:LYS:HE2	1:C:753:PHE:HB3	1.90	0.54
1:D:507:PRO:HG2	1:D:510:MET:HB3	1.88	0.54
1:A:786:ASP:O	1:A:790:GLU:HG2	2.07	0.54
1:A:432:MET:CE	1:B:400:LEU:HD11	2.38	0.54
1:A:532:ASN:HA	1:A:555:LYS:HE3	1.89	0.53
1:B:450:LYS:HA	1:B:473:CYS:HB3	1.89	0.53
1:C:447:GLN:HA	1:C:468:ASN:O	2.08	0.53
1:A:506:LEU:CD1	1:A:521:LEU:HD11	2.37	0.53
1:B:590:ASN:OD1	1:B:590:ASN:O	2.27	0.53
1:D:667:PHE:HE2	1:D:672:VAL:CG1	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:VAL:HG22	1:A:664:ARG:HD3	1.91	0.53
1:C:706:GLN:HG3	1:C:707:SER:H	1.74	0.53
1:D:446:LEU:HD11	1:D:466:LEU:HD13	1.90	0.53
1:D:588:MET:CB	1:D:591:LEU:HD13	2.29	0.53
1:A:618:ASP:HA	1:A:643:LYS:HB2	1.90	0.53
1:A:481:ILE:HD11	1:A:486:LEU:CD2	2.33	0.53
1:B:475:HIS:HA	1:B:499:LYS:HB2	1.91	0.53
1:B:551:SER:OG	1:B:552:ASN:N	2.40	0.53
1:A:481:ILE:CD1	1:A:486:LEU:HD22	2.35	0.52
1:C:486:LEU:HD11	1:C:490:LYS:HE3	1.90	0.52
1:C:627:ILE:HD13	1:C:649:ILE:HD13	1.90	0.52
1:A:476:GLN:NE2	1:A:501:ASP:OD2	2.40	0.52
1:D:640:THR:HG23	1:D:663:GLU:HB2	1.92	0.52
1:D:731:LEU:HD23	1:D:751:LEU:HD13	1.91	0.52
1:B:397:GLU:OE2	1:C:417:LYS:NZ	2.43	0.52
1:A:498:VAL:HB	1:A:521:LEU:HD13	1.92	0.52
1:B:432:MET:HG2	1:B:453:ILE:HB	1.92	0.52
1:B:645:TRP:CH2	1:C:799:GLN:OE1	2.62	0.52
1:C:459:ILE:HB	1:C:481:ILE:HG13	1.90	0.52
1:D:680:PHE:HE2	1:D:699:PRO:HG2	1.75	0.52
1:B:796:VAL:O	1:B:799:GLN:HG3	2.10	0.52
1:A:401:LYS:CE	1:A:434:SER:HB3	2.39	0.51
1:A:500:PHE:HB2	1:A:502:ASP:O	2.10	0.51
1:A:510:MET:CE	1:A:519:LEU:HD11	2.39	0.51
1:B:431:ILE:HA	1:B:452:GLU:HB2	1.92	0.51
1:C:522:VAL:HG22	1:C:550:LYS:HD2	1.92	0.51
1:A:447:GLN:HA	1:A:468:ASN:O	2.10	0.51
1:A:500:PHE:CE1	1:A:521:LEU:HD12	2.43	0.51
1:C:600:ASP:OD2	1:C:623:ASN:ND2	2.44	0.51
1:C:499:LYS:HE2	1:C:522:VAL:HG21	1.92	0.51
1:D:450:LYS:HE2	1:D:452:GLU:OE2	2.11	0.51
1:D:578:LYS:HE3	1:D:580:VAL:HG12	1.93	0.51
1:B:729:LYS:HE2	1:B:750:ASN:HB3	1.93	0.51
1:D:705:LEU:HD12	1:D:708:LEU:HD12	1.93	0.51
1:B:736:ILE:HG21	1:B:741:LEU:HD12	1.92	0.51
1:D:683:ASN:OD1	1:D:683:ASN:N	2.44	0.50
1:B:597:VAL:HG22	1:B:620:LYS:HB3	1.92	0.50
1:C:746:PRO:HB3	1:C:770:GLU:HG3	1.93	0.50
1:C:705:LEU:HD23	1:C:708:LEU:HD12	1.93	0.50
1:B:402:GLN:O	1:B:406:ASN:ND2	2.44	0.50
1:A:493:LEU:HD23	1:A:513:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:TYR:CE1	1:C:536:GLU:HB3	2.46	0.50
1:C:599:CYS:O	1:C:601:LEU:N	2.37	0.50
1:D:588:MET:O	1:D:611:LEU:HD22	2.12	0.50
1:B:408:GLU:HG3	1:D:408:GLU:OE1	2.12	0.49
1:A:663:GLU:OE1	1:A:686:ARG:NH1	2.45	0.49
1:B:557:PRO:O	1:B:560:VAL:HG12	2.12	0.49
1:B:731:LEU:HD21	1:B:734:LEU:HD13	1.94	0.49
1:C:452:GLU:HG2	1:C:475:HIS:HB2	1.95	0.49
1:C:766:VAL:HG23	1:C:791:THR:HB	1.94	0.49
1:D:525:LEU:HD22	1:D:535:LEU:HD13	1.94	0.49
1:A:450:LYS:HA	1:A:473:CYS:HB3	1.93	0.49
1:A:481:ILE:HD11	1:A:486:LEU:HD13	1.89	0.49
1:B:582:LEU:HD13	1:B:605:PRO:HB3	1.94	0.49
1:D:486:LEU:HG	1:D:490:LYS:HE2	1.94	0.49
1:D:656:ILE:HD12	1:D:657:LYS:N	2.27	0.49
1:A:511:TYR:CZ	1:A:536:GLU:HB2	2.48	0.49
1:A:709:GLN:HA	1:A:731:LEU:HA	1.95	0.49
1:B:430:LEU:HD11	1:B:440:VAL:HG21	1.95	0.48
1:B:696:ARG:HD2	1:B:697:PHE:CZ	2.48	0.48
1:B:799:GLN:NE2	1:B:800:MET:HG2	2.28	0.48
1:B:441:PHE:HA	1:B:466:LEU:HD21	1.95	0.48
1:C:532:ASN:OD1	1:C:555:LYS:HD3	2.14	0.48
1:C:663:GLU:OE2	1:C:686:ARG:NH1	2.46	0.48
1:B:459:ILE:HB	1:B:481:ILE:HG13	1.95	0.48
1:D:789:PHE:CZ	1:D:797:ARG:HG2	2.48	0.48
1:D:569:LYS:HD2	1:D:593:GLU:OE1	2.13	0.48
1:B:702:ILE:HG12	1:B:702:ILE:O	2.14	0.48
1:C:779:ARG:NH1	1:C:782:LEU:O	2.45	0.48
1:D:458:MET:HA	1:D:480:LYS:O	2.14	0.48
1:A:675:LEU:HD23	1:A:675:LEU:H	1.79	0.47
1:D:511:TYR:OH	1:D:536:GLU:HA	2.13	0.47
1:D:667:PHE:HB3	1:D:690:LEU:HD23	1.96	0.47
1:B:712:SER:HA	1:B:735:LYS:HB2	1.95	0.47
1:D:548:SER:HA	1:D:571:CYS:O	2.15	0.47
1:A:794:SER:HA	1:A:797:ARG:NE	2.30	0.47
1:C:534:THR:O	1:C:534:THR:HG22	2.14	0.47
1:D:651:TYR:HE1	1:D:674:VAL:HB	1.78	0.47
1:C:605:PRO:HG2	1:C:608:VAL:HG23	1.95	0.47
1:C:597:VAL:HG13	1:C:620:LYS:HB3	1.97	0.47
1:C:598:HIS:NE2	1:D:467:ASP:OD2	2.40	0.47
1:A:533:VAL:HB	1:A:557:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ARG:HA	1:C:418:LEU:HG	1.96	0.47
1:A:683:ASN:OD1	1:A:683:ASN:N	2.47	0.46
1:D:426:LEU:H	1:D:447:GLN:HB2	1.79	0.46
1:D:702:ILE:HD13	1:D:725:LEU:HD13	1.97	0.46
1:B:630:ILE:HG23	1:B:659:LEU:HD11	1.98	0.46
1:D:673:GLU:HG2	1:D:694:ASP:HB3	1.96	0.46
1:B:410:THR:HG23	1:B:413:LYS:H	1.79	0.46
1:C:641:VAL:HG22	1:C:664:ARG:HD3	1.98	0.46
1:D:699:PRO:HB2	1:D:701:GLU:OE1	2.16	0.46
1:B:493:LEU:HD23	1:B:513:LEU:HD13	1.98	0.46
1:A:627:ILE:O	1:A:630:ILE:HG12	2.16	0.46
1:B:799:GLN:HE21	1:B:800:MET:HG2	1.81	0.46
1:B:419:GLN:O	1:B:426:LEU:HD23	2.16	0.46
1:B:426:LEU:O	1:B:447:GLN:N	2.42	0.46
1:D:779:ARG:HD3	1:D:789:PHE:CZ	2.51	0.46
1:B:393:GLY:HA3	1:C:408:GLU:OE1	2.14	0.46
1:B:714:THR:HG22	1:B:737:GLY:HA3	1.98	0.46
1:D:553:VAL:HG22	1:D:555:LYS:O	2.16	0.46
1:A:419:GLN:O	1:A:426:LEU:HD12	2.15	0.46
1:C:413:LYS:HD2	1:C:413:LYS:N	2.31	0.45
1:C:580:VAL:HG23	1:C:581:MET:HG3	1.96	0.45
1:D:455:LYS:NZ	1:D:476:GLN:O	2.49	0.45
1:D:518:GLU:HG2	1:D:546:ILE:HB	1.98	0.45
1:A:557:PRO:HG2	1:A:560:VAL:HG23	1.98	0.45
1:D:737:GLY:O	1:D:762:ASN:ND2	2.50	0.45
1:A:605:PRO:HG2	1:A:608:VAL:HG23	1.99	0.45
1:C:758:ASP:CG	1:C:783:VAL:CG1	2.85	0.45
1:D:595:GLU:HG2	1:D:618:ASP:HB3	1.99	0.45
1:A:736:ILE:O	1:A:739:ASN:ND2	2.50	0.44
1:B:654:GLU:O	1:B:657:LYS:HG2	2.16	0.44
1:B:687:TYR:HA	1:B:710:TYR:HB3	1.98	0.44
1:D:759:ILE:HG13	1:D:784:VAL:HG12	1.99	0.44
1:B:588:MET:O	1:B:611:LEU:HD22	2.18	0.44
1:D:520:TYR:HD1	1:D:548:SER:HB3	1.82	0.44
1:D:643:LYS:HA	1:D:666:PHE:HB2	1.99	0.44
1:B:597:VAL:HG22	1:B:620:LYS:H	1.81	0.44
1:C:788:LEU:O	1:C:791:THR:OG1	2.31	0.44
1:D:452:GLU:HG2	1:D:475:HIS:HB2	2.00	0.44
1:A:680:PHE:HE2	1:A:699:PRO:HG2	1.83	0.44
1:A:551:SER:O	1:A:574:ASN:HA	2.18	0.44
1:C:433:LEU:O	1:C:454:ILE:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:ARG:NH2	1:C:717:LYS:HD3	2.33	0.44
1:A:643:LYS:HB3	1:A:645:TRP:NE1	2.33	0.44
1:C:421:ASN:ND2	1:C:471:GLU:OE1	2.50	0.44
1:C:777:LEU:HD21	1:C:782:LEU:HD12	2.00	0.44
1:D:598:HIS:HA	1:D:621:GLU:O	2.18	0.44
1:B:425:ARG:NH1	1:B:471:GLU:HB2	2.32	0.44
1:C:609:PHE:HA	1:C:636:LEU:HD11	2.00	0.44
1:A:673:GLU:HG2	1:A:694:ASP:HB3	2.00	0.43
1:B:425:ARG:HB2	1:B:447:GLN:HB2	2.00	0.43
1:B:657:LYS:HD3	1:B:678:HIS:CD2	2.53	0.43
1:C:525:LEU:HB3	1:C:533:VAL:HG13	1.99	0.43
1:A:740:SER:HA	1:A:763:HIS:ND1	2.33	0.43
1:B:595:GLU:HG2	1:B:618:ASP:HB3	2.00	0.43
1:D:794:SER:HA	1:D:797:ARG:HH21	1.83	0.43
1:B:799:GLN:HE21	1:B:800:MET:CG	2.31	0.43
1:B:663:GLU:HA	1:B:685:ILE:HA	1.99	0.43
1:D:736:ILE:HD12	1:D:759:ILE:HG22	2.00	0.43
1:B:643:LYS:HA	1:B:666:PHE:HB2	1.99	0.43
1:C:423:HIS:HB3	1:C:425:ARG:HH11	1.83	0.43
1:C:754:LEU:HD11	1:C:757:LEU:HB2	2.01	0.43
1:B:614:LEU:HB3	1:B:636:LEU:HD23	2.00	0.43
1:B:657:LYS:HD3	1:B:678:HIS:HD2	1.83	0.43
1:C:419:GLN:O	1:C:426:LEU:HD12	2.19	0.43
1:A:432:MET:SD	1:B:400:LEU:CD1	2.96	0.43
1:C:569:LYS:HG3	1:C:593:GLU:HB3	2.00	0.43
1:A:415:ARG:HA	1:A:418:LEU:HG	2.01	0.43
1:B:511:TYR:CZ	1:B:536:GLU:HB2	2.54	0.42
1:A:628:GLU:OE2	1:A:653:PRO:HG3	2.19	0.42
1:B:645:TRP:N	1:B:645:TRP:CD1	2.87	0.42
1:C:686:ARG:HG2	1:C:707:SER:O	2.19	0.42
1:D:538:LEU:HD23	1:D:559:ALA:HA	2.01	0.42
1:A:675:LEU:HD21	1:A:699:PRO:HD3	2.00	0.42
1:B:482:HIS:ND1	1:B:483:SER:N	2.67	0.42
1:B:633:PHE:HA	1:B:636:LEU:HD13	2.00	0.42
1:B:731:LEU:HD23	1:B:751:LEU:HD13	2.02	0.42
1:C:785:GLU:H	1:C:785:GLU:CD	2.08	0.42
1:B:683:ASN:OD1	1:B:683:ASN:N	2.49	0.42
1:B:796:VAL:O	1:B:800:MET:HG3	2.20	0.42
1:D:525:LEU:HD13	1:D:535:LEU:HD13	2.01	0.42
1:D:650:ALA:O	1:D:672:VAL:HA	2.20	0.42
1:D:760:LYS:HD2	1:D:783:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ALA:HA	1:B:485:ALA:HB2	2.00	0.42
1:B:569:LYS:NZ	1:B:571:CYS:SG	2.90	0.42
1:C:714:THR:HG22	1:C:737:GLY:HA3	2.01	0.42
1:D:787:ALA:O	1:D:791:THR:HG23	2.19	0.42
1:A:580:VAL:HG23	1:A:581:MET:HG3	2.01	0.42
1:D:433:LEU:O	1:D:454:ILE:HG23	2.20	0.42
1:A:736:ILE:HB	1:A:759:ILE:HG22	2.01	0.42
1:B:597:VAL:HG13	1:B:620:LYS:O	2.19	0.42
1:D:652:ILE:O	1:D:676:PRO:HG3	2.20	0.42
1:A:598:HIS:HA	1:A:621:GLU:O	2.20	0.42
1:B:567:LEU:O	1:B:590:ASN:OD1	2.38	0.42
1:D:429:PRO:HA	1:D:450:LYS:HB3	2.02	0.42
1:D:714:THR:HG22	1:D:737:GLY:HA3	2.01	0.41
1:A:551:SER:HB3	1:A:552:ASN:H	1.68	0.41
1:C:418:LEU:HD13	1:C:426:LEU:HD21	2.02	0.41
1:C:579:LEU:HB2	1:C:599:CYS:HB3	2.01	0.41
1:D:784:VAL:HG21	1:D:789:PHE:HB2	2.02	0.41
1:A:551:SER:CB	1:A:553:VAL:HG23	2.44	0.41
1:A:555:LYS:HZ2	1:A:557:PRO:HA	1.82	0.41
1:B:699:PRO:HA	1:B:700:PRO:HD3	1.51	0.41
1:C:503:MET:HB3	1:C:504:ARG:NH2	2.34	0.41
1:C:769:PRO:HB3	1:C:793:PRO:HG2	2.02	0.41
1:B:520:TYR:HD1	1:B:548:SER:HB3	1.86	0.41
1:A:414:LEU:HB3	1:A:443:ILE:HD11	2.03	0.41
1:A:525:LEU:O	1:A:534:THR:HG22	2.20	0.41
1:B:431:ILE:HB	1:B:452:GLU:OE1	2.21	0.41
1:D:651:TYR:CE1	1:D:674:VAL:HB	2.54	0.41
1:C:593:GLU:HG3	1:C:616:GLU:HB2	2.02	0.41
1:C:695:ILE:HD12	1:C:716:ASN:HD21	1.85	0.41
1:C:695:ILE:HD12	1:C:716:ASN:ND2	2.36	0.41
1:B:499:LYS:HG2	1:B:522:VAL:HB	2.02	0.41
1:B:633:PHE:HD1	1:B:636:LEU:HD13	1.86	0.41
1:B:708:LEU:HD21	1:B:711:PHE:HB2	2.02	0.41
1:C:654:GLU:HA	1:C:678:HIS:CD2	2.56	0.41
1:A:432:MET:HE3	1:B:400:LEU:HD11	2.02	0.41
1:C:529:ILE:HG13	1:C:530:SER:N	2.32	0.41
1:A:620:LYS:HZ2	1:A:645:TRP:HH2	0.61	0.40
1:A:739:ASN:HB3	1:A:740:SER:H	1.72	0.40
1:D:646:TYR:CE1	1:D:669:HIS:CG	3.10	0.40
1:A:506:LEU:CD1	1:A:521:LEU:CD1	2.99	0.40
1:A:713:ILE:HD12	1:A:718:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:LYS:HB2	1:D:581:MET:HB2	2.03	0.40
1:B:609:PHE:HA	1:B:636:LEU:HD11	2.03	0.40
1:B:415:ARG:HA	1:B:418:LEU:HG	2.02	0.40
1:C:713:ILE:HD11	1:C:736:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

## 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	399/412 (97%)	373 (94%)	26 (6%)	0	100	100
1	B	402/412 (98%)	373 (93%)	28 (7%)	1 (0%)	47	79
1	C	406/412 (98%)	380 (94%)	26 (6%)	0	100	100
1	D	397/412 (96%)	376 (95%)	20 (5%)	1 (0%)	41	73
All	All	1604/1648 (97%)	1502 (94%)	100 (6%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	627	ILE
1	B	429	PRO

### 5.3.2 Protein sidechains [i](#)

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	381/388 (98%)	380 (100%)	1 (0%)	92	96
1	B	383/388 (99%)	379 (99%)	4 (1%)	76	90
1	C	386/388 (100%)	383 (99%)	3 (1%)	81	92
1	D	380/388 (98%)	377 (99%)	3 (1%)	81	92
All	All	1530/1552 (99%)	1519 (99%)	11 (1%)	84	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	667	PHE
1	B	645	TRP
1	B	667	PHE
1	B	754	LEU
1	B	779	ARG
1	C	645	TRP
1	C	667	PHE
1	C	795	ASP
1	D	634	GLN
1	D	645	TRP
1	D	667	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	799	GLN
1	C	799	GLN
1	D	598	HIS

### 5.3.3 RNA [i](#)

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 monosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	403/412 (97%)	-0.19	0 <a href="#">100</a> <a href="#">100</a>	11, 22, 44, 104	0
1	B	406/412 (98%)	-0.15	0 <a href="#">100</a> <a href="#">100</a>	11, 25, 47, 67	0
1	C	408/412 (99%)	-0.17	4 (0%) <a href="#">82</a> <a href="#">67</a>	11, 23, 48, 88	0
1	D	401/412 (97%)	-0.10	1 (0%) <a href="#">95</a> <a href="#">90</a>	12, 25, 47, 63	0
All	All	1618/1648 (98%)	-0.15	5 (0%) <a href="#">94</a> <a href="#">88</a>	11, 24, 47, 104	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	527	HIS	2.8
1	D	613	SER	2.2
1	C	528	ASP	2.1
1	C	395	SER	2.1
1	C	396	SER	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.