



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:41 PM UTC

PDB ID : 8BEN / pdb_00008ben
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

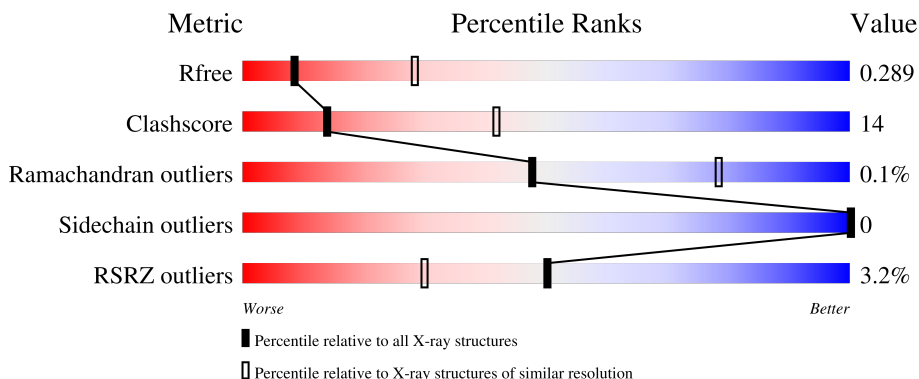
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 ≥ 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	2% 71% 25% ..
1	B	412	3% 65% 33% ..
1	C	412	3% 72% 27% .
1	D	412	5% 69% 28% .

2 Entry composition

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

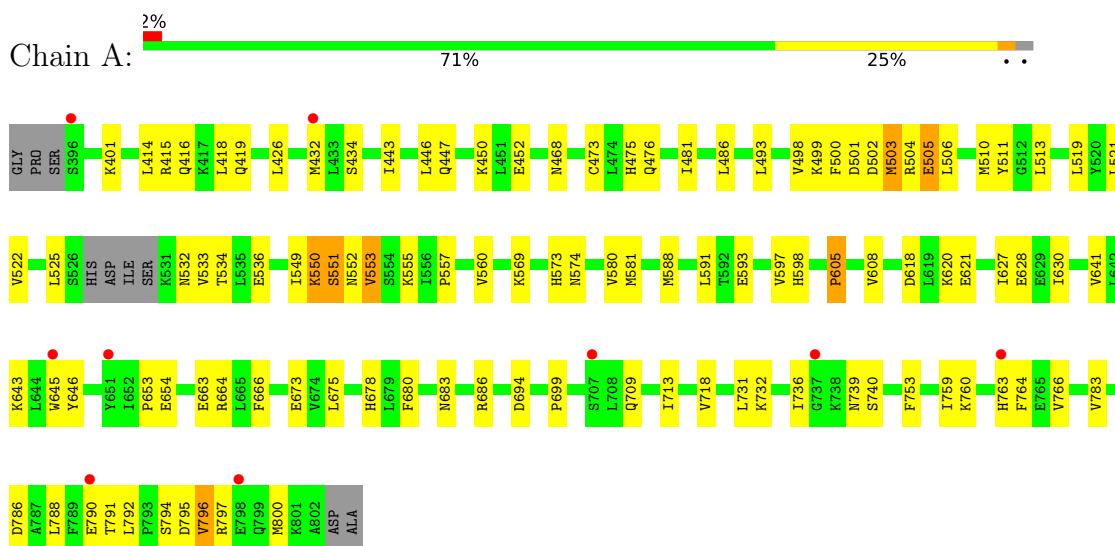
There are 16 discrepancies between the modelled and reference sequences:

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

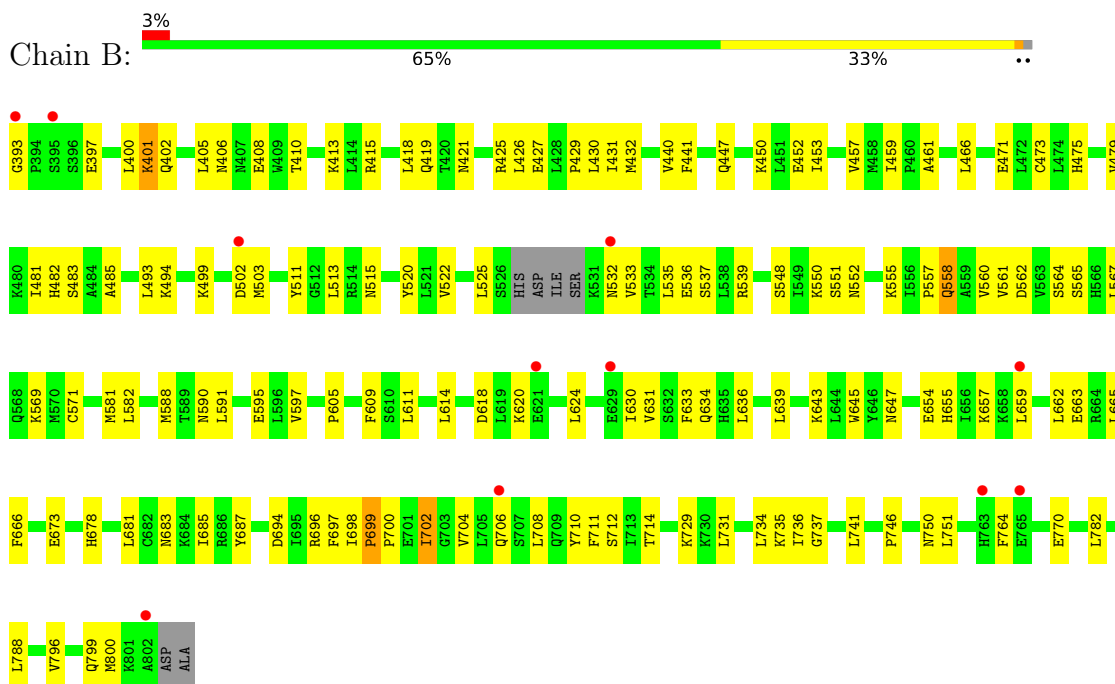
3 Residue-property plots

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.

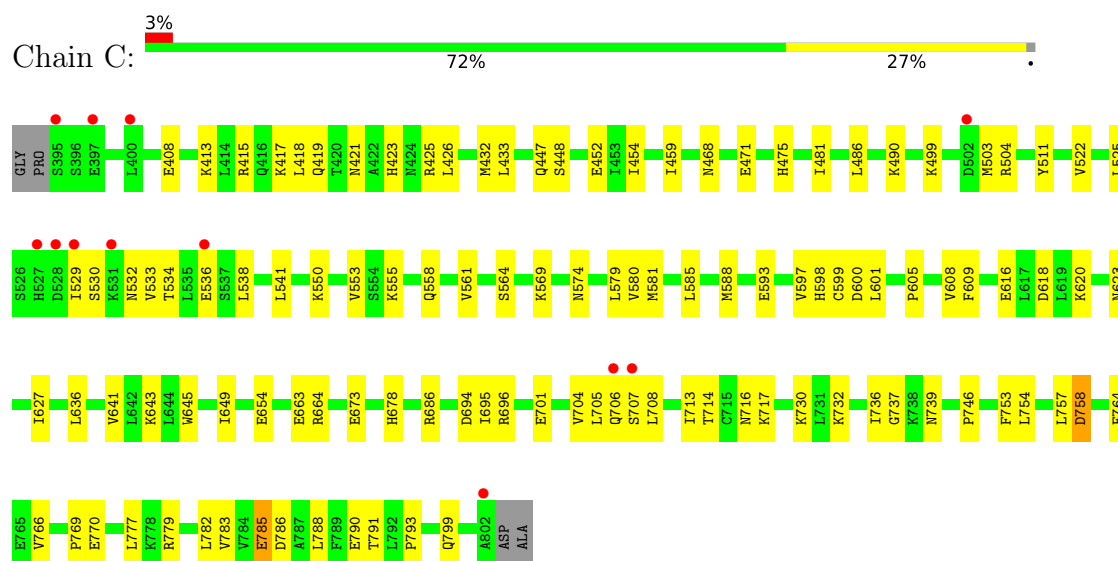
• Molecule 1: Volume-regulated anion channel subunit LRRC8C



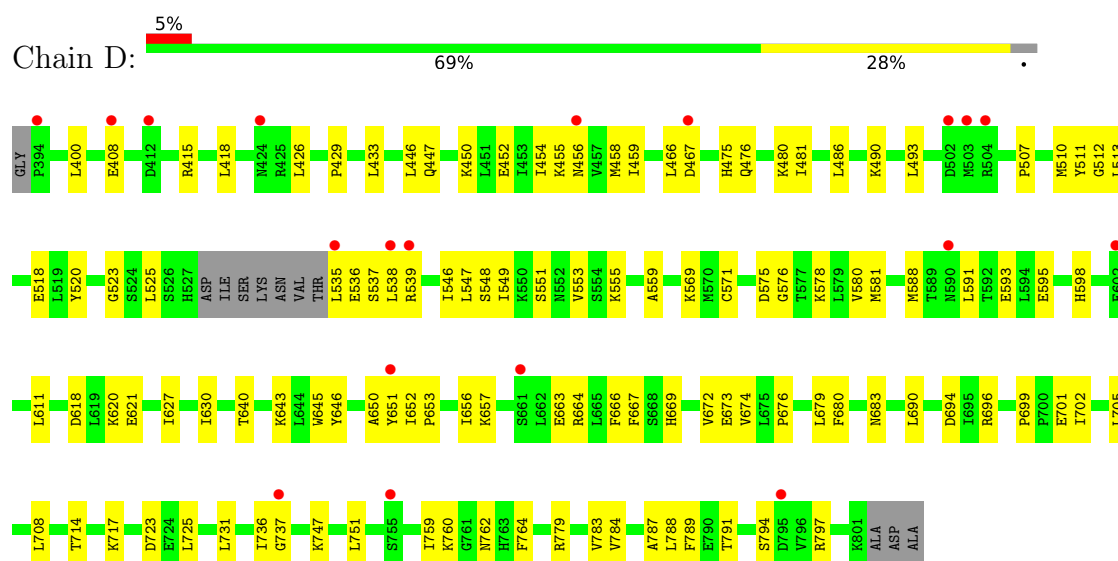
• Molecule 1: Volume-regulated anion channel subunit LRRC8C



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.241 , 0.290 0.240 , 0.289	Depositor DCC
R_{free} test set	2008 reflections (6.52%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13038	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage'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.*

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

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	0.46	6/3305 (0.2%)	0.52	4/4465 (0.1%)
1	B	0.49	8/3323 (0.2%)	0.64	5/4490 (0.1%)
1	C	0.35	2/3345 (0.1%)	0.43	0/4521
1	D	0.30	1/3294 (0.0%)	0.44	1/4450 (0.0%)
All	All	0.41	17/13267 (0.1%)	0.52	10/17926 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	699	PRO	C-O	-11.41	1.15	1.24
1	A	551	SER	C-O	-6.84	1.17	1.24
1	D	549	ILE	C-O	-6.82	1.16	1.24
1	A	549	ILE	C-O	-6.69	1.17	1.24
1	B	704	VAL	C-O	-5.57	1.17	1.24
1	A	553	VAL	C-O	-5.30	1.18	1.24
1	A	605	PRO	C-O	-5.26	1.17	1.23
1	B	558	GLN	CD-OE1	5.23	1.33	1.23
1	B	698	ILE	CA-C	-5.19	1.48	1.52
1	B	702	ILE	N-CA	-5.19	1.40	1.46
1	C	758	ASP	C-O	-5.17	1.18	1.24
1	B	702	ILE	C-O	-5.16	1.17	1.24
1	B	706	GLN	CD-OE1	5.16	1.33	1.23
1	A	550	LYS	C-O	-5.15	1.18	1.24
1	B	698	ILE	C-O	-5.11	1.18	1.24
1	C	785	GLU	C-O	-5.08	1.17	1.23
1	A	551	SER	CA-C	-5.06	1.47	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	699	PRO	CA-C-N	16.32	136.85	119.87
1	B	699	PRO	C-N-CA	16.32	136.85	119.87
1	A	503	MET	N-CA-C	-8.22	103.14	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	LYS	N-CA-C	-6.85	103.50	110.97
1	A	505	GLU	N-CA-C	6.58	120.91	113.02
1	A	796	VAL	N-CA-C	-6.39	104.29	110.42
1	A	505	GLU	N-CA-CB	-6.05	101.69	110.47
1	D	537	SER	N-CA-CB	-5.97	102.13	110.25
1	B	698	ILE	N-CA-C	-5.52	101.88	107.89
1	B	639	LEU	N-CA-C	5.42	117.54	109.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3249	0	3403	116	0
1	B	3266	0	3418	115	0
1	C	3287	0	3436	78	0
1	D	3236	0	3383	90	0
All	All	13038	0	13640	385	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 (385) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:645:TRP:CE3	1:A:646:TYR:CE1	2.42	1.07
1:B:561:VAL:HA	1:B:588:MET:HE1	1.41	1.02
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
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:B:555:LYS:HB3	1:B:581:MET:HE3	1.69	0.74
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:590:ASN:OD1	1:B:590:ASN:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:510:MET:HE2	1:A:519:LEU:HD11	1.82	0.60
1:B:565:SER:O	1:B:590:ASN:ND2	2.34	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:C:785:GLU:H	1:C:785:GLU:CD	2.08	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
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:561:VAL:HA	1:B:588:MET:CE	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:555:LYS:HZ2	1:A:557:PRO:HA	1.70	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:432:MET:HE1	1:D:400:LEU:HD22	1.90	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:569:LYS:NZ	1:A:593:GLU:OE1	2.41	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:A:645:TRP:CD1	1:A:645:TRP:H	2.29	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
1:C:511:TYR:CE1	1:C:536:GLU:HB3	2.46	0.50
1:C:564:SER:HB3	1:C:588:MET:HE2	1.94	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:A:796:VAL:HG12	1:A:800:MET:HE3	1.93	0.49
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:C:758:ASP:CG	1:C:783:VAL:CG1	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:792:LEU:HD13	1:A:800:MET:HE3	1.94	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
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:B:782:LEU:HD22	1:B:800:MET:HE1	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:645:TRP:H	1:B:645:TRP:CD1	2.33	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:B:564:SER:HB3	1:B:588:MET:HE1	1.98	0.45
1:A:476:GLN:HE21	1:A:501:ASP:CG	2.24	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:551:SER:OG	1:B:552:ASN:N	2.40	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:A:663:GLU:CD	1:A:686:ARG:NH1	2.77	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:624:LEU:HB2	1:B:647:ASN:CG	2.44	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:CD1	1:B:645:TRP:N	2.87	0.42
1:B:746:PRO:HB3	1:B:770:GLU:CD	2.44	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:D:575:ASP:C	1:D:598:HIS:CD2	2.97	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:758:ASP:CG	1:C:783:VAL:HG13	2.43	0.42
1:D:450:LYS:HE2	1:D:452:GLU:CD	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:539:ARG:HE	1:B:562:ASP:CG	2.28	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:539:ARG:NE	1:B:562:ASP:CG	2.77	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:532:ASN:CG	1:C:533:VAL:H	2.27	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: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:645:TRP:CD1	1:C:645:TRP:H	2.37	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:D:523:GLY:O	1:D:551:SER:OG	2.35	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:ND2	2.36	0.41
1:C:695:ILE:HD12	1:C:716:ASN:HD21	1.85	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: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:A:503:MET:HE1	1:A:506:LEU:HD23	2.03	0.40
1:D:646:TYR:CE1	1:D:669:HIS:CG	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:490:LYS:NZ	1:D:512:GLY:O	2.54	0.40
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%)	43	73
1	C	406/412 (98%)	380 (94%)	26 (6%)	0	100	100
1	D	397/412 (96%)	376 (95%)	20 (5%)	1 (0%)	36	67
All	All	1604/1648 (97%)	1502 (94%)	100 (6%)	2 (0%)	48	78

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%)	381 (100%)	0	100	100
1	B	383/388 (99%)	383 (100%)	0	100	100
1	C	386/388 (100%)	386 (100%)	0	100	100
1	D	380/388 (98%)	380 (100%)	0	100	100
All	All	1530/1552 (99%)	1530 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	HIS
1	A	573	HIS
1	A	669	HIS
1	B	492	ASN
1	B	558	GLN
1	B	763	HIS
1	B	799	GLN
1	C	476	GLN
1	C	590	ASN
1	C	669	HIS
1	C	683	ASN
1	C	762	ASN
1	C	799	GLN
1	D	573	HIS
1	D	598	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	403/412 (97%)	0.39	9 (2%) 62 41	11, 22, 44, 104	0
1	B	406/412 (98%)	0.44	11 (2%) 56 35	11, 25, 47, 67	0
1	C	408/412 (99%)	0.44	12 (2%) 53 32	11, 23, 48, 88	0
1	D	401/412 (97%)	0.52	19 (4%) 36 19	12, 25, 47, 63	0
All	All	1618/1648 (98%)	0.45	51 (3%) 50 30	11, 24, 47, 104	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	527	HIS	4.6
1	A	645	TRP	3.5
1	A	651	TYR	3.4
1	C	531	LYS	3.4
1	D	394	PRO	3.2
1	A	432	MET	3.2
1	B	502	ASP	3.2
1	D	424	ASN	3.2
1	C	802	ALA	3.2
1	D	661	SER	3.1
1	D	651	TYR	3.0
1	B	802	ALA	3.0
1	D	737	GLY	3.0
1	C	529	ILE	2.9
1	D	412	ASP	2.7
1	D	408	GLU	2.7
1	D	503	MET	2.7
1	C	528	ASP	2.6
1	C	395	SER	2.5
1	B	765	GLU	2.5
1	B	763	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	539	ARG	2.4
1	B	395	SER	2.4
1	B	659	LEU	2.4
1	D	755	SER	2.3
1	C	400	LEU	2.3
1	B	621	GLU	2.2
1	D	535	LEU	2.2
1	D	538	LEU	2.2
1	A	707	SER	2.2
1	C	707	SER	2.2
1	A	737	GLY	2.2
1	A	763	HIS	2.2
1	B	706	GLN	2.2
1	D	590	ASN	2.2
1	B	393	GLY	2.2
1	D	467	ASP	2.2
1	D	602	GLU	2.2
1	C	502	ASP	2.2
1	C	706	GLN	2.1
1	A	396	SER	2.1
1	C	536	GLU	2.1
1	D	795	ASP	2.1
1	A	790	GLU	2.1
1	A	798	GLU	2.1
1	C	397	GLU	2.1
1	B	532	ASN	2.1
1	D	502	ASP	2.1
1	B	629	GLU	2.1
1	D	456	ASN	2.0
1	D	504	ARG	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 oligosaccharides 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.