



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 09:29 PM EDT

PDB ID : 1C8B / pdb_00001c8b
Title : CRYSTAL STRUCTURE OF A NOVEL GERMINATION PROTEASE
FROM SPORES OF BACILLUS MEGATERIUM: STRUCTURAL REAR-
RANGEMENTS AND ZYMOGEN ACTIVATION
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Deposited on : 2000-05-03
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 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

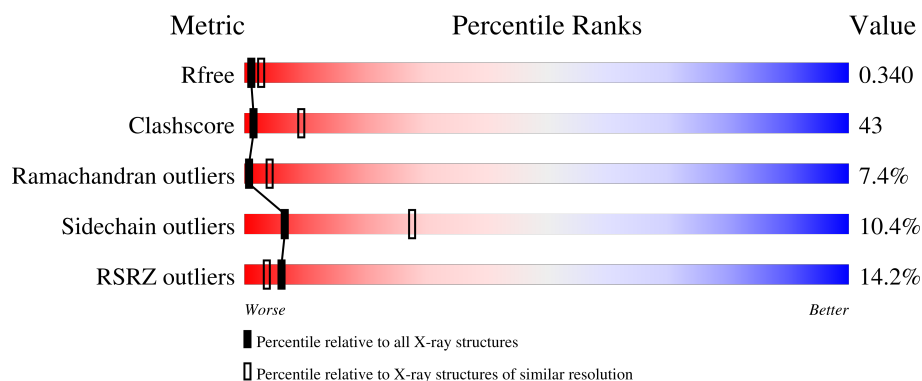
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	371	
1	B	371	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4454 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 SPORE PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2164	1354	372	430	8			
1	B	320	Total	C	N	O	S	0	0	0
			2164	1354	372	430	8			

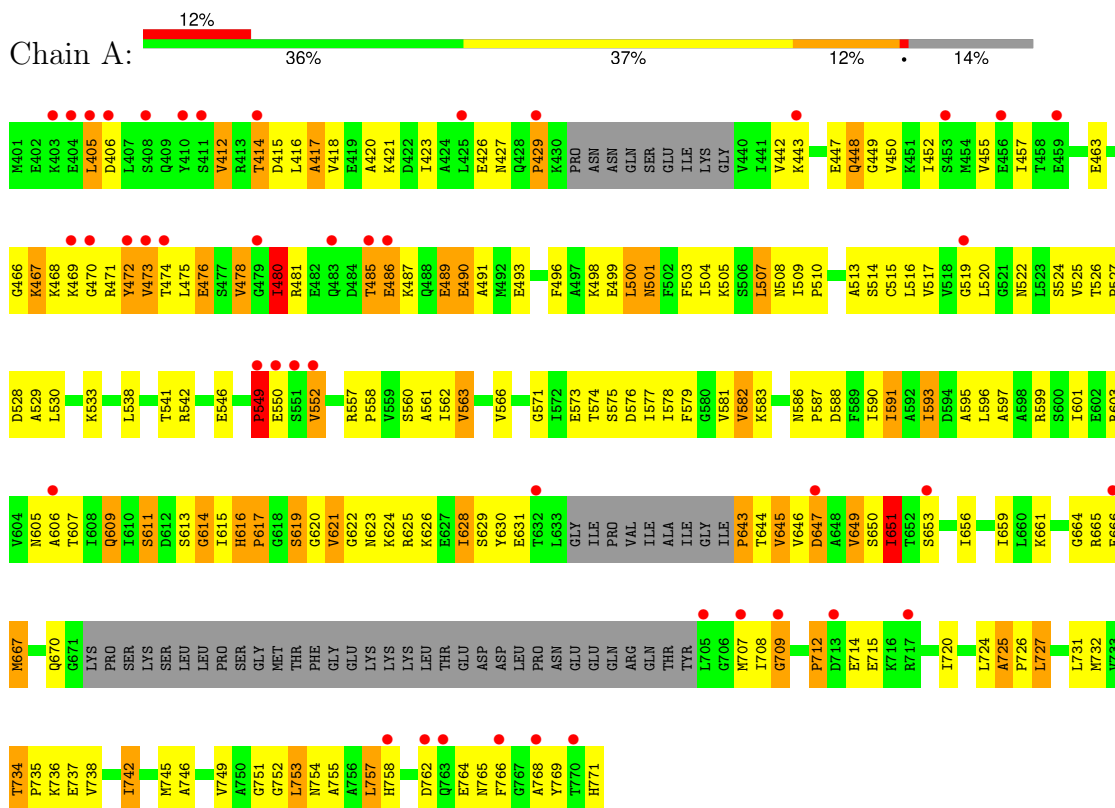
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	63	Total	O	0	0
			63	63		
2	B	63	Total	O	0	0
			63	63		

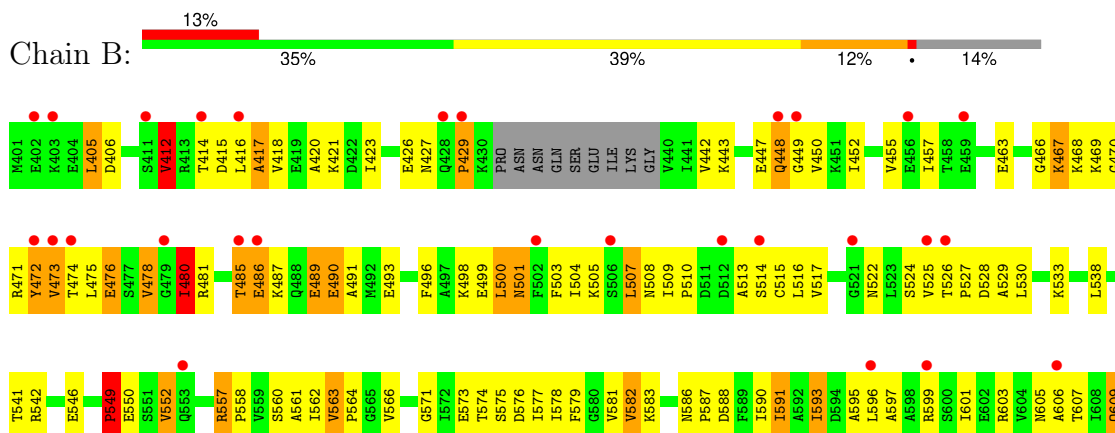
3 Residue-property plots [i](#)

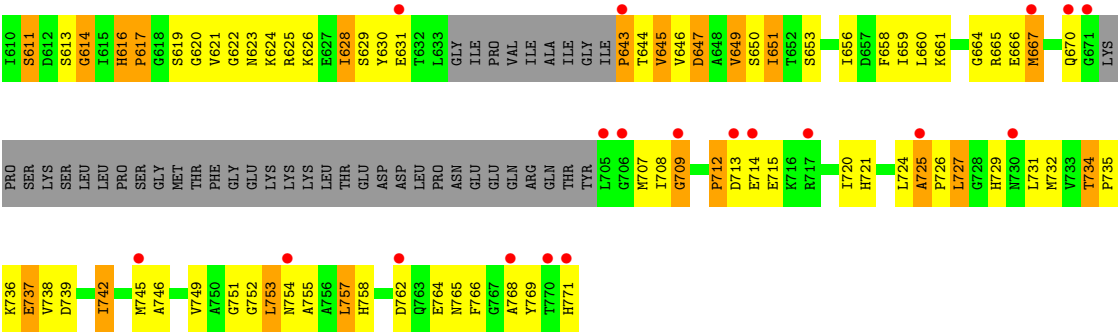
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SPORE PROTEASE



• Molecule 1: SPORE PROTEASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.41Å 77.41Å 313.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.0 (15.00-3.00) 91.3 (15.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.308 , 0.330 0.332 , 0.340	Depositor DCC
R_{free} test set	1927 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 126.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4454	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.33 % 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 3.9133e-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

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	0.87	0/2184	1.34	35/2976 (1.2%)
1	B	0.96	1/2184 (0.0%)	1.36	34/2976 (1.1%)
All	All	0.92	1/4368 (0.0%)	1.35	69/5952 (1.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	729	HIS	CD2-NE2	5.59	1.44	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	LYS	N-CA-C	-9.98	99.65	112.23
1	B	661	LYS	N-CA-C	-9.96	99.68	112.23
1	B	757	LEU	N-CA-C	-8.79	100.65	112.26
1	B	667	MET	N-CA-C	-8.74	101.68	111.82
1	A	757	LEU	N-CA-C	-8.72	100.75	112.26
1	A	667	MET	N-CA-C	-8.18	102.33	111.82
1	B	712	PRO	N-CA-CB	7.68	111.31	103.25
1	A	473	VAL	N-CA-C	7.59	118.83	107.51
1	A	712	PRO	N-CA-CB	7.56	111.19	103.25
1	B	768	ALA	N-CA-C	-7.45	102.53	111.69
1	A	715	GLU	N-CA-C	-7.42	104.23	113.28
1	B	480	ILE	N-CA-C	7.30	118.64	108.12
1	A	480	ILE	N-CA-C	7.27	118.59	108.12
1	B	473	VAL	N-CA-C	7.26	118.33	107.51
1	A	768	ALA	N-CA-C	-7.20	102.83	111.69
1	A	563	VAL	CA-C-N	7.06	126.31	118.97
1	A	563	VAL	C-N-CA	7.06	126.31	118.97
1	B	715	GLU	N-CA-C	-7.05	104.68	113.28
1	A	623	ASN	N-CA-C	7.02	120.07	108.49
1	B	737	GLU	N-CA-C	-7.01	104.65	112.57
1	B	501	ASN	N-CA-C	-7.00	102.48	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	764	GLU	N-CA-C	-6.94	104.81	113.28
1	A	501	ASN	N-CA-C	-6.76	102.78	111.02
1	A	571	GLY	N-CA-C	-6.75	105.87	114.37
1	B	563	VAL	CA-C-N	6.71	126.22	119.24
1	B	563	VAL	C-N-CA	6.71	126.22	119.24
1	B	528	ASP	N-CA-C	-6.71	103.69	112.41
1	B	764	GLU	N-CA-C	-6.64	105.18	113.28
1	A	415	ASP	N-CA-C	6.59	119.68	109.07
1	B	571	GLY	N-CA-C	-6.54	106.14	114.37
1	A	643	PRO	N-CA-CB	6.53	110.18	103.00
1	A	737	GLU	N-CA-C	-6.37	105.37	112.57
1	B	643	PRO	N-CA-CB	6.24	109.86	103.00
1	B	415	ASP	N-CA-C	6.19	119.04	109.07
1	A	528	ASP	N-CA-C	-6.05	104.54	112.41
1	B	490	GLU	N-CA-C	-5.96	105.11	112.38
1	A	549	PRO	N-CA-CB	5.95	109.49	103.25
1	B	742	ILE	N-CA-C	-5.94	104.72	110.72
1	B	709	GLY	N-CA-C	-5.93	105.42	113.37
1	A	616	HIS	CA-C-N	5.92	127.24	119.84
1	A	616	HIS	C-N-CA	5.92	127.24	119.84
1	A	709	GLY	N-CA-C	-5.79	105.61	113.37
1	A	490	GLU	N-CA-C	-5.73	105.39	112.38
1	B	616	HIS	CA-C-N	5.68	126.94	119.84
1	B	616	HIS	C-N-CA	5.68	126.94	119.84
1	B	734	THR	N-CA-C	5.61	117.30	108.55
1	B	623	ASN	N-CA-C	5.58	119.34	107.67
1	B	549	PRO	N-CA-CB	5.54	109.07	103.25
1	B	582	VAL	N-CA-C	-5.51	105.13	110.42
1	A	614	GLY	N-CA-C	-5.43	104.03	112.45
1	B	448	GLN	N-CA-C	5.42	118.31	109.59
1	B	489	GLU	N-CA-C	-5.37	106.86	113.41
1	A	448	GLN	N-CA-C	5.36	118.22	109.59
1	B	611	SER	N-CA-C	5.34	116.64	108.52
1	B	670	GLN	N-CA-C	-5.34	106.62	113.02
1	A	611	SER	N-CA-C	5.33	116.62	108.52
1	A	515	CYS	N-CA-C	5.32	118.13	109.24
1	A	582	VAL	N-CA-C	-5.32	105.19	110.62
1	A	734	THR	N-CA-C	5.26	116.76	108.55
1	A	742	ILE	N-CA-C	-5.21	105.45	110.72
1	B	515	CYS	N-CA-C	5.17	117.88	109.24
1	B	614	GLY	N-CA-C	-5.16	104.45	112.45
1	B	557	ARG	N-CA-C	-5.15	103.46	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	THR	N-CA-C	5.14	117.67	109.96
1	A	670	GLN	N-CA-C	-5.09	106.92	113.02
1	A	651	ILE	N-CA-C	5.07	115.27	108.17
1	B	478	VAL	N-CA-C	5.06	115.20	108.11
1	A	489	GLU	N-CA-C	-5.05	107.24	113.41
1	A	478	VAL	N-CA-C	5.02	115.14	108.11

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	2164	0	1943	181	5
1	B	2164	0	1943	185	8
2	A	63	0	0	12	14
2	B	63	0	0	10	11
All	All	4454	0	3886	356	19

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 43.

All (356) 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:B:442:VAL:HG12	1:B:443:LYS:H	1.12	1.13
1:A:442:VAL:HG12	1:A:443:LYS:H	1.13	1.09
1:A:510:PRO:HG2	1:A:513:ALA:HB2	1.39	1.04
1:B:510:PRO:HG2	1:B:513:ALA:HB2	1.39	1.03
1:B:416:LEU:HA	2:B:106:HOH:O	1.61	0.99
1:A:463:GLU:HA	1:A:473:VAL:HG11	1.41	0.97
1:B:463:GLU:HA	1:B:473:VAL:HG11	1.43	0.97
1:B:481:ARG:O	1:B:606:ALA:HB1	1.66	0.95
1:A:481:ARG:O	1:A:606:ALA:HB1	1.66	0.95
1:B:530:LEU:CD1	1:B:593:ILE:HD11	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:CD1	1:A:593:ILE:HD11	1.98	0.92
1:A:725:ALA:HB1	1:A:726:PRO:HD3	1.53	0.89
1:B:725:ALA:HB1	1:B:726:PRO:HD3	1.52	0.88
1:B:522:ASN:HD21	1:B:524:SER:HB2	1.38	0.87
1:A:522:ASN:HD21	1:A:524:SER:HB2	1.38	0.86
1:A:442:VAL:HG12	1:A:443:LYS:N	1.92	0.84
1:A:516:LEU:HB3	1:A:590:ILE:HG22	1.59	0.84
1:A:579:PHE:O	1:A:582:VAL:HG22	1.79	0.82
1:B:725:ALA:HB1	1:B:726:PRO:CD	2.08	0.82
1:B:516:LEU:HB3	1:B:590:ILE:HG22	1.62	0.82
1:B:579:PHE:O	1:B:582:VAL:HG22	1.79	0.82
1:A:725:ALA:HB1	1:A:726:PRO:CD	2.09	0.81
1:A:522:ASN:ND2	1:A:524:SER:HB2	1.96	0.80
1:A:563:VAL:O	1:A:566:VAL:HG22	1.83	0.78
1:B:522:ASN:ND2	1:B:524:SER:HB2	1.97	0.78
1:B:442:VAL:HG12	1:B:443:LYS:N	1.91	0.78
1:B:563:VAL:O	1:B:566:VAL:HG22	1.84	0.77
1:A:651:ILE:CG2	1:A:745:MET:HE3	2.15	0.77
1:B:651:ILE:CG2	1:B:745:MET:HE3	2.15	0.77
1:A:476:GLU:HG3	1:A:611:SER:HB3	1.66	0.76
1:B:476:GLU:HG3	1:B:611:SER:HB3	1.66	0.76
1:B:575:SER:HA	1:B:578:ILE:HG12	1.67	0.75
1:B:614:GLY:HA3	1:B:628:ILE:HG22	1.69	0.75
1:A:651:ILE:HG21	1:A:745:MET:HG2	1.69	0.74
1:A:736:LYS:HA	1:B:732:MET:HE2	1.68	0.74
1:A:514:SER:HA	1:A:558:PRO:HG2	1.69	0.74
1:A:591:ILE:HB	1:A:647:ASP:HB3	1.70	0.74
1:A:414:THR:HA	2:A:101:HOH:O	1.87	0.74
1:B:414:THR:HA	2:B:1101:HOH:O	1.86	0.74
1:A:575:SER:HA	1:A:578:ILE:HG12	1.67	0.73
1:A:417:ALA:HB2	1:A:609:GLN:OE1	1.89	0.73
1:B:417:ALA:HB2	1:B:609:GLN:OE1	1.89	0.73
1:B:514:SER:HA	1:B:558:PRO:HG2	1.70	0.73
1:A:614:GLY:HA3	1:A:628:ILE:HG22	1.69	0.73
1:B:651:ILE:HG21	1:B:745:MET:HG2	1.71	0.72
1:B:530:LEU:HD13	1:B:593:ILE:HD11	1.71	0.72
1:B:476:GLU:HG3	1:B:611:SER:CB	2.20	0.72
1:A:476:GLU:HG3	1:A:611:SER:CB	2.20	0.72
1:B:505:LYS:O	1:B:508:ASN:N	2.21	0.71
1:A:732:MET:HE2	1:B:736:LYS:HA	1.69	0.71
1:B:562:ILE:HD13	1:B:581:VAL:HG21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ILE:HB	1:B:647:ASP:HB3	1.73	0.71
1:A:562:ILE:HD13	1:A:581:VAL:HG21	1.72	0.71
1:A:505:LYS:O	1:A:508:ASN:N	2.21	0.71
1:A:530:LEU:HD13	1:A:593:ILE:HD11	1.72	0.71
1:A:651:ILE:N	1:A:651:ILE:HD12	2.06	0.71
1:A:659:ILE:HB	1:A:720:ILE:HD12	1.73	0.70
1:B:651:ILE:HD12	1:B:651:ILE:N	2.06	0.70
1:B:653:SER:O	1:B:734:THR:HG22	1.92	0.70
1:A:517:VAL:HB	1:A:561:ALA:HB2	1.73	0.69
1:B:448:GLN:HB3	1:B:457:ILE:HG23	1.74	0.69
1:B:517:VAL:HB	1:B:561:ALA:HB2	1.75	0.68
1:A:653:SER:O	1:A:734:THR:HG22	1.92	0.68
1:A:448:GLN:HB3	1:A:457:ILE:HG23	1.75	0.68
1:B:738:VAL:O	1:B:742:ILE:HG12	1.93	0.67
1:A:738:VAL:O	1:A:742:ILE:HG12	1.95	0.67
1:B:593:ILE:HD13	1:B:749:VAL:HG11	1.76	0.67
1:B:651:ILE:HG21	1:B:745:MET:HE3	1.77	0.67
1:A:651:ILE:HG21	1:A:745:MET:HE3	1.77	0.67
1:A:513:ALA:HB3	1:A:557:ARG:HH12	1.60	0.66
1:A:517:VAL:HB	1:A:561:ALA:CB	2.25	0.66
1:A:659:ILE:HA	2:A:116:HOH:O	1.95	0.66
1:A:593:ILE:HD13	1:A:749:VAL:HG11	1.76	0.66
1:B:659:ILE:HB	1:B:720:ILE:HD12	1.76	0.66
1:B:480:ILE:HG22	2:B:1107:HOH:O	1.95	0.65
1:A:480:ILE:HG22	2:A:107:HOH:O	1.95	0.65
1:B:442:VAL:CG1	1:B:443:LYS:H	1.97	0.65
1:A:727:LEU:HD12	1:A:731:LEU:HD13	1.79	0.64
1:A:498:LYS:HE3	1:A:499:GLU:OE2	1.97	0.64
1:A:538:LEU:HD11	1:A:753:LEU:HD12	1.78	0.64
1:B:517:VAL:HB	1:B:561:ALA:CB	2.27	0.64
1:B:659:ILE:HA	2:B:1116:HOH:O	1.97	0.64
1:B:727:LEU:HD12	1:B:731:LEU:HD13	1.79	0.64
1:B:498:LYS:HE3	1:B:499:GLU:OE2	1.98	0.64
1:B:449:GLY:HA3	2:B:1110:HOH:O	1.97	0.64
1:B:651:ILE:HG23	1:B:745:MET:HE3	1.80	0.64
1:B:507:LEU:HD13	1:B:509:ILE:HD11	1.80	0.64
1:B:513:ALA:HB3	1:B:557:ARG:HH12	1.60	0.64
1:A:563:VAL:O	1:A:563:VAL:HG13	1.96	0.64
1:A:591:ILE:HD11	1:A:753:LEU:HD11	1.80	0.64
1:A:427:ASN:O	1:A:429:PRO:HD3	1.98	0.63
1:B:563:VAL:O	1:B:563:VAL:HG13	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ILE:HG23	1:A:745:MET:HE3	1.80	0.62
1:A:480:ILE:HG21	1:A:603:ARG:NH2	2.15	0.62
1:B:605:ASN:ND2	1:B:735:PRO:HG2	2.15	0.62
1:A:507:LEU:HD13	1:A:509:ILE:HD11	1.82	0.62
1:B:427:ASN:O	1:B:429:PRO:HD3	2.00	0.62
1:B:480:ILE:HG21	1:B:603:ARG:NH2	2.15	0.62
1:A:619:SER:HA	2:A:1131:HOH:O	1.99	0.61
1:B:591:ILE:HD11	1:B:753:LEU:HD11	1.82	0.61
1:A:449:GLY:HA3	2:A:110:HOH:O	1.99	0.61
1:B:725:ALA:CB	1:B:726:PRO:CD	2.79	0.61
1:A:442:VAL:CG1	1:A:443:LYS:H	1.98	0.61
1:B:538:LEU:HD11	1:B:753:LEU:HD12	1.81	0.61
1:A:455:VAL:HB	1:A:480:ILE:HG23	1.83	0.60
1:A:605:ASN:ND2	1:A:735:PRO:HG2	2.17	0.60
1:A:725:ALA:CB	1:A:726:PRO:CD	2.80	0.60
1:A:504:ILE:HG22	1:A:509:ILE:HB	1.84	0.60
1:A:664:GLY:C	1:A:666:GLU:H	2.09	0.60
1:B:504:ILE:HG22	1:B:509:ILE:HB	1.83	0.60
1:A:628:ILE:HD13	1:A:628:ILE:H	1.67	0.59
1:B:455:VAL:HB	1:B:480:ILE:HG23	1.83	0.59
1:B:575:SER:OG	1:B:625:ARG:HD2	2.02	0.59
1:B:664:GLY:C	1:B:666:GLU:H	2.10	0.59
1:B:423:ILE:O	1:B:426:GLU:HB3	2.03	0.59
1:B:596:LEU:HG	1:B:650:SER:HB2	1.84	0.59
1:A:726:PRO:O	1:A:727:LEU:HG	2.03	0.59
1:B:644:THR:O	1:B:646:VAL:HG23	2.03	0.59
1:B:628:ILE:HD13	1:B:631:GLU:CB	2.34	0.58
1:B:405:LEU:H	1:B:405:LEU:HD23	1.67	0.58
1:B:582:VAL:HG23	1:B:583:LYS:N	2.18	0.58
1:A:478:VAL:HG22	1:A:609:GLN:HG3	1.86	0.58
1:B:629:SER:O	1:B:643:PRO:HA	2.04	0.57
1:B:749:VAL:O	1:B:753:LEU:HB2	2.04	0.57
1:A:405:LEU:HD23	1:A:405:LEU:H	1.68	0.57
1:A:510:PRO:HG2	1:A:513:ALA:CB	2.26	0.57
1:A:596:LEU:HG	1:A:650:SER:HB2	1.86	0.57
1:A:516:LEU:HD23	1:A:582:VAL:HG12	1.86	0.57
1:B:414:THR:O	1:B:599:ARG:HB2	2.05	0.57
1:B:478:VAL:HG22	1:B:609:GLN:HG3	1.85	0.57
1:A:644:THR:O	1:A:646:VAL:HG23	2.04	0.57
1:B:628:ILE:HD13	1:B:628:ILE:H	1.68	0.57
1:A:726:PRO:C	1:A:727:LEU:HG	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:LYS:O	1:B:490:GLU:HG2	2.05	0.57
1:B:714:GLU:OE1	1:B:714:GLU:HA	2.04	0.57
1:B:470:GLY:O	1:B:472:TYR:N	2.38	0.57
1:A:575:SER:OG	1:A:625:ARG:HD2	2.05	0.57
1:A:582:VAL:HG23	1:A:583:LYS:N	2.19	0.57
1:B:463:GLU:HA	1:B:473:VAL:CG1	2.27	0.56
1:A:423:ILE:O	1:A:426:GLU:HB3	2.05	0.56
1:A:470:GLY:O	1:A:472:TYR:N	2.39	0.56
1:B:726:PRO:C	1:B:727:LEU:HG	2.31	0.56
1:B:726:PRO:O	1:B:727:LEU:HG	2.04	0.56
1:A:529:ALA:O	1:A:533:LYS:HG3	2.06	0.56
1:B:516:LEU:HD23	1:B:582:VAL:HG12	1.87	0.56
1:A:628:ILE:HD13	1:A:631:GLU:CB	2.36	0.56
1:A:629:SER:O	1:A:643:PRO:HA	2.05	0.56
1:A:414:THR:O	1:A:599:ARG:HB2	2.05	0.56
1:B:510:PRO:HG2	1:B:513:ALA:CB	2.27	0.56
1:A:463:GLU:HA	1:A:473:VAL:CG1	2.25	0.55
1:B:582:VAL:O	1:B:586:ASN:N	2.37	0.55
1:A:714:GLU:HA	1:A:714:GLU:OE1	2.05	0.55
1:B:724:LEU:O	1:B:725:ALA:C	2.50	0.55
1:B:562:ILE:CD1	1:B:581:VAL:HG21	2.35	0.55
1:A:749:VAL:O	1:A:753:LEU:HB2	2.07	0.55
1:A:487:LYS:O	1:A:490:GLU:HG2	2.07	0.54
1:B:613:SER:HB3	1:B:616:HIS:NE2	2.22	0.54
1:A:735:PRO:HA	1:B:731:LEU:HD12	1.88	0.54
1:A:562:ILE:CD1	1:A:581:VAL:HG21	2.37	0.54
1:A:664:GLY:C	1:A:666:GLU:N	2.63	0.54
1:A:514:SER:HB3	1:A:588:ASP:H	1.72	0.54
1:A:517:VAL:HG21	1:A:538:LEU:HD21	1.90	0.54
1:B:514:SER:HB3	1:B:588:ASP:H	1.72	0.54
1:A:522:ASN:HD21	1:A:524:SER:CB	2.16	0.54
1:A:582:VAL:O	1:A:586:ASN:N	2.37	0.54
1:B:529:ALA:O	1:B:533:LYS:HG3	2.08	0.54
1:B:574:THR:O	1:B:578:ILE:HG23	2.08	0.54
1:B:599:ARG:HH11	1:B:599:ARG:HG2	1.73	0.54
1:B:530:LEU:HD11	1:B:593:ILE:HD11	1.88	0.53
1:A:513:ALA:HB3	1:A:557:ARG:NH1	2.22	0.53
1:A:650:SER:C	1:A:651:ILE:HD12	2.33	0.53
1:A:724:LEU:O	1:A:725:ALA:C	2.50	0.53
1:B:664:GLY:C	1:B:666:GLU:N	2.64	0.53
1:A:499:GLU:O	1:A:503:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PHE:HD2	1:A:752:GLY:HA3	1.73	0.53
1:A:613:SER:HB3	1:A:616:HIS:NE2	2.24	0.53
1:A:485:THR:O	1:A:486:GLU:HB3	2.09	0.53
1:A:651:ILE:N	1:A:651:ILE:CD1	2.72	0.53
1:A:574:THR:O	1:A:578:ILE:HG23	2.08	0.53
1:B:485:THR:O	1:B:486:GLU:HB3	2.08	0.53
1:B:499:GLU:O	1:B:503:PHE:HB2	2.09	0.53
1:B:751:GLY:HA2	1:B:754:ASN:HD22	1.74	0.53
1:B:563:VAL:HG13	1:B:566:VAL:CG2	2.39	0.53
1:B:450:VAL:HG22	1:B:455:VAL:HG22	1.91	0.53
1:A:448:GLN:HB3	1:A:457:ILE:HG12	1.91	0.52
1:A:450:VAL:HG22	1:A:455:VAL:HG22	1.91	0.52
1:B:513:ALA:HB3	1:B:557:ARG:NH1	2.23	0.52
1:B:550:GLU:N	2:B:1100:HOH:O	2.43	0.52
1:B:650:SER:C	1:B:651:ILE:HD12	2.35	0.52
1:A:563:VAL:HG13	1:A:566:VAL:CG2	2.39	0.52
1:B:496:PHE:HD2	1:B:752:GLY:HA3	1.74	0.52
1:A:599:ARG:HG2	1:A:599:ARG:HH11	1.75	0.52
1:B:412:VAL:HB	2:B:190:HOH:O	2.09	0.52
1:A:550:GLU:N	2:A:100:HOH:O	2.42	0.52
1:A:751:GLY:HA2	1:A:754:ASN:HD22	1.76	0.51
1:B:651:ILE:N	1:B:651:ILE:CD1	2.72	0.51
1:A:546:GLU:O	1:A:549:PRO:N	2.44	0.51
1:A:557:ARG:HG2	1:A:558:PRO:N	2.25	0.51
1:B:522:ASN:HD21	1:B:524:SER:CB	2.18	0.51
1:B:595:ALA:HA	1:B:651:ILE:O	2.11	0.51
1:B:448:GLN:HB3	1:B:457:ILE:HG12	1.92	0.51
1:B:517:VAL:HG21	1:B:538:LEU:HD21	1.92	0.51
1:B:587:PRO:HG3	1:B:590:ILE:HG22	1.92	0.51
1:B:557:ARG:HG2	1:B:558:PRO:N	2.26	0.51
1:B:418:VAL:C	1:B:420:ALA:N	2.66	0.50
1:B:596:LEU:HD11	1:B:650:SER:OG	2.11	0.50
1:B:546:GLU:O	1:B:549:PRO:N	2.44	0.50
1:A:591:ILE:HB	1:A:647:ASP:CB	2.40	0.50
1:A:644:THR:O	1:A:645:VAL:C	2.54	0.50
1:A:525:VAL:HG12	1:A:527:PRO:HD2	1.94	0.50
1:B:582:VAL:CG2	1:B:583:LYS:N	2.74	0.50
1:A:452:ILE:HG22	1:A:452:ILE:O	2.11	0.50
1:A:500:LEU:O	1:A:501:ASN:C	2.55	0.50
1:B:504:ILE:CG2	1:B:509:ILE:HB	2.42	0.50
1:B:644:THR:O	1:B:645:VAL:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:VAL:C	1:A:420:ALA:N	2.66	0.49
1:A:595:ALA:HA	1:A:651:ILE:O	2.12	0.49
1:A:621:VAL:HA	1:B:736:LYS:HD3	1.94	0.49
1:A:480:ILE:HG21	1:A:603:ARG:CZ	2.42	0.49
1:A:617:PRO:HA	1:A:624:LYS:O	2.12	0.49
1:B:513:ALA:H	1:B:557:ARG:NH1	2.10	0.49
1:A:418:VAL:O	1:A:421:LYS:N	2.44	0.49
1:A:659:ILE:HD12	1:A:724:LEU:HG	1.94	0.49
1:A:738:VAL:O	1:A:738:VAL:HG22	2.12	0.49
1:B:452:ILE:HG22	1:B:452:ILE:O	2.12	0.49
1:B:525:VAL:HG12	1:B:527:PRO:HD2	1.94	0.49
1:B:738:VAL:O	1:B:738:VAL:HG22	2.13	0.49
1:B:480:ILE:HG21	1:B:603:ARG:CZ	2.42	0.49
1:A:596:LEU:HD11	1:A:650:SER:OG	2.13	0.48
1:B:573:GLU:O	1:B:576:ASP:HB2	2.14	0.48
1:A:504:ILE:CG2	1:A:509:ILE:HB	2.43	0.48
1:B:591:ILE:HB	1:B:647:ASP:CB	2.43	0.48
1:A:557:ARG:H	1:A:757:LEU:HD23	1.78	0.48
1:A:582:VAL:CG2	1:A:583:LYS:N	2.76	0.48
1:B:500:LEU:O	1:B:501:ASN:C	2.55	0.48
1:B:659:ILE:HD12	1:B:724:LEU:HG	1.93	0.48
1:A:587:PRO:HG3	1:A:590:ILE:HG22	1.95	0.48
1:B:617:PRO:HA	1:B:624:LYS:O	2.13	0.48
1:A:480:ILE:HG21	1:A:603:ARG:HH22	1.77	0.48
1:A:573:GLU:O	1:A:576:ASP:HB2	2.14	0.48
1:B:557:ARG:H	1:B:757:LEU:HD23	1.78	0.48
1:B:628:ILE:HG12	1:B:630:TYR:N	2.28	0.48
1:A:516:LEU:HA	1:A:560:SER:O	2.14	0.47
1:A:601:ILE:HB	1:B:725:ALA:HB3	1.96	0.47
1:B:418:VAL:C	1:B:420:ALA:H	2.21	0.47
1:B:476:GLU:HG3	1:B:611:SER:HB2	1.97	0.47
1:A:418:VAL:C	1:A:420:ALA:H	2.21	0.47
1:B:480:ILE:HG21	1:B:603:ARG:HH22	1.78	0.47
1:A:496:PHE:CD2	1:A:752:GLY:HA3	2.48	0.47
1:A:667:MET:HE2	1:A:667:MET:HA	1.96	0.47
1:B:496:PHE:CD2	1:B:752:GLY:HA3	2.49	0.47
1:A:527:PRO:HB3	1:A:738:VAL:HG21	1.97	0.47
1:B:614:GLY:CA	1:B:628:ILE:HG22	2.42	0.47
1:B:416:LEU:O	1:B:417:ALA:C	2.58	0.46
1:B:480:ILE:CG2	1:B:603:ARG:NH1	2.78	0.46
1:B:667:MET:HE2	1:B:667:MET:HA	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ILE:CG2	1:A:603:ARG:NH1	2.78	0.46
1:A:513:ALA:H	1:A:557:ARG:NH1	2.13	0.46
1:A:552:VAL:HG12	1:A:552:VAL:O	2.16	0.46
1:B:664:GLY:O	1:B:666:GLU:N	2.49	0.46
1:A:417:ALA:HB2	1:A:609:GLN:HG3	1.97	0.46
1:A:573:GLU:HG2	2:A:1153:HOH:O	2.16	0.46
1:A:530:LEU:HD11	1:A:651:ILE:HD13	1.97	0.46
1:A:628:ILE:HG12	1:A:630:TYR:N	2.30	0.46
1:A:664:GLY:O	1:A:666:GLU:N	2.48	0.46
1:B:418:VAL:O	1:B:421:LYS:N	2.46	0.46
1:A:731:LEU:HD21	1:B:601:ILE:HD13	1.98	0.45
1:B:466:GLY:C	1:B:468:LYS:H	2.25	0.45
1:B:467:LYS:HB2	2:B:1169:HOH:O	2.17	0.45
1:A:416:LEU:O	1:A:417:ALA:C	2.59	0.45
1:A:736:LYS:HG2	1:B:732:MET:HB3	1.98	0.45
1:A:735:PRO:CA	1:B:731:LEU:HD12	2.47	0.45
1:B:557:ARG:CG	1:B:558:PRO:HD2	2.46	0.45
1:B:516:LEU:HA	1:B:560:SER:O	2.16	0.45
1:B:507:LEU:HB3	1:B:509:ILE:HG13	1.98	0.45
1:A:577:ILE:C	1:A:579:PHE:N	2.74	0.45
1:A:473:VAL:HG23	1:A:473:VAL:O	2.17	0.45
1:B:527:PRO:HB3	1:B:738:VAL:HG21	1.98	0.45
1:A:628:ILE:HD13	1:A:628:ILE:N	2.32	0.45
1:A:614:GLY:CA	1:A:628:ILE:HG22	2.42	0.44
1:B:597:ALA:HB1	1:B:656:ILE:HG13	2.00	0.44
1:A:476:GLU:HG3	1:A:611:SER:HB2	1.97	0.44
1:B:480:ILE:HG21	1:B:603:ARG:NH1	2.32	0.44
1:B:530:LEU:HD11	1:B:651:ILE:HD13	1.99	0.44
1:B:552:VAL:O	1:B:552:VAL:HG12	2.17	0.44
1:B:742:ILE:O	1:B:746:ALA:HB2	2.18	0.44
1:A:466:GLY:O	1:A:468:LYS:N	2.50	0.44
1:B:541:THR:O	1:B:542:ARG:C	2.59	0.44
1:B:656:ILE:O	1:B:658:PHE:N	2.47	0.44
1:B:480:ILE:CG2	1:B:603:ARG:HH12	2.31	0.44
1:B:737:GLU:C	1:B:739:ASP:N	2.75	0.44
1:A:480:ILE:CG2	1:A:603:ARG:HH12	2.30	0.44
1:A:507:LEU:HB3	1:A:509:ILE:HG13	1.99	0.44
1:A:541:THR:O	1:A:542:ARG:C	2.59	0.44
1:B:466:GLY:O	1:B:468:LYS:N	2.50	0.44
1:B:599:ARG:HG2	1:B:599:ARG:NH1	2.33	0.44
1:B:490:GLU:O	1:B:493:GLU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ILE:HD11	1:B:753:LEU:HD21	2.00	0.43
1:A:485:THR:OG1	1:A:486:GLU:N	2.51	0.43
1:A:563:VAL:HG13	1:A:566:VAL:HG21	2.00	0.43
1:B:620:GLY:HA2	2:B:1146:HOH:O	2.18	0.43
1:B:563:VAL:HA	1:B:564:PRO:HD2	1.84	0.43
1:B:605:ASN:HD21	1:B:735:PRO:HG2	1.82	0.43
1:B:755:ALA:O	1:B:758:HIS:HA	2.19	0.43
1:A:732:MET:CE	1:B:736:LYS:HA	2.44	0.43
1:A:416:LEU:HD12	2:A:1106:HOH:O	2.19	0.43
1:A:520:LEU:HD11	1:A:615:ILE:HG13	2.00	0.43
1:B:417:ALA:HB2	1:B:609:GLN:HG3	2.00	0.43
1:B:563:VAL:HG13	1:B:566:VAL:HG22	2.00	0.43
1:A:466:GLY:C	1:A:468:LYS:H	2.27	0.43
1:A:490:GLU:O	1:A:493:GLU:HB3	2.18	0.43
1:A:599:ARG:HG2	1:A:599:ARG:NH1	2.34	0.43
1:B:466:GLY:C	1:B:468:LYS:N	2.76	0.43
1:A:620:GLY:HA2	2:A:146:HOH:O	2.19	0.43
1:A:480:ILE:HG21	1:A:603:ARG:NH1	2.33	0.42
1:B:563:VAL:HG13	1:B:566:VAL:HG21	2.01	0.42
1:A:563:VAL:HG13	1:A:566:VAL:HG22	2.00	0.42
1:A:593:ILE:HA	1:A:649:VAL:O	2.20	0.42
1:B:489:GLU:C	1:B:491:ALA:N	2.76	0.42
1:B:593:ILE:HA	1:B:649:VAL:O	2.20	0.42
1:A:557:ARG:CG	1:A:558:PRO:HD2	2.49	0.42
1:A:467:LYS:HB2	2:A:169:HOH:O	2.18	0.42
1:A:526:THR:HB	1:A:527:PRO:HD3	2.01	0.42
1:A:597:ALA:HB1	1:A:656:ILE:HG13	2.02	0.42
1:B:550:GLU:CB	2:B:1100:HOH:O	2.68	0.42
1:B:755:ALA:O	1:B:758:HIS:N	2.53	0.42
1:B:473:VAL:HG23	1:B:473:VAL:O	2.19	0.42
1:B:485:THR:OG1	1:B:486:GLU:N	2.51	0.42
1:A:480:ILE:HB	1:A:603:ARG:NH1	2.34	0.41
1:A:742:ILE:O	1:A:746:ALA:HB2	2.20	0.41
1:A:755:ALA:O	1:A:758:HIS:HA	2.20	0.41
1:B:478:VAL:HG22	1:B:609:GLN:CG	2.49	0.41
1:A:724:LEU:O	1:A:725:ALA:O	2.39	0.41
1:B:707:MET:O	1:B:709:GLY:N	2.53	0.41
1:A:550:GLU:CB	2:A:100:HOH:O	2.68	0.41
1:A:591:ILE:HD11	1:A:753:LEU:HD21	2.01	0.41
1:B:507:LEU:HD13	1:B:509:ILE:CD1	2.50	0.41
1:B:577:ILE:C	1:B:579:PHE:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLY:HA3	2:A:173:HOH:O	2.20	0.41
1:A:478:VAL:HG22	1:A:609:GLN:CG	2.50	0.41
1:B:628:ILE:HD13	1:B:628:ILE:N	2.33	0.41
1:B:660:LEU:HA	1:B:660:LEU:HD23	1.72	0.41
1:A:519:GLY:O	1:A:563:VAL:HG23	2.20	0.41
1:A:466:GLY:C	1:A:468:LYS:N	2.78	0.41
1:A:489:GLU:C	1:A:491:ALA:N	2.77	0.41
1:A:736:LYS:HE3	1:B:731:LEU:C	2.46	0.41
1:B:480:ILE:HB	1:B:603:ARG:NH1	2.36	0.41
1:A:516:LEU:CD2	1:A:582:VAL:HG12	2.51	0.40
1:A:530:LEU:HD11	1:A:593:ILE:HD11	1.90	0.40
1:B:721:HIS:ND1	1:B:721:HIS:C	2.79	0.40
1:B:753:LEU:HD22	1:B:753:LEU:HA	1.89	0.40
1:B:417:ALA:HB2	1:B:609:GLN:CD	2.47	0.40
1:B:575:SER:CA	1:B:578:ILE:HG12	2.46	0.40
1:A:707:MET:O	1:A:709:GLY:N	2.54	0.40
1:A:418:VAL:O	1:A:420:ALA:N	2.55	0.40
1:B:526:THR:HG21	1:B:738:VAL:HG13	2.03	0.40

All (19) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:177:HOH:O	2:B:1174:HOH:O[1_655]	0.20	2.00
2:A:174:HOH:O	2:B:1177:HOH:O[1_655]	0.36	1.84
2:A:112:HOH:O	2:B:1107:HOH:O[1_655]	0.44	1.76
2:A:144:HOH:O	2:B:1105:HOH:O[8_555]	0.48	1.72
2:A:105:HOH:O	2:B:1144:HOH:O[8_555]	0.61	1.59
2:A:132:HOH:O	2:B:1110:HOH:O[1_655]	0.62	1.58
2:A:110:HOH:O	2:B:1132:HOH:O[1_655]	0.67	1.53
2:A:107:HOH:O	2:B:1112:HOH:O[1_655]	0.70	1.50
1:A:769:TYR:CB	1:B:769:TYR:CB[1_655]	1.14	1.06
2:A:108:HOH:O	2:B:1113:HOH:O[8_555]	1.31	0.89
2:A:113:HOH:O	2:B:1108:HOH:O[8_555]	1.54	0.66
1:A:771:HIS:CB	1:B:475:LEU:CB[1_655]	1.77	0.43
1:A:475:LEU:CB	1:B:771:HIS:CB[1_655]	1.84	0.36
1:B:755:ALA:O	2:A:149:HOH:O[1_455]	1.95	0.25
1:B:755:ALA:C	2:A:149:HOH:O[1_455]	1.99	0.21
1:B:713:ASP:OD1	2:A:193:HOH:O[5_455]	1.99	0.21
2:A:188:HOH:O	2:B:1158:HOH:O[1_655]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:HIS:CB	1:B:475:LEU:CG[1_655]	2.14	0.06
1:A:475:LEU:CG	1:B:771:HIS:CB[1_655]	2.16	0.04

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	312/371 (84%)	238 (76%)	51 (16%)	23 (7%)	1	4
1	B	312/371 (84%)	236 (76%)	53 (17%)	23 (7%)	1	4
All	All	624/742 (84%)	474 (76%)	104 (17%)	46 (7%)	1	4

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASP
1	A	417	ALA
1	A	429	PRO
1	A	469	LYS
1	A	471	ARG
1	A	485	THR
1	A	549	PRO
1	A	619	SER
1	A	708	ILE
1	A	725	ALA
1	A	762	ASP
1	B	406	ASP
1	B	417	ALA
1	B	429	PRO
1	B	469	LYS
1	B	471	ARG
1	B	485	THR
1	B	549	PRO

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Mol	Chain	Res	Type
1	B	619	SER
1	B	708	ILE
1	B	725	ALA
1	B	762	ASP
1	A	712	PRO
1	B	712	PRO
1	A	467	LYS
1	A	486	GLU
1	A	617	PRO
1	B	467	LYS
1	B	486	GLU
1	A	474	THR
1	A	622	GLY
1	A	765	ASN
1	A	766	PHE
1	B	474	THR
1	B	617	PRO
1	B	622	GLY
1	B	765	ASN
1	B	766	PHE
1	A	412	VAL
1	B	412	VAL
1	A	665	ARG
1	B	665	ARG
1	A	552	VAL
1	B	552	VAL
1	A	621	VAL
1	B	621	VAL

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	192/317 (61%)	172 (90%)	20 (10%)	7	28
1	B	192/317 (61%)	172 (90%)	20 (10%)	7	28
All	All	384/634 (61%)	344 (90%)	40 (10%)	7	28

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	LEU
1	A	412	VAL
1	A	447	GLU
1	A	472	TYR
1	A	476	GLU
1	A	480	ILE
1	A	500	LEU
1	A	507	LEU
1	A	591	ILE
1	A	593	ILE
1	A	607	THR
1	A	609	GLN
1	A	626	LYS
1	A	628	ILE
1	A	645	VAL
1	A	647	ASP
1	A	649	VAL
1	A	651	ILE
1	A	727	LEU
1	A	753	LEU
1	B	405	LEU
1	B	412	VAL
1	B	447	GLU
1	B	472	TYR
1	B	476	GLU
1	B	480	ILE
1	B	500	LEU
1	B	507	LEU
1	B	591	ILE
1	B	593	ILE
1	B	607	THR
1	B	609	GLN
1	B	626	LYS
1	B	628	ILE
1	B	645	VAL
1	B	647	ASP
1	B	649	VAL
1	B	651	ILE
1	B	727	LEU
1	B	753	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	448	GLN
1	A	522	ASN
1	A	543	HIS
1	A	730	ASN
1	A	765	ASN
1	B	448	GLN
1	B	522	ASN
1	B	543	HIS
1	B	730	ASN
1	B	765	ASN

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 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	320/371 (86%)	0.83	44 (13%) 6 4	19, 59, 98, 103	0
1	B	320/371 (86%)	1.05	47 (14%) 6 3	19, 59, 98, 103	0
All	All	640/742 (86%)	0.94	91 (14%) 6 4	19, 59, 98, 103	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	709	GLY	11.9
1	B	717	ARG	7.3
1	A	551	SER	6.4
1	A	414	THR	5.9
1	B	486	GLU	5.8
1	A	474	THR	5.1
1	A	453	SER	4.8
1	B	456	GLU	4.6
1	A	456	GLU	4.5
1	B	414	THR	4.5
1	B	473	VAL	4.4
1	B	606	ALA	4.3
1	A	552	VAL	4.2
1	A	470	GLY	4.1
1	B	474	THR	4.0
1	A	486	GLU	3.9
1	A	549	PRO	3.9
1	A	770	THR	3.9
1	B	485	THR	3.6
1	A	666	GLU	3.6
1	B	472	TYR	3.6
1	B	402	GLU	3.5
1	B	403	LYS	3.5
1	A	472	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	762	ASP	3.4
1	B	705	LEU	3.4
1	B	643	PRO	3.4
1	A	473	VAL	3.4
1	A	405	LEU	3.3
1	A	469	LYS	3.1
1	A	647	ASP	3.1
1	B	525	VAL	3.1
1	B	730	ASN	3.0
1	B	667	MET	3.0
1	A	758	HIS	3.0
1	A	763	GLN	3.0
1	A	632	THR	2.9
1	B	506	SER	2.9
1	A	707	MET	2.9
1	B	428	GLN	2.8
1	A	403	LYS	2.8
1	A	485	THR	2.8
1	B	502	PHE	2.8
1	B	706	GLY	2.8
1	A	410	TYR	2.8
1	A	425	LEU	2.8
1	A	483	GLN	2.6
1	A	713	ASP	2.6
1	B	762	ASP	2.6
1	A	705	LEU	2.6
1	B	411	SER	2.5
1	B	713	ASP	2.5
1	B	521	GLY	2.5
1	A	429	PRO	2.4
1	B	514	SER	2.4
1	B	768	ALA	2.4
1	A	479	GLY	2.4
1	A	606	ALA	2.4
1	A	653	SER	2.4
1	A	768	ALA	2.4
1	B	416	LEU	2.4
1	B	429	PRO	2.3
1	A	404	GLU	2.3
1	A	408	SER	2.3
1	B	671	GLY	2.3
1	A	411	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	766	PHE	2.3
1	B	771	HIS	2.2
1	A	443	LYS	2.2
1	B	631	GLU	2.2
1	B	725	ALA	2.2
1	B	670	GLN	2.2
1	A	550	GLU	2.2
1	B	448	GLN	2.2
1	B	459	GLU	2.2
1	B	745	MET	2.2
1	B	526	THR	2.1
1	A	519	GLY	2.1
1	A	709	GLY	2.1
1	B	449	GLY	2.1
1	B	714	GLU	2.1
1	A	406	ASP	2.1
1	B	599	ARG	2.1
1	B	512	ASP	2.1
1	A	459	GLU	2.1
1	B	479	GLY	2.0
1	A	717	ARG	2.0
1	B	596	LEU	2.0
1	B	754	ASN	2.0
1	B	770	THR	2.0
1	B	553	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 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.