



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:59 AM UTC

PDB ID : 3KWV / pdb_00003kwv
Title : Structural basis for the unfolding of anthrax lethal factor by protective antigen oligomers
Authors : Feld, G.K.; Kintzer, A.F.; Krantz, B.A.
Deposited on : 2009-12-01
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

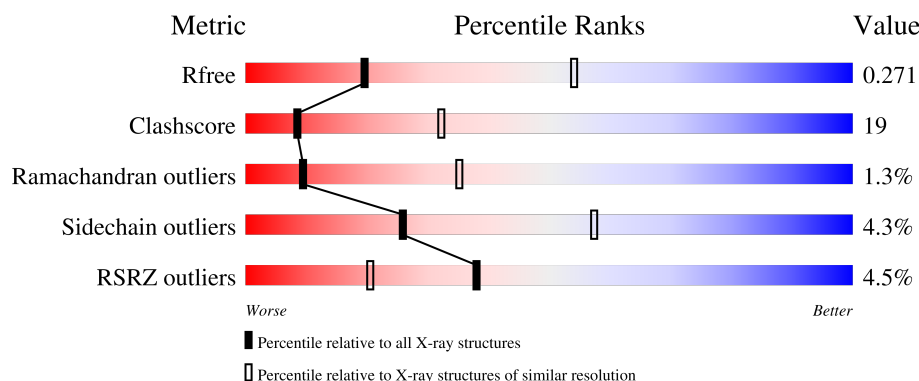
1 Overall quality at a glance

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	548	2% 57% 36% • •
1	B	548	4% 61% 32% • •
1	D	548	5% 57% 35% • •
1	E	548	5% 59% 33% • •
2	C	263	3% 49% 32% • 16%

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Mol	Chain	Length	Quality of chain
2	F	263	6% 48% 33% • 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20349 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 Protective antigen PA-63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4178	2617	718	837	6			
1	B	526	Total	C	N	O	S	0	0	0
			4169	2612	717	834	6			
1	D	526	Total	C	N	O	S	0	0	0
			4171	2613	717	835	6			
1	E	528	Total	C	N	O	S	0	0	0
			4187	2622	720	839	6			

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	PRO	VAL	engineered mutation	UNP P13423
A	304	GLY	HIS	engineered mutation	UNP P13423
A	?	-	GLY	deletion	UNP P13423
A	?	-	ASN	deletion	UNP P13423
A	?	-	ALA	deletion	UNP P13423
A	?	-	GLU	deletion	UNP P13423
A	?	-	VAL	deletion	UNP P13423
A	?	-	HIS	deletion	UNP P13423
A	?	-	ALA	deletion	UNP P13423
A	?	-	SER	deletion	UNP P13423
A	?	-	PHE	deletion	UNP P13423
A	?	-	PHE	deletion	UNP P13423
A	?	-	ASP	deletion	UNP P13423
A	?	-	ILE	deletion	UNP P13423
A	?	-	GLY	deletion	UNP P13423
A	?	-	GLY	deletion	UNP P13423
A	?	-	SER	deletion	UNP P13423
A	?	-	VAL	deletion	UNP P13423
A	?	-	SER	deletion	UNP P13423
A	?	-	ALA	deletion	UNP P13423
A	?	-	GLY	deletion	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP P13423
B	303	PRO	VAL	engineered mutation	UNP P13423
B	304	GLY	HIS	engineered mutation	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	ASN	deletion	UNP P13423
B	?	-	ALA	deletion	UNP P13423
B	?	-	GLU	deletion	UNP P13423
B	?	-	VAL	deletion	UNP P13423
B	?	-	HIS	deletion	UNP P13423
B	?	-	ALA	deletion	UNP P13423
B	?	-	SER	deletion	UNP P13423
B	?	-	PHE	deletion	UNP P13423
B	?	-	PHE	deletion	UNP P13423
B	?	-	ASP	deletion	UNP P13423
B	?	-	ILE	deletion	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	SER	deletion	UNP P13423
B	?	-	VAL	deletion	UNP P13423
B	?	-	SER	deletion	UNP P13423
B	?	-	ALA	deletion	UNP P13423
B	?	-	GLY	deletion	UNP P13423
B	?	-	PHE	deletion	UNP P13423
D	303	PRO	VAL	engineered mutation	UNP P13423
D	304	GLY	HIS	engineered mutation	UNP P13423
D	?	-	GLY	deletion	UNP P13423
D	?	-	ASN	deletion	UNP P13423
D	?	-	ALA	deletion	UNP P13423
D	?	-	GLU	deletion	UNP P13423
D	?	-	VAL	deletion	UNP P13423
D	?	-	HIS	deletion	UNP P13423
D	?	-	ALA	deletion	UNP P13423
D	?	-	SER	deletion	UNP P13423
D	?	-	PHE	deletion	UNP P13423
D	?	-	PHE	deletion	UNP P13423
D	?	-	ASP	deletion	UNP P13423
D	?	-	ILE	deletion	UNP P13423
D	?	-	GLY	deletion	UNP P13423
D	?	-	GLY	deletion	UNP P13423
D	?	-	SER	deletion	UNP P13423
D	?	-	VAL	deletion	UNP P13423
D	?	-	SER	deletion	UNP P13423

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ALA	deletion	UNP P13423
D	?	-	GLY	deletion	UNP P13423
E	303	PRO	VAL	engineered mutation	UNP P13423
E	304	GLY	HIS	engineered mutation	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	ASN	deletion	UNP P13423
E	?	-	ALA	deletion	UNP P13423
E	?	-	GLU	deletion	UNP P13423
E	?	-	VAL	deletion	UNP P13423
E	?	-	HIS	deletion	UNP P13423
E	?	-	ALA	deletion	UNP P13423
E	?	-	SER	deletion	UNP P13423
E	?	-	PHE	deletion	UNP P13423
E	?	-	PHE	deletion	UNP P13423
E	?	-	ASP	deletion	UNP P13423
E	?	-	ILE	deletion	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	SER	deletion	UNP P13423
E	?	-	VAL	deletion	UNP P13423
E	?	-	SER	deletion	UNP P13423
E	?	-	ALA	deletion	UNP P13423
E	?	-	GLY	deletion	UNP P13423
E	?	-	PHE	deletion	UNP P13423

- Molecule 2 is a protein called Lethal factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	222	Total	C	N	O	S	0	0	0
			1816	1164	290	359	3			
2	F	222	Total	C	N	O	S	0	0	0
			1816	1164	290	359	3			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Ca	0	0
			2	2		

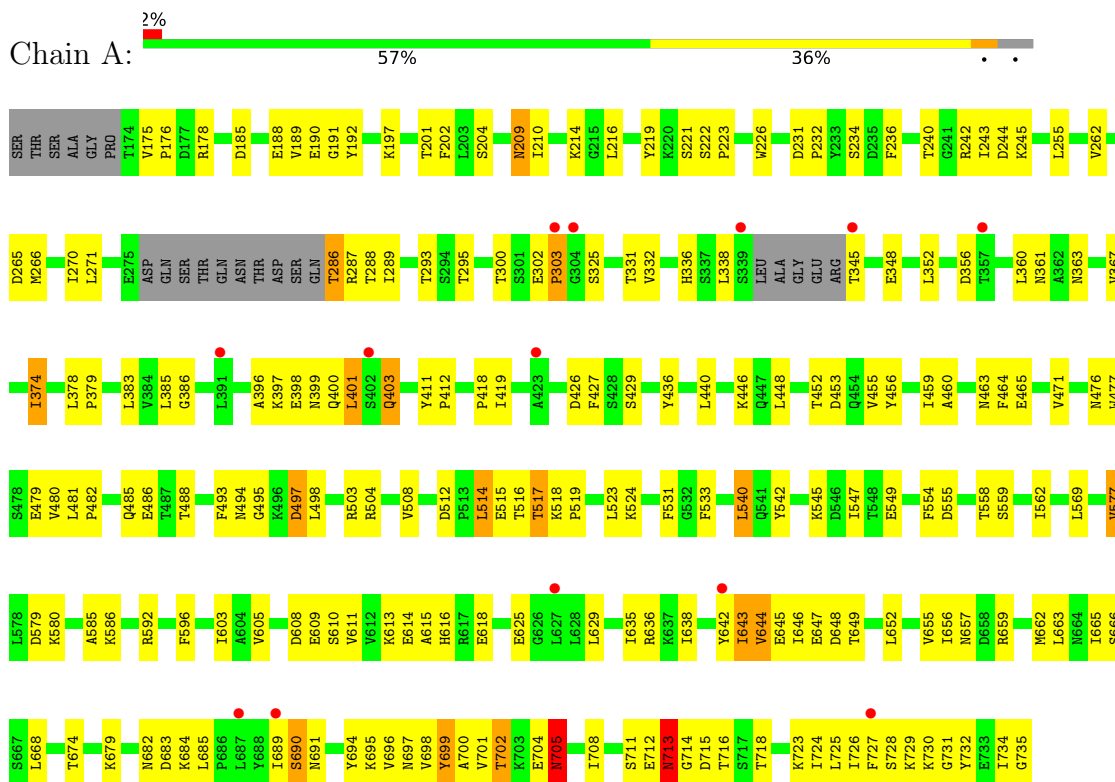
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

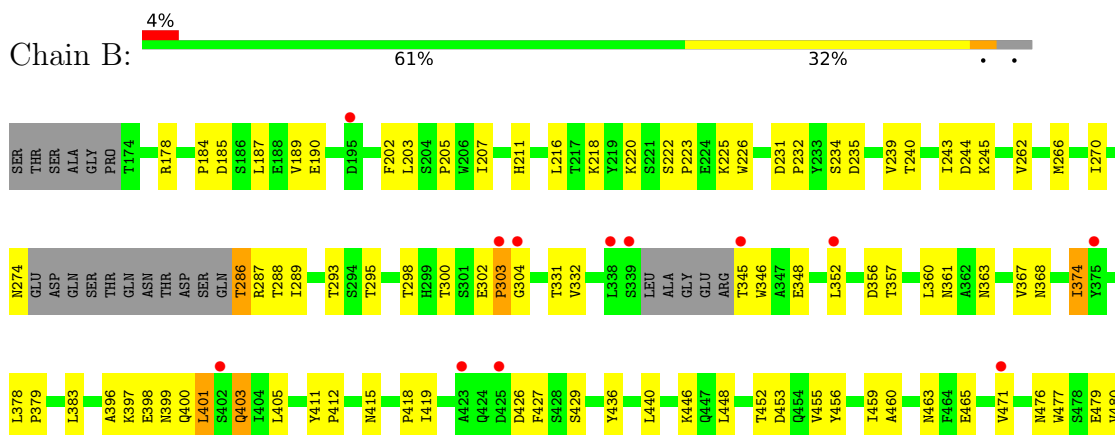
3 Residue-property plots [i](#)

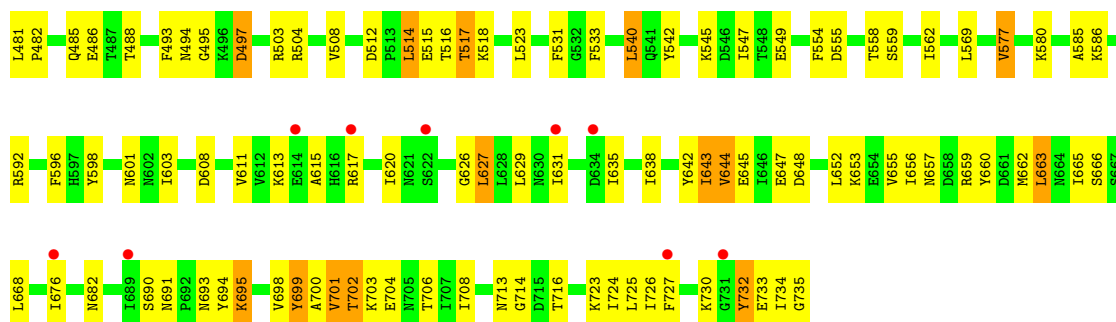
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protective antigen PA-63

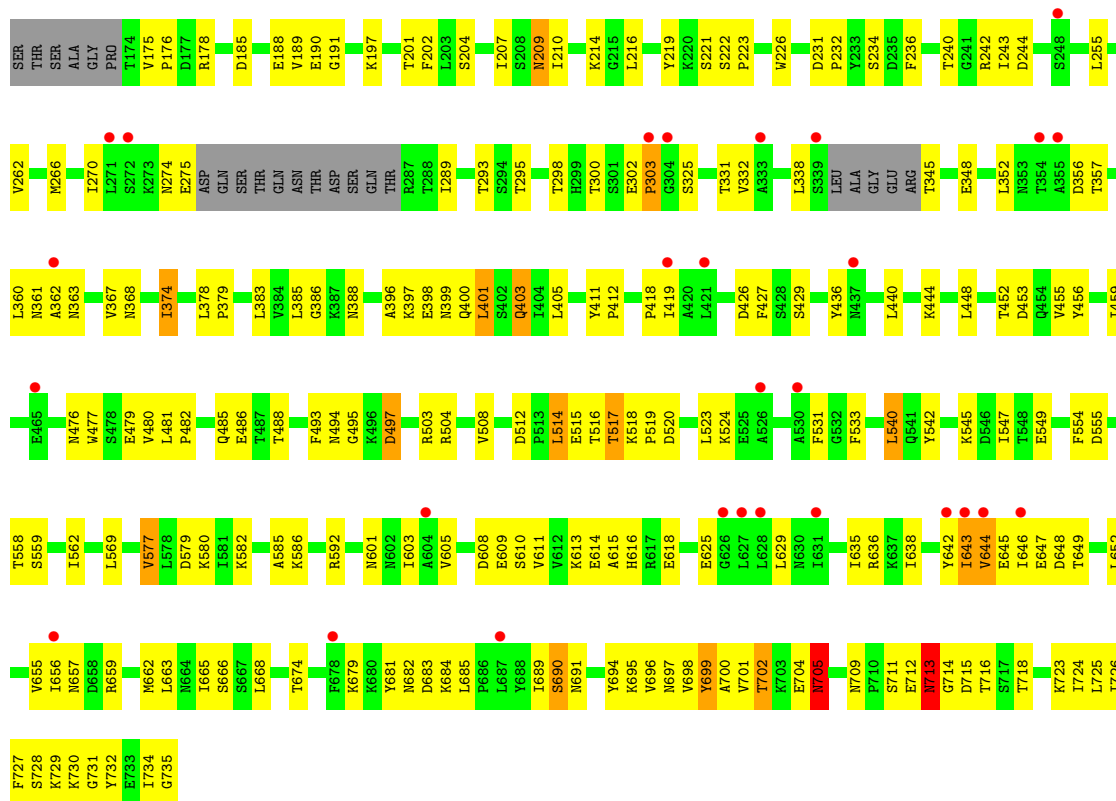


• Molecule 1: Protective antigen PA-63

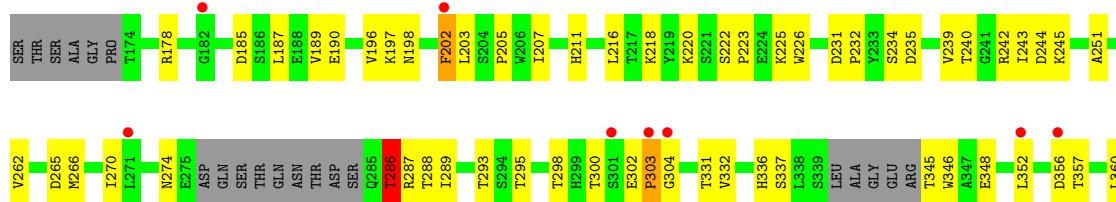


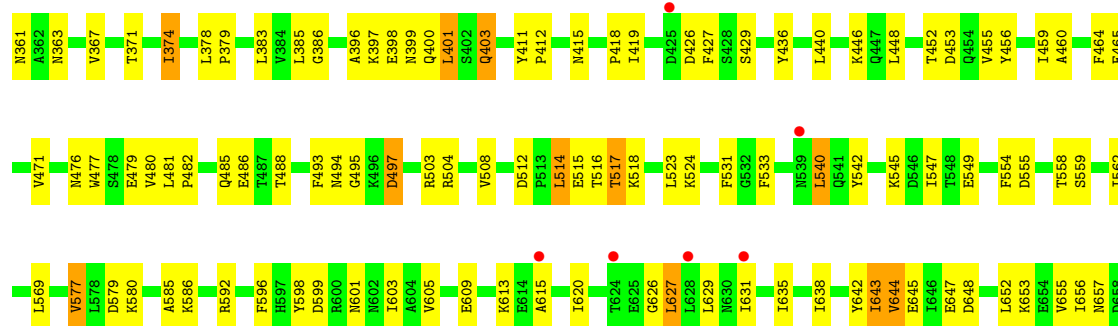


• Molecule 1: Protective antigen PA-63

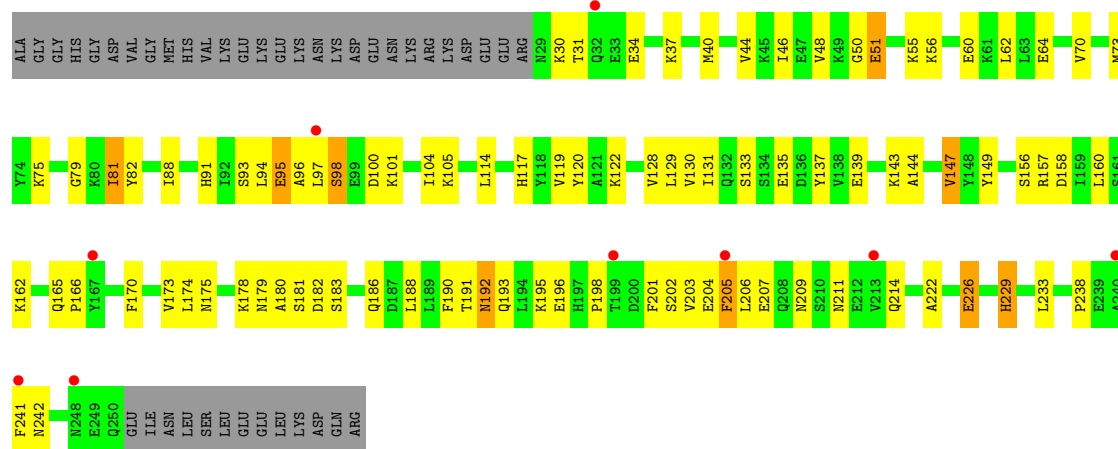


• Molecule 1: Protective antigen PA-63

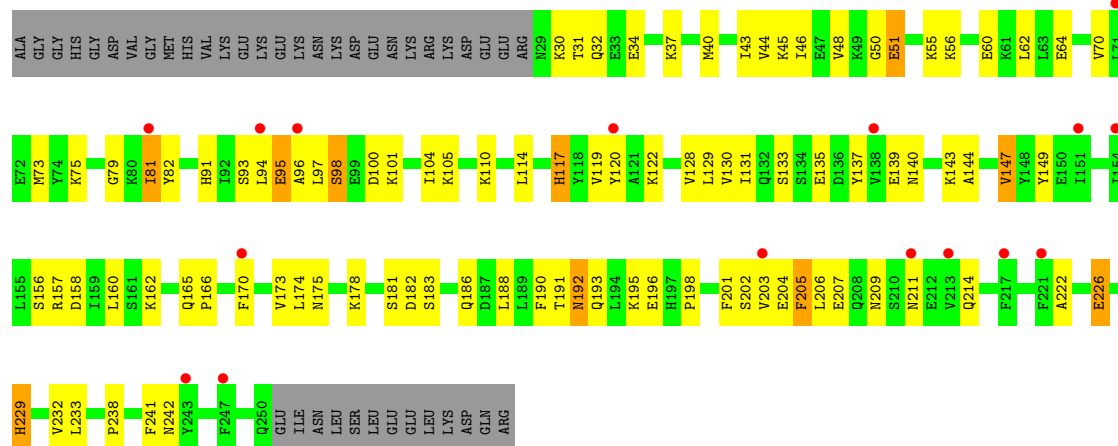




• Molecule 2: Lethal factor



• Molecule 2: Lethal factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.38Å 178.38Å 240.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.10 49.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.1 (49.84-3.10) 92.0 (49.84-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.249 , 0.281 0.240 , 0.271	Depositor DCC
R_{free} test set	2000 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20349	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.32	3/4249 (0.1%)	0.71	1/5764 (0.0%)
1	B	0.28	1/4240 (0.0%)	0.70	2/5752 (0.0%)
1	D	0.32	3/4242 (0.1%)	0.71	1/5754 (0.0%)
1	E	0.30	2/4258 (0.0%)	0.70	2/5776 (0.0%)
2	C	0.31	1/1850 (0.1%)	0.71	4/2493 (0.2%)
2	F	0.31	1/1850 (0.1%)	0.71	4/2493 (0.2%)
All	All	0.31	11/20689 (0.1%)	0.71	14/28032 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	229	HIS	ND1-CE1	5.42	1.38	1.32
2	C	229	HIS	ND1-CE1	5.39	1.38	1.32
1	A	485	GLN	CD-OE1	5.23	1.33	1.23
1	D	485	GLN	CD-OE1	5.23	1.33	1.23
1	E	485	GLN	CD-OE1	5.20	1.33	1.23
1	B	485	GLN	CD-OE1	5.19	1.33	1.23
1	A	713	ASN	CG-OD1	5.17	1.33	1.23
1	D	713	ASN	CG-OD1	5.15	1.33	1.23
1	D	705	ASN	CG-OD1	5.10	1.33	1.23
1	A	705	ASN	CG-OD1	5.07	1.33	1.23
1	E	198	ASN	CG-OD1	5.04	1.33	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	229	HIS	CB-CG-CD2	-6.65	122.56	131.20
2	C	229	HIS	CB-CG-CD2	-6.54	122.69	131.20
2	F	229	HIS	CB-CG-ND1	5.69	131.23	122.70
2	C	229	HIS	CB-CG-ND1	5.68	131.21	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	714	GLY	N-CA-C	-5.64	107.00	114.95
1	D	714	GLY	N-CA-C	-5.62	107.02	114.95
1	E	695	LYS	N-CA-C	5.42	117.53	110.53
1	B	695	LYS	N-CA-C	5.40	117.49	110.53
2	F	226	GLU	CA-C-N	5.12	125.16	119.32
2	F	226	GLU	C-N-CA	5.12	125.16	119.32
2	C	226	GLU	CA-C-N	5.07	125.10	119.32
2	C	226	GLU	C-N-CA	5.07	125.10	119.32
1	E	714	GLY	N-CA-C	-5.04	108.30	115.30
1	B	714	GLY	N-CA-C	-5.03	108.31	115.30

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	4178	0	4149	174	0
1	B	4169	0	4143	152	0
1	D	4171	0	4142	175	0
1	E	4187	0	4157	159	0
2	C	1816	0	1797	62	0
2	F	1816	0	1797	70	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	20349	0	20185	771	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 19.

All (771) 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:266:MET:H	1:A:295:THR:HG21	1.36	0.90
1:D:699:TYR:HA	1:D:726:ILE:HG12	1.58	0.86
1:A:699:TYR:HA	1:A:726:ILE:HG12	1.58	0.85
1:D:210:ILE:HD11	2:F:188:LEU:HB2	1.59	0.84
1:D:625:GLU:HB3	1:D:679:LYS:HE3	1.57	0.84
1:A:625:GLU:HB3	1:A:679:LYS:HE3	1.58	0.83
1:B:266:MET:H	1:B:295:THR:HG21	1.45	0.82
1:A:554:PHE:HB3	1:A:558:THR:HG23	1.62	0.82
1:E:554:PHE:HB3	1:E:558:THR:HG23	1.62	0.81
1:D:554:PHE:HB3	1:D:558:THR:HG23	1.62	0.81
1:D:266:MET:H	1:D:295:THR:HG21	1.45	0.81
1:B:554:PHE:HB3	1:B:558:THR:HG23	1.62	0.81
1:A:336:HIS:CD2	1:A:708:ILE:HA	2.18	0.78
1:E:266:MET:H	1:E:295:THR:HG21	1.49	0.78
1:D:648:ASP:HB2	1:D:652:LEU:HB3	1.65	0.77
1:A:648:ASP:HB2	1:A:652:LEU:HB3	1.65	0.77
1:A:266:MET:N	1:A:295:THR:HG21	1.99	0.77
2:F:55:LYS:HB3	2:F:133:SER:HB2	1.67	0.76
2:C:55:LYS:HB3	2:C:133:SER:HB2	1.68	0.76
1:E:231:ASP:HB2	1:E:232:PRO:CD	2.17	0.75
1:B:659:ARG:HE	1:B:716:THR:HG21	1.52	0.75
1:E:231:ASP:HB2	1:E:232:PRO:HD3	1.69	0.75
1:B:463:ASN:HB3	1:B:465:GLU:OE2	1.87	0.75
1:B:231:ASP:HB2	1:B:232:PRO:CD	2.17	0.74
1:E:659:ARG:HE	1:E:716:THR:HG21	1.52	0.74
1:B:231:ASP:HB2	1:B:232:PRO:HD3	1.69	0.74
2:F:157:ARG:HG3	2:F:158:ASP:H	1.52	0.73
1:B:298:THR:HB	1:B:601:ASN:HB3	1.71	0.73
2:C:157:ARG:HG3	2:C:158:ASP:H	1.51	0.73
1:E:577:VAL:HG22	1:E:580:LYS:HB2	1.71	0.72
1:A:231:ASP:HB2	1:A:232:PRO:CD	2.21	0.71
1:D:231:ASP:HB2	1:D:232:PRO:CD	2.21	0.71
1:D:300:THR:HG21	1:E:415:ASN:HD22	1.56	0.70
1:E:699:TYR:HB3	1:E:725:LEU:HA	1.73	0.70
1:A:577:VAL:HG22	1:A:580:LYS:HB2	1.71	0.70
1:D:577:VAL:HG22	1:D:580:LYS:HB2	1.72	0.70
1:D:695:LYS:HD2	1:D:728:SER:HB2	1.73	0.70
1:B:577:VAL:HG22	1:B:580:LYS:HB2	1.72	0.70
1:B:699:TYR:HB3	1:B:725:LEU:HA	1.73	0.70
1:E:274:ASN:HB3	1:E:357:THR:HG23	1.73	0.70
2:C:156:SER:HB2	2:C:214:GLN:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:156:SER:HB2	2:F:214:GLN:HB2	1.74	0.69
2:F:48:VAL:HG12	2:F:50:GLY:H	1.58	0.69
1:A:695:LYS:HD2	1:A:728:SER:HB2	1.73	0.69
1:B:663:LEU:HD13	1:B:701:VAL:HG11	1.73	0.69
1:D:656:ILE:HD11	1:D:682:ASN:HB2	1.75	0.68
1:A:202:PHE:CE2	1:A:204:SER:HB3	2.27	0.68
1:D:266:MET:N	1:D:295:THR:HG21	2.07	0.68
1:B:274:ASN:HB3	1:B:357:THR:HG23	1.76	0.68
2:F:40:MET:O	2:F:44:VAL:HG12	1.94	0.68
1:D:202:PHE:CE2	1:D:204:SER:HB3	2.28	0.68
1:B:730:LYS:HB2	1:B:734:ILE:HD11	1.75	0.67
1:E:663:LEU:HD13	1:E:701:VAL:HG11	1.74	0.67
1:A:656:ILE:HD11	1:A:682:ASN:HB2	1.75	0.67
2:C:40:MET:O	2:C:44:VAL:HG12	1.95	0.67
1:A:360:LEU:HD23	1:A:361:ASN:N	2.10	0.67
1:B:266:MET:N	1:B:295:THR:HG21	2.09	0.67
2:F:75:LYS:HA	2:F:79:GLY:H	1.60	0.67
2:C:75:LYS:HA	2:C:79:GLY:H	1.61	0.66
2:C:48:VAL:HG12	2:C:50:GLY:H	1.58	0.66
1:D:274:ASN:HB3	1:D:357:THR:HG23	1.76	0.66
1:D:493:PHE:CZ	1:D:495:GLY:HA3	2.31	0.66
1:D:240:THR:HG23	1:D:242:ARG:H	1.61	0.66
1:E:730:LYS:HB2	1:E:734:ILE:HD11	1.76	0.66
1:E:493:PHE:CZ	1:E:495:GLY:HA3	2.31	0.66
1:A:659:ARG:HB2	1:A:662:MET:HG3	1.78	0.66
1:E:266:MET:N	1:E:295:THR:HG21	2.09	0.65
1:E:298:THR:HG22	1:E:603:ILE:HD11	1.77	0.65
1:A:240:THR:HG23	1:A:242:ARG:H	1.60	0.65
1:A:493:PHE:CZ	1:A:495:GLY:HA3	2.32	0.65
1:B:298:THR:HG22	1:B:603:ILE:HD11	1.79	0.65
1:A:210:ILE:HD11	2:C:188:LEU:HB2	1.79	0.65
1:A:262:VAL:HG21	1:A:374:ILE:HD12	1.79	0.65
1:D:659:ARG:HB2	1:D:662:MET:HG3	1.78	0.65
1:B:401:LEU:HB2	1:B:403:GLN:OE1	1.98	0.64
1:B:493:PHE:CZ	1:B:495:GLY:HA3	2.32	0.64
1:E:401:LEU:HB2	1:E:403:GLN:OE1	1.98	0.64
1:A:401:LEU:HB2	1:A:403:GLN:OE1	1.98	0.64
1:A:514:LEU:O	1:A:517:THR:HG22	1.98	0.64
1:D:401:LEU:HB2	1:D:403:GLN:OE1	1.98	0.64
1:D:702:THR:CG2	1:D:704:GLU:HG2	2.27	0.64
1:E:659:ARG:NE	1:E:716:THR:HG21	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:702:THR:CG2	1:E:704:GLU:HG2	2.28	0.63
1:B:702:THR:CG2	1:B:704:GLU:HG2	2.28	0.63
1:A:702:THR:CG2	1:A:704:GLU:HG2	2.27	0.63
1:D:699:TYR:HB2	1:D:724:ILE:O	1.98	0.63
1:D:729:LYS:HD3	1:D:734:ILE:O	1.98	0.63
1:A:729:LYS:HD3	1:A:734:ILE:O	1.98	0.63
1:D:396:ALA:HB1	1:D:401:LEU:HD21	1.80	0.63
1:D:514:LEU:O	1:D:517:THR:HG22	1.99	0.63
1:B:514:LEU:O	1:B:517:THR:HG22	1.99	0.63
1:A:699:TYR:HB2	1:A:724:ILE:O	1.99	0.62
1:D:555:ASP:OD1	1:D:558:THR:HG22	1.99	0.62
1:B:659:ARG:NE	1:B:716:THR:HG21	2.13	0.62
1:B:295:THR:HB	1:B:332:VAL:HG22	1.82	0.62
1:E:295:THR:HB	1:E:332:VAL:HG22	1.82	0.62
1:A:704:GLU:HG3	1:A:705:ASN:ND2	2.14	0.62
1:D:704:GLU:HG3	1:D:705:ASN:ND2	2.15	0.62
1:E:655:VAL:HG12	1:E:657:ASN:H	1.64	0.62
1:A:295:THR:HB	1:A:332:VAL:HG22	1.82	0.62
1:D:295:THR:HB	1:D:332:VAL:HG22	1.82	0.62
1:A:659:ARG:HA	1:A:716:THR:O	2.00	0.62
2:C:119:VAL:HG23	2:C:131:ILE:HG22	1.82	0.62
1:D:691:ASN:HB3	1:D:694:TYR:CZ	2.35	0.62
1:E:514:LEU:O	1:E:517:THR:HG22	1.99	0.62
1:B:699:TYR:HA	1:B:726:ILE:HG12	1.82	0.62
1:D:659:ARG:HG3	1:D:662:MET:HE2	1.81	0.62
1:E:396:ALA:HB1	1:E:401:LEU:HD21	1.80	0.62
1:E:555:ASP:OD1	1:E:558:THR:HG22	1.99	0.61
1:B:396:ALA:HB1	1:B:401:LEU:HD21	1.80	0.61
1:D:659:ARG:HA	1:D:716:THR:O	2.00	0.61
2:F:119:VAL:HG23	2:F:131:ILE:HG22	1.82	0.61
2:F:157:ARG:HG3	2:F:158:ASP:N	2.15	0.61
1:D:444:LYS:HA	1:D:709:ASN:HD21	1.65	0.61
1:D:444:LYS:HA	1:D:709:ASN:ND2	2.15	0.61
2:C:157:ARG:HG3	2:C:158:ASP:N	2.14	0.61
1:A:555:ASP:OD1	1:A:558:THR:HG22	2.00	0.61
1:A:338:LEU:HD12	1:A:662:MET:HG2	1.81	0.61
1:A:691:ASN:HB3	1:A:694:TYR:CZ	2.35	0.61
1:B:555:ASP:OD1	1:B:558:THR:HG22	2.01	0.61
1:A:396:ALA:HB1	1:A:401:LEU:HD21	1.80	0.61
1:A:659:ARG:HG3	1:A:662:MET:HE2	1.81	0.61
1:B:655:VAL:HG12	1:B:657:ASN:H	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:702:THR:HG22	1:E:704:GLU:HG2	1.83	0.60
1:A:642:TYR:CE1	1:A:700:ALA:HB2	2.36	0.60
1:E:620:ILE:HG12	1:E:629:LEU:HA	1.83	0.60
1:B:702:THR:HG22	1:B:704:GLU:HG2	1.83	0.60
1:E:699:TYR:HA	1:E:726:ILE:HG12	1.82	0.60
1:B:508:VAL:HG13	1:B:516:THR:HA	1.84	0.60
1:E:699:TYR:N	1:E:699:TYR:CD2	2.69	0.60
2:C:211:ASN:O	2:C:214:GLN:HG2	2.02	0.60
2:F:192:ASN:HA	2:F:195:LYS:HE2	1.83	0.60
1:E:642:TYR:CE2	1:E:666:SER:HB2	2.38	0.59
1:A:663:LEU:HD13	1:A:701:VAL:HG11	1.84	0.59
1:B:302:GLU:HB3	1:B:303:PRO:HD2	1.85	0.59
1:D:642:TYR:CE1	1:D:700:ALA:HB2	2.37	0.59
1:A:463:ASN:HB3	1:A:465:GLU:OE2	2.02	0.59
1:D:302:GLU:HB3	1:D:303:PRO:HD2	1.84	0.59
2:F:211:ASN:O	2:F:214:GLN:HG2	2.03	0.59
1:B:642:TYR:CE2	1:B:666:SER:HB2	2.38	0.59
1:E:302:GLU:HB3	1:E:303:PRO:HD2	1.85	0.59
1:A:302:GLU:HB3	1:A:303:PRO:HD2	1.85	0.59
1:A:699:TYR:N	1:A:699:TYR:HD2	2.01	0.59
1:D:190:GLU:CD	2:F:140:ASN:HA	2.28	0.59
2:F:70:VAL:HA	2:F:73:MET:HE2	1.84	0.59
1:D:338:LEU:HD12	1:D:681:TYR:HE1	1.66	0.59
2:F:170:PHE:O	2:F:173:VAL:HG12	2.02	0.59
1:E:555:ASP:CG	1:E:558:THR:HG22	2.28	0.58
1:B:620:ILE:HG12	1:B:629:LEU:HA	1.83	0.58
2:C:70:VAL:HA	2:C:73:MET:HE2	1.84	0.58
2:C:170:PHE:O	2:C:173:VAL:HG12	2.03	0.58
2:C:192:ASN:HA	2:C:195:LYS:HE2	1.84	0.58
2:F:178:LYS:HB2	2:F:201:PHE:CE2	2.38	0.58
1:D:555:ASP:CG	1:D:558:THR:HG22	2.29	0.58
1:D:644:VAL:HB	1:D:698:VAL:HG22	1.84	0.58
1:A:645:GLU:HA	1:A:655:VAL:HA	1.84	0.58
1:D:663:LEU:HD13	1:D:701:VAL:HG11	1.84	0.58
1:E:508:VAL:HG13	1:E:516:THR:HA	1.84	0.58
1:A:508:VAL:HG13	1:A:516:THR:HA	1.85	0.58
1:A:659:ARG:HE	1:A:716:THR:HG21	1.69	0.58
1:A:555:ASP:CG	1:A:558:THR:HG22	2.28	0.58
1:A:644:VAL:HB	1:A:698:VAL:HG22	1.85	0.58
2:F:186:GLN:O	2:F:190:PHE:HB2	2.03	0.58
2:C:186:GLN:O	2:C:190:PHE:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:178:LYS:HB2	2:C:201:PHE:CE2	2.38	0.58
2:C:175:ASN:OD1	2:C:201:PHE:HB2	2.04	0.58
1:D:645:GLU:HA	1:D:655:VAL:HA	1.85	0.58
1:D:508:VAL:HG13	1:D:516:THR:HA	1.85	0.58
1:A:699:TYR:N	1:A:699:TYR:CD2	2.72	0.57
1:A:608:ASP:O	1:A:611:VAL:HG22	2.04	0.57
2:C:94:LEU:HB2	2:C:122:LYS:NZ	2.19	0.57
1:D:699:TYR:CD2	1:D:699:TYR:N	2.72	0.57
1:D:232:PRO:CG	1:D:459:ILE:HD13	2.34	0.57
1:D:699:TYR:N	1:D:699:TYR:HD2	2.02	0.57
1:B:262:VAL:HG21	1:B:374:ILE:HD12	1.86	0.57
1:B:555:ASP:CG	1:B:558:THR:HG22	2.29	0.57
1:B:615:ALA:HB1	1:B:631:ILE:HG13	1.86	0.57
1:D:659:ARG:HE	1:D:716:THR:HG21	1.68	0.57
1:A:635:ILE:O	1:A:638:ILE:HG12	2.04	0.57
1:D:635:ILE:O	1:D:638:ILE:HG12	2.04	0.57
2:F:175:ASN:OD1	2:F:201:PHE:HB2	2.05	0.57
1:B:699:TYR:N	1:B:699:TYR:CD2	2.69	0.57
2:F:191:THR:C	2:F:193:GLN:H	2.13	0.57
1:D:608:ASP:O	1:D:611:VAL:HG22	2.04	0.57
1:D:647:GLU:O	1:D:694:TYR:HB2	2.05	0.57
1:A:683:ASP:O	1:A:684:LYS:HG2	2.05	0.56
1:B:476:ASN:O	1:B:479:GLU:HG2	2.05	0.56
1:A:647:GLU:O	1:A:694:TYR:HB2	2.05	0.56
1:D:345:THR:HB	1:D:348:GLU:HB3	1.88	0.56
1:D:683:ASP:O	1:D:684:LYS:HG2	2.05	0.56
1:E:262:VAL:HG21	1:E:374:ILE:HD12	1.87	0.56
1:E:656:ILE:HD11	1:E:682:ASN:CG	2.30	0.56
1:E:627:LEU:HD11	1:E:727:PHE:CD1	2.40	0.56
2:F:94:LEU:HB2	2:F:122:LYS:NZ	2.20	0.56
1:D:298:THR:HG22	1:D:603:ILE:HD11	1.87	0.56
1:D:188:GLU:HB3	1:D:221:SER:O	2.06	0.56
1:D:476:ASN:O	1:D:479:GLU:HG2	2.05	0.56
2:F:186:GLN:HB2	2:F:190:PHE:CD2	2.41	0.56
1:D:262:VAL:HG21	1:D:374:ILE:HD12	1.88	0.56
1:A:476:ASN:O	1:A:479:GLU:HG2	2.06	0.56
2:C:81:ILE:HD12	2:C:81:ILE:O	2.06	0.56
2:C:156:SER:CB	2:C:214:GLN:HB2	2.35	0.56
1:E:345:THR:HB	1:E:348:GLU:HB3	1.88	0.56
2:F:156:SER:CB	2:F:214:GLN:HB2	2.35	0.56
1:A:302:GLU:HG3	1:B:415:ASN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:HB	1:A:348:GLU:HB3	1.88	0.56
2:C:186:GLN:HB2	2:C:190:PHE:CD2	2.41	0.56
2:C:191:THR:C	2:C:193:GLN:H	2.13	0.56
1:B:345:THR:HB	1:B:348:GLU:HB3	1.88	0.55
2:C:202:SER:C	2:C:204:GLU:H	2.14	0.55
1:E:298:THR:HB	1:E:601:ASN:HB3	1.86	0.55
2:F:81:ILE:HD12	2:F:81:ILE:O	2.06	0.55
1:A:647:GLU:HA	1:A:652:LEU:O	2.06	0.55
1:D:647:GLU:HA	1:D:652:LEU:O	2.06	0.55
1:B:656:ILE:HD11	1:B:682:ASN:CG	2.31	0.55
1:E:270:ILE:HA	1:E:289:ILE:O	2.06	0.55
1:A:188:GLU:HB3	1:A:221:SER:O	2.07	0.55
1:A:724:ILE:O	1:A:726:ILE:HG23	2.07	0.55
2:F:202:SER:C	2:F:204:GLU:H	2.14	0.55
1:B:627:LEU:HD11	1:B:727:PHE:CD1	2.41	0.54
1:D:699:TYR:CZ	1:D:723:LYS:HD2	2.43	0.54
1:D:724:ILE:O	1:D:726:ILE:HG23	2.07	0.54
1:E:476:ASN:O	1:E:479:GLU:HG2	2.07	0.54
1:A:705:ASN:N	1:A:705:ASN:HD22	2.05	0.54
1:B:346:TRP:CZ2	1:B:446:LYS:HE3	2.43	0.54
2:C:205:PHE:HD2	2:C:209:ASN:HD22	1.55	0.54
1:B:512:ASP:O	1:B:516:THR:HG23	2.08	0.54
1:D:643:ILE:HG22	1:D:663:LEU:HD22	1.89	0.54
1:B:644:VAL:HB	1:B:698:VAL:HG22	1.90	0.54
1:A:699:TYR:CZ	1:A:723:LYS:HD2	2.43	0.54
1:B:360:LEU:HD23	1:B:361:ASN:N	2.22	0.54
1:A:643:ILE:HG22	1:A:663:LEU:HD22	1.89	0.54
1:B:401:LEU:H	1:B:401:LEU:HD22	1.73	0.54
1:D:705:ASN:N	1:D:705:ASN:HD22	2.05	0.54
1:E:401:LEU:H	1:E:401:LEU:HD22	1.73	0.54
2:F:205:PHE:HD2	2:F:209:ASN:HD22	1.55	0.54
1:A:643:ILE:HD12	1:A:718:THR:HG21	1.90	0.53
1:B:642:TYR:HE2	1:B:666:SER:HB2	1.73	0.53
1:D:643:ILE:HD12	1:D:718:THR:HG21	1.90	0.53
1:B:648:ASP:HB2	1:B:652:LEU:HB3	1.90	0.53
1:E:642:TYR:HE2	1:E:666:SER:HB2	1.73	0.53
1:B:613:LYS:O	1:B:617:ARG:N	2.42	0.53
1:D:512:ASP:O	1:D:516:THR:HG23	2.08	0.53
1:E:379:PRO:HB2	1:E:452:THR:HG23	1.90	0.53
1:E:644:VAL:HB	1:E:698:VAL:HG22	1.89	0.53
1:E:648:ASP:HB2	1:E:652:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TYR:CE2	1:A:440:LEU:HD11	2.43	0.53
1:D:379:PRO:HB2	1:D:452:THR:HG23	1.91	0.53
1:D:698:VAL:HB	1:D:727:PHE:HB3	1.91	0.53
1:E:189:VAL:HG13	1:E:223:PRO:HG3	1.91	0.53
1:A:642:TYR:HB2	1:A:665:ILE:HD11	1.89	0.53
1:A:656:ILE:HD11	1:A:682:ASN:CB	2.39	0.53
1:B:189:VAL:HG13	1:B:223:PRO:HG3	1.91	0.53
1:D:642:TYR:HB2	1:D:665:ILE:HD11	1.89	0.53
1:D:730:LYS:HB2	1:D:734:ILE:HG21	1.90	0.53
1:D:615:ALA:HB2	1:D:635:ILE:HD12	1.91	0.53
1:A:189:VAL:HG23	1:A:190:GLU:HG3	1.90	0.53
1:A:698:VAL:HB	1:A:727:PHE:HB3	1.91	0.53
1:D:436:TYR:CE2	1:D:440:LEU:HD11	2.43	0.53
1:D:656:ILE:HD11	1:D:682:ASN:CB	2.39	0.53
1:E:436:TYR:CE2	1:E:440:LEU:HD11	2.43	0.53
1:D:398:GLU:C	1:D:400:GLN:H	2.17	0.53
1:D:494:ASN:OD1	1:D:592:ARG:HA	2.09	0.53
1:B:436:TYR:CE2	1:B:440:LEU:HD11	2.43	0.52
1:B:481:LEU:N	1:B:482:PRO:HD2	2.24	0.52
1:D:699:TYR:CD1	1:D:725:LEU:HD23	2.44	0.52
1:D:401:LEU:H	1:D:401:LEU:HD22	1.74	0.52
2:F:144:ALA:O	2:F:147:VAL:HG22	2.10	0.52
1:A:401:LEU:HD22	1:A:401:LEU:H	1.74	0.52
1:B:644:VAL:HG13	1:B:656:ILE:HG22	1.91	0.52
1:E:494:ASN:OD1	1:E:592:ARG:HA	2.10	0.52
1:A:730:LYS:HB2	1:A:734:ILE:HG21	1.90	0.52
1:D:642:TYR:CD1	1:D:700:ALA:HB2	2.45	0.52
1:E:615:ALA:HB1	1:E:631:ILE:HG13	1.90	0.52
1:A:699:TYR:CD1	1:A:725:LEU:HD23	2.44	0.52
1:D:189:VAL:HG23	1:D:190:GLU:HG3	1.90	0.52
1:B:383:LEU:HD11	1:B:448:LEU:HD13	1.92	0.52
1:A:481:LEU:N	1:A:482:PRO:HD2	2.25	0.52
1:E:659:ARG:HB2	1:E:662:MET:HG3	1.91	0.52
1:B:398:GLU:C	1:B:400:GLN:H	2.17	0.52
2:C:144:ALA:O	2:C:147:VAL:HG22	2.10	0.52
1:B:659:ARG:HB2	1:B:662:MET:HG3	1.91	0.52
2:C:181:SER:O	2:C:182:ASP:HB2	2.10	0.52
1:D:656:ILE:HD11	1:D:682:ASN:CG	2.34	0.52
1:E:398:GLU:C	1:E:400:GLN:H	2.17	0.52
1:E:659:ARG:HA	1:E:716:THR:O	2.09	0.52
1:A:379:PRO:HB2	1:A:452:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:C	1:A:400:GLN:H	2.17	0.52
1:A:656:ILE:HD11	1:A:682:ASN:CG	2.35	0.52
1:A:702:THR:HG21	1:A:704:GLU:HG2	1.92	0.52
1:B:187:LEU:HD21	1:B:205:PRO:HG3	1.92	0.51
1:B:379:PRO:HB2	1:B:452:THR:HG23	1.91	0.51
1:A:383:LEU:HD11	1:A:448:LEU:HD13	1.92	0.51
1:A:642:TYR:CD1	1:A:700:ALA:HB2	2.45	0.51
1:E:242:ARG:NH2	2:F:43:ILE:HD11	2.25	0.51
1:E:481:LEU:N	1:E:482:PRO:HD2	2.26	0.51
1:A:712:GLU:HG3	1:A:713:ASN:ND2	2.25	0.51
1:D:702:THR:HG22	1:D:704:GLU:HG2	1.91	0.51
1:E:202:PHE:CE2	2:F:45:LYS:HG3	2.46	0.51
1:A:494:ASN:OD1	1:A:592:ARG:HA	2.10	0.51
1:B:494:ASN:OD1	1:B:592:ARG:HA	2.11	0.51
1:B:585:ALA:O	1:B:586:LYS:HB2	2.10	0.51
1:B:659:ARG:HE	1:B:716:THR:CG2	2.20	0.51
1:B:659:ARG:HA	1:B:716:THR:O	2.09	0.51
2:C:97:LEU:O	2:C:101:LYS:HE2	2.10	0.51
1:A:512:ASP:O	1:A:516:THR:HG23	2.11	0.51
1:D:712:GLU:HG3	1:D:713:ASN:ND2	2.25	0.51
1:E:265:ASP:HA	1:E:295:THR:HG21	1.92	0.51
1:A:649:THR:N	1:A:694:TYR:HB3	2.26	0.51
1:A:702:THR:HG22	1:A:704:GLU:HG2	1.92	0.51
1:D:222:SER:OG	1:D:517:THR:HG23	2.11	0.51
1:D:481:LEU:N	1:D:482:PRO:HD2	2.25	0.51
1:A:615:ALA:HB2	1:A:635:ILE:HD12	1.91	0.51
1:B:592:ARG:HB3	1:B:598:TYR:CZ	2.46	0.51
1:D:702:THR:HG22	1:D:704:GLU:H	1.76	0.51
1:A:585:ALA:O	1:A:586:LYS:HB2	2.11	0.51
1:A:702:THR:HG22	1:A:704:GLU:H	1.76	0.51
1:E:644:VAL:HG13	1:E:656:ILE:HG22	1.92	0.51
1:A:610:SER:O	1:A:614:GLU:HG2	2.11	0.51
1:D:610:SER:O	1:D:614:GLU:HG2	2.11	0.51
1:D:644:VAL:HG13	1:D:656:ILE:CG2	2.41	0.51
2:F:165:GLN:HA	2:F:166:PRO:C	2.35	0.51
1:B:455:VAL:HG23	1:B:455:VAL:O	2.11	0.50
1:B:645:GLU:OE1	1:B:653:LYS:HD3	2.11	0.50
1:E:642:TYR:CE1	1:E:700:ALA:HB2	2.46	0.50
1:B:286:THR:O	1:B:288:THR:HG23	2.11	0.50
2:C:165:GLN:HA	2:C:166:PRO:C	2.35	0.50
1:D:585:ALA:O	1:D:586:LYS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:648:ASP:HA	1:E:694:TYR:CG	2.46	0.50
2:C:94:LEU:HB2	2:C:122:LYS:HZ1	1.77	0.50
1:D:255:LEU:HD21	1:D:519:PRO:HG2	1.94	0.50
1:D:488:THR:OG1	1:D:504:ARG:HD3	2.12	0.50
1:E:187:LEU:HD21	1:E:205:PRO:HG3	1.93	0.50
1:E:512:ASP:O	1:E:516:THR:HG23	2.10	0.50
1:B:691:ASN:HB3	1:B:694:TYR:CE1	2.47	0.50
1:E:645:GLU:OE1	1:E:653:LYS:HD3	2.11	0.50
1:E:691:ASN:HB3	1:E:694:TYR:CE1	2.46	0.50
1:A:446:LYS:CG	1:A:708:ILE:HD12	2.40	0.50
1:A:545:LYS:HE2	1:A:549:GLU:HB3	1.94	0.50
1:D:655:VAL:HG22	1:D:657:ASN:H	1.77	0.50
1:E:734:ILE:HG13	1:E:735:GLY:H	1.77	0.50
2:F:238:PRO:O	2:F:242:ASN:HB2	2.12	0.50
1:E:383:LEU:HD11	1:E:448:LEU:HD13	1.93	0.50
1:E:460:ALA:HA	1:E:471:VAL:HA	1.94	0.50
1:E:545:LYS:HE2	1:E:549:GLU:HB3	1.94	0.50
1:E:659:ARG:HE	1:E:716:THR:CG2	2.21	0.50
1:A:455:VAL:O	1:A:455:VAL:HG23	2.11	0.50
1:B:232:PRO:CG	1:B:459:ILE:HD13	2.41	0.50
1:B:734:ILE:HG13	1:B:735:GLY:H	1.77	0.50
1:D:545:LYS:HE2	1:D:549:GLU:HB3	1.94	0.50
1:E:286:THR:O	1:E:288:THR:HG23	2.11	0.50
1:E:488:THR:OG1	1:E:504:ARG:HD3	2.12	0.50
2:F:97:LEU:O	2:F:101:LYS:HE2	2.11	0.50
2:F:181:SER:O	2:F:182:ASP:HB2	2.10	0.50
1:A:644:VAL:HG13	1:A:656:ILE:CG2	2.41	0.50
1:B:226:TRP:CE2	1:B:234:SER:HB3	2.47	0.49
1:B:648:ASP:HA	1:B:694:TYR:CG	2.46	0.49
1:E:455:VAL:HG23	1:E:455:VAL:O	2.12	0.49
1:E:585:ALA:O	1:E:586:LYS:HB2	2.12	0.49
2:F:94:LEU:HB2	2:F:122:LYS:HZ1	1.77	0.49
1:B:286:THR:HG22	1:B:287:ARG:H	1.77	0.49
1:E:226:TRP:CE2	1:E:234:SER:HB3	2.47	0.49
1:B:545:LYS:HE2	1:B:549:GLU:HB3	1.94	0.49
1:D:388:ASN:HB2	1:E:418:PRO:HD2	1.93	0.49
1:A:695:LYS:HE3	1:A:697:ASN:HD21	1.78	0.49
1:D:649:THR:N	1:D:694:TYR:HB3	2.26	0.49
1:D:695:LYS:HE3	1:D:697:ASN:HD21	1.78	0.49
1:E:596:PHE:HD1	1:E:638:ILE:HD13	1.77	0.49
1:E:642:TYR:HB2	1:E:665:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:THR:HG23	2:F:34:GLU:H	1.77	0.49
1:A:403:GLN:HG2	1:A:411:TYR:CZ	2.48	0.49
1:A:734:ILE:HG23	1:A:735:GLY:N	2.28	0.49
1:D:383:LEU:HD11	1:D:448:LEU:HD13	1.93	0.49
1:E:286:THR:HG22	1:E:287:ARG:H	1.76	0.49
1:A:286:THR:HG22	1:A:287:ARG:H	1.77	0.49
2:C:238:PRO:O	2:C:242:ASN:HB2	2.12	0.49
1:A:286:THR:O	1:A:288:THR:HG23	2.12	0.49
1:A:325:SER:CB	1:B:415:ASN:HD21	2.26	0.49
1:A:338:LEU:CD1	1:A:662:MET:HG2	2.42	0.49
1:A:655:VAL:HG22	1:A:657:ASN:H	1.76	0.49
1:B:515:GLU:OE1	1:B:518:LYS:HE3	2.13	0.49
1:B:558:THR:O	1:B:562:ILE:HG12	2.13	0.49
1:B:642:TYR:CE1	1:B:700:ALA:HB2	2.48	0.49
1:B:642:TYR:HB2	1:B:665:ILE:HD11	1.93	0.49
1:D:702:THR:HG21	1:D:704:GLU:HG2	1.93	0.49
1:D:734:ILE:HG23	1:D:735:GLY:N	2.28	0.49
1:D:191:GLY:HA2	1:D:219:TYR:O	2.13	0.49
1:E:403:GLN:HG2	1:E:411:TYR:CZ	2.48	0.48
1:D:603:ILE:O	1:D:605:VAL:HG13	2.13	0.48
1:E:235:ASP:O	1:E:239:VAL:HG22	2.13	0.48
2:C:31:THR:HG23	2:C:34:GLU:H	1.78	0.48
1:D:455:VAL:HG23	1:D:455:VAL:O	2.13	0.48
1:E:453:ASP:OD1	1:E:455:VAL:HG22	2.13	0.48
1:A:231:ASP:HB2	1:A:232:PRO:HD3	1.96	0.48
1:A:374:ILE:HD11	1:A:456:TYR:CD1	2.49	0.48
1:D:302:GLU:HG3	1:E:415:ASN:HB3	1.96	0.48
1:D:689:ILE:HG13	1:D:689:ILE:O	2.13	0.48
1:E:401:LEU:HD22	1:E:401:LEU:N	2.29	0.48
1:A:689:ILE:O	1:A:689:ILE:HG13	2.14	0.48
1:B:235:ASP:O	1:B:239:VAL:HG22	2.13	0.48
1:B:403:GLN:HG2	1:B:411:TYR:CZ	2.48	0.48
1:D:515:GLU:OE1	1:D:518:LYS:HE3	2.14	0.48
1:A:488:THR:OG1	1:A:504:ARG:HD3	2.13	0.48
1:E:698:VAL:HB	1:E:727:PHE:HB3	1.96	0.48
1:A:222:SER:OG	1:A:517:THR:HG23	2.13	0.48
1:D:403:GLN:HG2	1:D:411:TYR:CZ	2.49	0.48
1:A:232:PRO:CG	1:A:459:ILE:HD13	2.44	0.48
1:A:453:ASP:OD1	1:A:455:VAL:HG22	2.14	0.48
1:A:683:ASP:O	1:A:685:LEU:HG	2.13	0.48
1:B:698:VAL:HB	1:B:727:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLU:OE1	1:A:518:LYS:HE3	2.14	0.47
2:C:37:LYS:HA	2:C:40:MET:HG2	1.96	0.47
1:D:374:ILE:HD11	1:D:456:TYR:CD1	2.50	0.47
1:D:401:LEU:HD22	1:D:401:LEU:N	2.29	0.47
1:D:683:ASP:O	1:D:685:LEU:HG	2.14	0.47
1:A:231:ASP:HB2	1:A:232:PRO:HD2	1.96	0.47
1:B:379:PRO:HB2	1:B:452:THR:CG2	2.44	0.47
1:D:231:ASP:HB2	1:D:232:PRO:HD2	1.94	0.47
1:D:338:LEU:HD12	1:D:681:TYR:CE1	2.48	0.47
1:E:397:LYS:C	1:E:399:ASN:H	2.22	0.47
1:A:397:LYS:C	1:A:399:ASN:H	2.22	0.47
1:A:558:THR:O	1:A:562:ILE:HG12	2.14	0.47
1:B:488:THR:OG1	1:B:504:ARG:HD3	2.14	0.47
2:C:196:GLU:O	2:C:198:PRO:HD3	2.14	0.47
1:D:397:LYS:C	1:D:399:ASN:H	2.22	0.47
2:C:95:GLU:HB2	2:C:96:ALA:H	1.46	0.47
1:E:222:SER:OG	1:E:225:LYS:HG3	2.15	0.47
1:E:643:ILE:HD11	1:E:723:LYS:HD3	1.97	0.47
1:E:724:ILE:O	1:E:726:ILE:HG23	2.15	0.47
1:A:191:GLY:HA2	1:A:219:TYR:O	2.14	0.47
1:B:222:SER:OG	1:B:225:LYS:HG3	2.15	0.47
1:D:453:ASP:OD1	1:D:455:VAL:HG22	2.14	0.47
1:D:615:ALA:CB	1:D:635:ILE:HD12	2.44	0.47
2:F:196:GLU:O	2:F:198:PRO:HD3	2.14	0.47
1:A:401:LEU:HD22	1:A:401:LEU:N	2.29	0.47
1:A:446:LYS:HG3	1:A:708:ILE:HD12	1.96	0.47
1:A:615:ALA:CB	1:A:635:ILE:HD12	2.44	0.47
1:B:453:ASP:OD1	1:B:455:VAL:HG22	2.14	0.47
1:D:360:LEU:C	1:D:360:LEU:HD23	2.40	0.47
1:D:558:THR:O	1:D:562:ILE:HG12	2.15	0.47
1:B:374:ILE:HD11	1:B:456:TYR:CD1	2.49	0.47
1:B:643:ILE:HG23	1:B:663:LEU:HD22	1.96	0.47
1:E:515:GLU:OE1	1:E:518:LYS:HE3	2.15	0.47
1:E:643:ILE:HG23	1:E:663:LEU:HD22	1.96	0.47
1:E:734:ILE:HG13	1:E:735:GLY:N	2.29	0.47
1:A:603:ILE:O	1:A:605:VAL:HG13	2.14	0.47
1:B:730:LYS:HD2	1:B:732:TYR:OH	2.15	0.47
2:C:104:ILE:HG22	2:C:105:LYS:H	1.80	0.47
2:F:37:LYS:HA	2:F:40:MET:HG2	1.96	0.47
1:B:231:ASP:CB	1:B:232:PRO:CD	2.91	0.47
1:B:659:ARG:HG3	1:B:662:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:558:THR:O	1:E:562:ILE:HG12	2.14	0.47
2:F:104:ILE:HG22	2:F:105:LYS:H	1.80	0.47
1:A:379:PRO:HB2	1:A:452:THR:CG2	2.44	0.46
1:B:695:LYS:HB3	1:B:730:LYS:HA	1.96	0.46
1:E:660:TYR:CE2	1:E:716:THR:HG23	2.50	0.46
2:F:157:ARG:HB3	2:F:214:GLN:OE1	2.15	0.46
1:A:271:LEU:CD2	1:A:360:LEU:HG	2.45	0.46
1:B:401:LEU:HD22	1:B:401:LEU:N	2.29	0.46
2:C:157:ARG:HB3	2:C:214:GLN:OE1	2.15	0.46
1:D:274:ASN:O	1:D:275:GLU:HB2	2.15	0.46
1:D:642:TYR:HA	1:D:700:ALA:HA	1.97	0.46
1:E:379:PRO:HB2	1:E:452:THR:CG2	2.44	0.46
1:E:503:ARG:HB2	1:E:531:PHE:CZ	2.51	0.46
2:F:100:ASP:OD1	2:F:101:LYS:N	2.48	0.46
1:A:460:ALA:HA	1:A:471:VAL:HA	1.98	0.46
1:A:644:VAL:HG13	1:A:656:ILE:HG22	1.97	0.46
1:E:426:ASP:OD2	1:E:429:SER:HB3	2.15	0.46
1:B:185:ASP:O	1:B:189:VAL:HG22	2.15	0.46
1:B:643:ILE:HD11	1:B:723:LYS:HD3	1.97	0.46
2:C:100:ASP:OD1	2:C:101:LYS:N	2.49	0.46
1:A:498:LEU:HD11	1:A:596:PHE:CE2	2.50	0.46
1:A:646:ILE:HG23	1:A:696:VAL:HG22	1.98	0.46
1:B:608:ASP:O	1:B:611:VAL:HG22	2.15	0.46
1:E:226:TRP:CZ2	1:E:234:SER:HB3	2.50	0.46
1:B:734:ILE:HG13	1:B:735:GLY:N	2.30	0.46
1:E:203:LEU:HD22	2:F:44:VAL:HG23	1.98	0.46
1:E:374:ILE:HD11	1:E:456:TYR:CD1	2.50	0.46
2:F:122:LYS:HE3	2:F:122:LYS:HB2	1.77	0.46
1:B:207:ILE:HB	1:B:211:HIS:CE1	2.50	0.46
1:B:660:TYR:CE2	1:B:716:THR:HG23	2.50	0.46
1:D:379:PRO:HB2	1:D:452:THR:CG2	2.44	0.46
1:E:626:GLY:HA3	1:E:676:ILE:O	2.15	0.46
1:E:695:LYS:HB3	1:E:730:LYS:HA	1.96	0.46
1:A:486:GLU:OE1	1:A:586:LYS:HE2	2.16	0.46
1:B:724:ILE:O	1:B:726:ILE:HG23	2.15	0.46
2:C:62:LEU:HD11	2:C:137:TYR:CD1	2.51	0.46
1:E:659:ARG:HG3	1:E:662:MET:HE2	1.98	0.46
1:A:265:ASP:HA	1:A:295:THR:HG21	1.97	0.46
1:D:426:ASP:OD2	1:D:429:SER:HB3	2.16	0.46
1:E:185:ASP:O	1:E:189:VAL:HG22	2.15	0.46
1:E:207:ILE:HB	1:E:211:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:60:GLU:O	2:F:64:GLU:HG3	2.16	0.46
1:B:397:LYS:C	1:B:399:ASN:H	2.22	0.45
2:F:143:LYS:O	2:F:147:VAL:HG13	2.16	0.45
1:A:503:ARG:HB2	1:A:531:PHE:CZ	2.51	0.45
1:E:730:LYS:HD2	1:E:732:TYR:OH	2.15	0.45
1:A:426:ASP:OD2	1:A:429:SER:HB3	2.16	0.45
1:B:226:TRP:CZ2	1:B:234:SER:HB3	2.50	0.45
1:B:426:ASP:OD2	1:B:429:SER:HB3	2.16	0.45
1:D:243:ILE:HG12	1:D:244:ASP:N	2.31	0.45
2:F:62:LEU:HD11	2:F:137:TYR:CD1	2.52	0.45
2:F:226:GLU:HB3	2:F:229:HIS:HB2	1.99	0.45
1:B:189:VAL:HG23	1:B:190:GLU:HG3	1.98	0.45
1:B:270:ILE:HA	1:B:289:ILE:O	2.16	0.45
1:B:503:ARG:HB2	1:B:531:PHE:CZ	2.51	0.45
1:A:243:ILE:HG12	1:A:244:ASP:N	2.31	0.45
1:E:222:SER:HA	1:E:223:PRO:HD3	1.82	0.45
1:E:609:GLU:O	1:E:613:LYS:HG3	2.16	0.45
1:A:226:TRP:CZ2	1:A:234:SER:HB3	2.52	0.45
1:A:711:SER:OG	1:A:715:ASP:HB3	2.17	0.45
1:D:644:VAL:HG13	1:D:656:ILE:HG22	1.97	0.45
1:D:691:ASN:HB3	1:D:694:TYR:CE1	2.51	0.45
1:A:691:ASN:HB3	1:A:694:TYR:CE1	2.51	0.45
1:D:646:ILE:HG23	1:D:696:VAL:HG22	1.98	0.45
1:B:300:THR:HB	1:B:302:GLU:HB2	1.99	0.45
1:B:486:GLU:OE1	1:B:586:LYS:HE2	2.17	0.45
1:B:626:GLY:HA3	1:B:676:ILE:O	2.16	0.45
2:C:98:SER:O	2:C:101:LYS:HG2	2.16	0.45
1:D:300:THR:HB	1:D:302:GLU:HB2	1.99	0.45
1:B:648:ASP:OD2	1:B:652:LEU:HB3	2.17	0.45
2:C:60:GLU:O	2:C:64:GLU:HG3	2.17	0.45
1:D:352:LEU:HB3	1:D:356:ASP:OD2	2.17	0.45
1:D:503:ARG:HB2	1:D:531:PHE:CZ	2.52	0.45
1:E:643:ILE:HD11	1:E:723:LYS:HB3	1.98	0.45
1:B:243:ILE:HG12	1:B:244:ASP:N	2.32	0.45
1:D:486:GLU:OE1	1:D:586:LYS:HE2	2.16	0.45
2:C:143:LYS:O	2:C:147:VAL:HG13	2.16	0.44
2:C:226:GLU:HB3	2:C:229:HIS:HB2	1.99	0.44
1:E:189:VAL:HG23	1:E:190:GLU:HG3	1.98	0.44
1:E:648:ASP:OD2	1:E:652:LEU:HB3	2.17	0.44
2:F:98:SER:O	2:F:101:LYS:HG2	2.16	0.44
1:B:554:PHE:HB2	1:B:559:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:SER:HB2	2:C:204:GLU:HG2	1.99	0.44
1:D:226:TRP:CZ2	1:D:234:SER:HB3	2.52	0.44
1:E:352:LEU:HB3	1:E:356:ASP:OD2	2.17	0.44
1:A:214:LYS:HB2	1:A:216:LEU:HG	1.99	0.44
1:A:300:THR:HB	1:A:302:GLU:HB2	1.99	0.44
1:B:184:PRO:CD	2:C:44:VAL:HG21	2.47	0.44
1:E:412:PRO:HD3	1:E:419:ILE:HG13	1.99	0.44
1:A:175:VAL:HA	1:A:176:PRO:HD3	1.83	0.44
1:B:643:ILE:CG2	1:B:663:LEU:HD22	2.48	0.44
1:D:214:LYS:HB2	1:D:216:LEU:HG	1.99	0.44
1:E:243:ILE:HG12	1:E:244:ASP:N	2.32	0.44
1:E:690:SER:HB3	1:E:694:TYR:OH	2.17	0.44
1:B:352:LEU:HB3	1:B:356:ASP:OD2	2.16	0.44
2:C:135:GLU:O	2:C:135:GLU:HG3	2.18	0.44
1:E:300:THR:HB	1:E:302:GLU:HB2	1.99	0.44
1:A:642:TYR:HA	1:A:700:ALA:HA	1.98	0.44
1:A:699:TYR:HB3	1:A:725:LEU:HA	2.00	0.44
1:B:643:ILE:HD11	1:B:723:LYS:HB3	1.98	0.44
1:B:690:SER:HB3	1:B:694:TYR:OH	2.17	0.44
1:D:412:PRO:HD3	1:D:419:ILE:HG13	1.98	0.44
1:E:486:GLU:OE1	1:E:586:LYS:HE2	2.18	0.44
1:A:352:LEU:HB3	1:A:356:ASP:OD2	2.17	0.44
1:B:412:PRO:HD3	1:B:419:ILE:HG13	1.99	0.44
1:E:197:LYS:HE2	2:F:135:GLU:HG2	2.00	0.44
1:E:211:HIS:HB3	1:E:216:LEU:HD12	2.00	0.44
2:F:104:ILE:HD11	2:F:114:LEU:HB2	2.00	0.44
1:B:596:PHE:HD1	1:B:638:ILE:HD13	1.81	0.44
1:D:555:ASP:OD1	1:D:555:ASP:C	2.61	0.44
1:D:690:SER:HB3	1:D:694:TYR:OH	2.18	0.44
1:E:303:PRO:HB2	1:E:304:GLY:H	1.61	0.44
1:E:464:PHE:HD2	2:F:32:GLN:HE21	1.66	0.44
1:E:605:VAL:O	1:E:702:THR:HG23	2.18	0.44
1:E:732:TYR:O	1:E:733:GLU:C	2.61	0.44
1:A:236:PHE:O	1:A:240:THR:HG22	2.18	0.44
2:C:50:GLY:O	2:C:51:GLU:C	2.61	0.44
1:D:629:LEU:N	1:D:629:LEU:HD23	2.33	0.44
1:A:412:PRO:HD3	1:A:419:ILE:HG13	1.99	0.43
1:A:629:LEU:N	1:A:629:LEU:HD23	2.33	0.43
1:A:690:SER:HB3	1:A:694:TYR:OH	2.18	0.43
1:B:211:HIS:HB3	1:B:216:LEU:HD12	2.00	0.43
1:B:446:LYS:HB2	1:B:708:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:TRP:HA	1:B:480:VAL:HG12	2.00	0.43
1:B:555:ASP:OD1	1:B:555:ASP:C	2.61	0.43
1:D:209:ASN:OD1	1:D:209:ASN:N	2.49	0.43
1:D:636:ARG:HD3	1:D:674:THR:HG21	2.00	0.43
1:D:704:GLU:HG3	1:D:705:ASN:HD22	1.83	0.43
1:A:378:LEU:HA	1:A:379:PRO:HD3	1.90	0.43
2:C:30:LYS:HD2	2:C:34:GLU:HB3	1.99	0.43
2:F:233:LEU:HG	2:F:241:PHE:HB2	2.00	0.43
1:B:732:TYR:O	1:B:733:GLU:C	2.61	0.43
1:D:554:PHE:HB2	1:D:559:SER:HB2	2.00	0.43
1:E:337:SER:HA	1:E:661:ASP:HB2	1.99	0.43
2:F:174:LEU:HD23	2:F:174:LEU:O	2.18	0.43
1:B:222:SER:HA	1:B:223:PRO:HD3	1.81	0.43
1:D:516:THR:OG1	1:E:196:VAL:HG21	2.19	0.43
1:E:242:ARG:HH22	2:F:43:ILE:HD11	1.83	0.43
1:E:346:TRP:CZ2	1:E:446:LYS:HE3	2.53	0.43
1:A:477:TRP:HA	1:A:480:VAL:HG12	2.01	0.43
1:A:555:ASP:OD1	1:A:555:ASP:C	2.61	0.43
2:C:122:LYS:HE3	2:C:122:LYS:HB2	1.77	0.43
1:D:222:SER:HA	1:D:223:PRO:HD3	1.77	0.43
1:E:270:ILE:CG1	1:E:361:ASN:HB3	2.49	0.43
2:F:30:LYS:HD2	2:F:34:GLU:HB3	2.00	0.43
2:F:135:GLU:O	2:F:135:GLU:HG3	2.18	0.43
1:A:209:ASN:OD1	1:A:209:ASN:N	2.49	0.43
1:A:222:SER:HA	1:A:223:PRO:HD3	1.77	0.43
2:C:82:TYR:HB2	2:C:130:VAL:HG23	2.00	0.43
1:D:711:SER:OG	1:D:715:ASP:HB3	2.17	0.43
1:E:232:PRO:CG	1:E:459:ILE:HD13	2.48	0.43
1:E:555:ASP:OD1	1:E:555:ASP:C	2.61	0.43
1:A:255:LEU:HD21	1:A:519:PRO:HG2	2.00	0.43
1:B:374:ILE:HD11	1:B:456:TYR:CG	2.54	0.43
2:F:202:SER:HB2	2:F:204:GLU:HG2	2.00	0.43
1:A:374:ILE:HD11	1:A:456:TYR:CG	2.54	0.43
1:B:178:ARG:HG3	1:B:185:ASP:OD2	2.19	0.43
1:B:460:ALA:HA	1:B:471:VAL:HA	2.01	0.43
1:A:609:GLU:O	1:A:613:LYS:HG3	2.19	0.43
1:D:609:GLU:O	1:D:613:LYS:HG3	2.18	0.43
1:E:477:TRP:HA	1:E:480:VAL:HG12	2.01	0.43
1:E:652:LEU:HD23	1:E:652:LEU:C	2.43	0.43
2:F:50:GLY:O	2:F:51:GLU:C	2.61	0.43
1:B:363:ASN:HB3	1:B:418:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:LYS:O	2:C:60:GLU:HG3	2.19	0.43
2:C:206:LEU:HD23	2:C:207:GLU:H	1.82	0.43
1:D:295:THR:HA	1:D:331:THR:O	2.19	0.43
1:E:554:PHE:HB2	1:E:559:SER:HB2	2.01	0.43
1:A:554:PHE:HB2	1:A:559:SER:HB2	2.01	0.42
1:A:636:ARG:HD3	1:A:674:THR:HG21	2.00	0.42
1:A:705:ASN:ND2	1:A:705:ASN:N	2.67	0.42
1:B:295:THR:HA	1:B:331:THR:O	2.18	0.42
1:B:352:LEU:HD22	1:B:356:ASP:OD2	2.19	0.42
1:D:293:THR:HB	1:D:332:VAL:HG13	2.01	0.42
1:D:352:LEU:HD22	1:D:356:ASP:OD2	2.19	0.42
1:D:477:TRP:HA	1:D:480:VAL:HG12	2.01	0.42
1:A:569:LEU:HD13	1:A:577:VAL:HG21	2.01	0.42
1:B:702:THR:HG21	1:B:704:GLU:HG2	2.01	0.42
2:C:104:ILE:HD11	2:C:114:LEU:HB2	2.00	0.42
2:C:174:LEU:HD23	2:C:174:LEU:O	2.18	0.42
1:D:189:VAL:HG13	1:D:223:PRO:HG3	2.00	0.42
1:D:363:ASN:HB3	1:D:418:PRO:HB2	2.02	0.42
1:E:178:ARG:HG3	1:E:185:ASP:OD2	2.19	0.42
1:E:569:LEU:HD13	1:E:577:VAL:HG21	2.01	0.42
1:E:647:GLU:O	1:E:694:TYR:HB2	2.19	0.42
1:D:231:ASP:HB2	1:D:232:PRO:HD3	1.97	0.42
1:D:569:LEU:HD13	1:D:577:VAL:HG21	2.02	0.42
1:E:643:ILE:CD1	1:E:723:LYS:HD3	2.49	0.42
2:F:206:LEU:HD23	2:F:207:GLU:H	1.82	0.42
1:A:363:ASN:HB3	1:A:418:PRO:HB2	2.01	0.42
1:A:533:PHE:CE1	1:A:542:TYR:HB2	2.55	0.42
1:B:647:GLU:O	1:B:694:TYR:HB2	2.19	0.42
2:C:233:LEU:HG	2:C:241:PHE:HB2	2.00	0.42
1:D:731:GLY:H	1:D:734:ILE:HG23	1.84	0.42
2:F:82:TYR:HB2	2:F:130:VAL:HG23	2.00	0.42
1:B:293:THR:HB	1:B:332:VAL:HG13	2.02	0.42
1:B:652:LEU:HD23	1:B:652:LEU:C	2.44	0.42
1:D:236:PHE:O	1:D:240:THR:HG22	2.20	0.42
1:E:251:ALA:HB2	1:E:371:THR:HB	2.00	0.42
1:E:643:ILE:CG2	1:E:663:LEU:HD22	2.48	0.42
2:F:91:HIS:CD2	2:F:93:SER:HB3	2.54	0.42
1:A:609:GLU:HA	1:A:724:ILE:HD13	2.02	0.42
1:D:642:TYR:CE2	1:D:666:SER:HB2	2.55	0.42
1:D:649:THR:OG1	1:D:694:TYR:HB3	2.20	0.42
1:D:659:ARG:HE	1:D:716:THR:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:HIS:CD2	1:E:708:ILE:HA	2.54	0.42
1:E:363:ASN:HB3	1:E:418:PRO:HB2	2.01	0.42
1:E:497:ASP:OD1	1:E:497:ASP:N	2.53	0.42
1:E:533:PHE:CE1	1:E:542:TYR:HB2	2.55	0.42
2:F:104:ILE:HG22	2:F:105:LYS:N	2.35	0.42
1:A:642:TYR:CE2	1:A:666:SER:HB2	2.55	0.42
1:A:731:GLY:H	1:A:734:ILE:HG23	1.84	0.42
1:B:644:VAL:HG13	1:B:656:ILE:CG2	2.50	0.42
2:C:91:HIS:CD2	2:C:93:SER:HB3	2.54	0.42
1:D:325:SER:CB	1:E:415:ASN:HD21	2.33	0.42
2:F:120:TYR:O	2:F:129:LEU:HD12	2.19	0.42
2:F:160:LEU:HD13	2:F:160:LEU:C	2.45	0.42
1:A:270:ILE:HA	1:A:289:ILE:O	2.20	0.42
1:A:295:THR:HA	1:A:331:THR:O	2.19	0.42
1:A:649:THR:OG1	1:A:694:TYR:HB3	2.20	0.42
2:F:95:GLU:HB2	2:F:96:ALA:H	1.46	0.42
1:A:352:LEU:HD22	1:A:356:ASP:OD2	2.19	0.42
1:A:497:ASP:OD1	1:A:497:ASP:N	2.53	0.42
1:B:703:LYS:HA	1:B:706:THR:OG1	2.19	0.42
1:D:497:ASP:OD1	1:D:497:ASP:N	2.53	0.42
1:E:703:LYS:HA	1:E:706:THR:OG1	2.19	0.42
2:C:120:TYR:O	2:C:129:LEU:HD12	2.19	0.41
1:D:222:SER:OG	1:D:517:THR:CG2	2.68	0.41
1:D:374:ILE:HD11	1:D:456:TYR:CG	2.55	0.41
1:D:609:GLU:HA	1:D:724:ILE:HD13	2.02	0.41
1:E:293:THR:HB	1:E:332:VAL:HG13	2.02	0.41
2:F:183:SER:O	2:F:186:GLN:HG2	2.20	0.41
1:A:189:VAL:HG13	1:A:223:PRO:HG3	2.01	0.41
1:D:659:ARG:CG	1:D:662:MET:HE2	2.48	0.41
1:D:699:TYR:HB3	1:D:725:LEU:HA	2.00	0.41
2:F:56:LYS:O	2:F:60:GLU:HG3	2.19	0.41
1:A:385:LEU:HD12	1:A:386:GLY:H	1.85	0.41
1:A:515:GLU:OE2	1:B:245:LYS:HE3	2.20	0.41
2:C:183:SER:O	2:C:186:GLN:HG2	2.20	0.41
2:C:191:THR:C	2:C:193:GLN:N	2.79	0.41
1:D:270:ILE:HA	1:D:289:ILE:O	2.20	0.41
1:D:625:GLU:HB3	1:D:679:LYS:CE	2.40	0.41
1:E:374:ILE:HD11	1:E:456:TYR:CG	2.56	0.41
1:A:293:THR:HB	1:A:332:VAL:HG13	2.02	0.41
1:A:659:ARG:HE	1:A:716:THR:CG2	2.32	0.41
1:B:533:PHE:CE1	1:B:542:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:TYR:N	1:B:699:TYR:HD2	2.16	0.41
1:D:524:LYS:CE	1:D:579:ASP:HB3	2.50	0.41
1:D:705:ASN:ND2	1:D:705:ASN:N	2.67	0.41
1:E:295:THR:HA	1:E:331:THR:O	2.19	0.41
1:A:403:GLN:HG2	1:A:411:TYR:OH	2.20	0.41
1:B:569:LEU:HD13	1:B:577:VAL:HG21	2.02	0.41
1:B:629:LEU:N	1:B:629:LEU:HD23	2.35	0.41
2:C:160:LEU:HD13	2:C:160:LEU:C	2.45	0.41
1:D:298:THR:HB	1:D:601:ASN:HB3	2.01	0.41
1:D:385:LEU:HD12	1:D:386:GLY:H	1.86	0.41
1:D:533:PHE:CE1	1:D:542:TYR:HB2	2.55	0.41
1:E:403:GLN:HG2	1:E:411:TYR:OH	2.20	0.41
1:E:524:LYS:CE	1:E:579:ASP:HB3	2.50	0.41
1:A:300:THR:HG21	1:B:415:ASN:HD22	1.86	0.41
1:A:616:HIS:C	1:A:618:GLU:H	2.29	0.41
1:D:178:ARG:HG3	1:D:185:ASP:OD2	2.20	0.41
1:E:245:LYS:HA	1:E:245:LYS:HD3	1.89	0.41
1:E:732:TYR:HB2	1:E:733:GLU:H	1.72	0.41
2:F:191:THR:C	2:F:193:GLN:N	2.79	0.41
1:A:178:ARG:HG3	1:A:185:ASP:OD2	2.21	0.41
1:B:533:PHE:HB3	1:B:540:LEU:HD21	2.02	0.41
1:B:631:ILE:HD11	1:B:635:ILE:HG21	2.03	0.41
1:D:533:PHE:HB3	1:D:540:LEU:HD21	2.03	0.41
1:E:352:LEU:HD22	1:E:356:ASP:OD2	2.19	0.41
1:E:596:PHE:CD1	1:E:638:ILE:HD13	2.54	0.41
1:A:524:LYS:CE	1:A:579:ASP:HB3	2.51	0.41
2:C:88:ILE:H	2:C:88:ILE:HG13	1.71	0.41
1:D:616:HIS:C	1:D:618:GLU:H	2.29	0.41
1:E:385:LEU:HD12	1:E:386:GLY:H	1.86	0.41
1:A:533:PHE:HB3	1:A:540:LEU:HD21	2.03	0.41
1:B:378:LEU:HB2	1:B:396:ALA:HB2	2.03	0.41
1:B:453:ASP:OD1	1:B:453:ASP:C	2.64	0.41
1:B:463:ASN:HB3	1:B:465:GLU:CD	2.45	0.41
1:B:497:ASP:OD1	1:B:497:ASP:N	2.53	0.41
1:D:368:ASN:HB2	1:D:405:LEU:HG	2.03	0.41
1:A:188:GLU:HA	1:A:192:TYR:CE2	2.56	0.41
1:B:303:PRO:HB2	1:B:304:GLY:H	1.61	0.41
1:D:713:ASN:ND2	1:D:713:ASN:H	2.19	0.41
1:A:245:LYS:HA	1:A:245:LYS:HD3	1.90	0.40
1:A:713:ASN:ND2	1:A:713:ASN:N	2.69	0.40
1:B:203:LEU:C	1:B:203:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ASN:OD1	1:D:362:ALA:N	2.54	0.40
1:D:378:LEU:HB2	1:D:396:ALA:HB2	2.02	0.40
1:D:453:ASP:OD1	1:D:453:ASP:C	2.64	0.40
1:E:218:LYS:HE2	1:E:220:LYS:HE3	2.03	0.40
1:E:512:ASP:CG	1:E:515:GLU:HG2	2.46	0.40
1:A:378:LEU:HB2	1:A:396:ALA:HB2	2.03	0.40
1:B:403:GLN:HG2	1:B:411:TYR:OH	2.21	0.40
2:C:104:ILE:HG22	2:C:105:LYS:N	2.35	0.40
1:D:190:GLU:OE2	2:F:140:ASN:HA	2.21	0.40
2:F:149:TYR:HA	2:F:222:ALA:HB2	2.03	0.40
1:A:704:GLU:HG3	1:A:705:ASN:HD22	1.83	0.40
1:B:643:ILE:CD1	1:B:723:LYS:HD3	2.50	0.40
2:C:149:TYR:HA	2:C:222:ALA:HB2	2.03	0.40
1:D:175:VAL:HA	1:D:176:PRO:HD3	1.83	0.40
1:E:533:PHE:HB3	1:E:540:LEU:HD21	2.03	0.40
1:E:592:ARG:HB3	1:E:598:TYR:CZ	2.56	0.40
1:E:629:LEU:HD23	1:E:629:LEU:N	2.36	0.40
1:A:453:ASP:OD1	1:A:453:ASP:C	2.64	0.40
1:A:464:PHE:O	1:A:465:GLU:C	2.64	0.40
1:B:218:LYS:HE2	1:B:220:LYS:HE3	2.02	0.40
1:B:368:ASN:HB2	1:B:405:LEU:HG	2.03	0.40
1:D:545:LYS:HE2	1:D:549:GLU:CB	2.52	0.40
1:E:360:LEU:HD23	1:E:361:ASN:N	2.37	0.40
1:E:631:ILE:HD11	1:E:635:ILE:HG21	2.03	0.40
2:F:44:VAL:O	2:F:44:VAL:HG13	2.22	0.40
2:F:105:LYS:HA	2:F:110:LYS:O	2.21	0.40
1:A:659:ARG:CG	1:A:662:MET:HE2	2.48	0.40
1:B:691:ASN:C	1:B:693:ASN:H	2.29	0.40
2:C:179:ASN:O	2:C:180:ALA:HB2	2.22	0.40
1:D:207:ILE:HD11	2:F:232:VAL:HG11	2.03	0.40
1:D:520:ASP:HB3	1:D:582:LYS:NZ	2.37	0.40
1:E:378:LEU:HB2	1:E:396:ALA:HB2	2.02	0.40
1:E:453:ASP:OD1	1:E:453:ASP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/548 (95%)	471 (90%)	45 (9%)	5 (1%)	12	41
1	B	520/548 (95%)	462 (89%)	54 (10%)	4 (1%)	16	47
1	D	520/548 (95%)	468 (90%)	47 (9%)	5 (1%)	12	41
1	E	522/548 (95%)	469 (90%)	47 (9%)	6 (1%)	11	39
2	C	220/263 (84%)	183 (83%)	30 (14%)	7 (3%)	3	18
2	F	220/263 (84%)	183 (83%)	30 (14%)	7 (3%)	3	18
All	All	2523/2718 (93%)	2236 (89%)	253 (10%)	34 (1%)	9	35

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	732	TYR
2	C	162	LYS
1	D	732	TYR
2	F	162	LYS
1	A	303	PRO
1	A	497	ASP
1	B	303	PRO
1	B	497	ASP
1	B	732	TYR
2	C	98	SER
1	D	303	PRO
1	D	497	ASP
1	E	303	PRO
1	E	497	ASP
1	E	732	TYR
2	F	98	SER
2	C	192	ASN
2	C	203	VAL
1	E	286	THR
2	F	192	ASN

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Mol	Chain	Res	Type
2	F	203	VAL
1	A	690	SER
1	D	690	SER
2	C	51	GLU
2	C	117	HIS
2	F	117	HIS
1	A	577	VAL
1	B	577	VAL
1	D	577	VAL
1	E	577	VAL
1	E	599	ASP
2	F	51	GLU
2	C	46	ILE
2	F	46	ILE

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	474/491 (96%)	453 (96%)	21 (4%)	25	56
1	B	473/491 (96%)	451 (95%)	22 (5%)	23	55
1	D	473/491 (96%)	453 (96%)	20 (4%)	26	58
1	E	475/491 (97%)	452 (95%)	23 (5%)	23	54
2	C	200/236 (85%)	194 (97%)	6 (3%)	36	65
2	F	200/236 (85%)	193 (96%)	7 (4%)	32	62
All	All	2295/2436 (94%)	2196 (96%)	99 (4%)	26	57

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	A	201	THR
1	A	209	ASN
1	A	286	THR

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Mol	Chain	Res	Type
1	A	367	VAL
1	A	374	ILE
1	A	401	LEU
1	A	403	GLN
1	A	427	PHE
1	A	514	LEU
1	A	517	THR
1	A	523	LEU
1	A	540	LEU
1	A	547	ILE
1	A	643	ILE
1	A	644	VAL
1	A	668	LEU
1	A	699	TYR
1	A	702	THR
1	A	705	ASN
1	A	713	ASN
1	B	202	PHE
1	B	240	THR
1	B	286	THR
1	B	367	VAL
1	B	374	ILE
1	B	401	LEU
1	B	403	GLN
1	B	427	PHE
1	B	514	LEU
1	B	517	THR
1	B	523	LEU
1	B	540	LEU
1	B	547	ILE
1	B	627	LEU
1	B	643	ILE
1	B	644	VAL
1	B	663	LEU
1	B	668	LEU
1	B	699	TYR
1	B	701	VAL
1	B	702	THR
1	B	713	ASN
2	C	81	ILE
2	C	95	GLU
2	C	128	VAL

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Mol	Chain	Res	Type
2	C	139	GLU
2	C	147	VAL
2	C	205	PHE
1	D	197	LYS
1	D	201	THR
1	D	209	ASN
1	D	367	VAL
1	D	374	ILE
1	D	401	LEU
1	D	403	GLN
1	D	427	PHE
1	D	514	LEU
1	D	517	THR
1	D	523	LEU
1	D	540	LEU
1	D	547	ILE
1	D	643	ILE
1	D	644	VAL
1	D	668	LEU
1	D	699	TYR
1	D	702	THR
1	D	705	ASN
1	D	713	ASN
1	E	202	PHE
1	E	240	THR
1	E	286	THR
1	E	367	VAL
1	E	374	ILE
1	E	401	LEU
1	E	403	GLN
1	E	427	PHE
1	E	465	GLU
1	E	514	LEU
1	E	517	THR
1	E	523	LEU
1	E	540	LEU
1	E	547	ILE
1	E	627	LEU
1	E	643	ILE
1	E	644	VAL
1	E	663	LEU
1	E	668	LEU

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Mol	Chain	Res	Type
1	E	699	TYR
1	E	701	VAL
1	E	702	THR
1	E	713	ASN
2	F	81	ILE
2	F	95	GLU
2	F	117	HIS
2	F	128	VAL
2	F	139	GLU
2	F	147	VAL
2	F	205	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	HIS
2	C	186	GLN
1	E	361	ASN
2	F	32	GLN
2	F	186	GLN
2	F	229	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	527/548 (96%)	0.20	13 (2%)	58	37	46, 82, 173, 206	0
1	B	526/548 (95%)	0.28	21 (3%)	42	23	45, 83, 158, 206	0
1	D	526/548 (95%)	0.29	28 (5%)	32	17	47, 82, 171, 206	0
1	E	528/548 (96%)	0.36	27 (5%)	33	18	46, 84, 160, 205	0
2	C	222/263 (84%)	0.48	9 (4%)	41	23	69, 126, 169, 201	0
2	F	222/263 (84%)	0.66	16 (7%)	21	11	68, 126, 170, 198	0
All	All	2551/2718 (93%)	0.33	114 (4%)	38	20	45, 92, 169, 206	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	674	THR	5.8
1	B	304	GLY	4.2
2	C	213	VAL	3.7
1	A	687	LEU	3.6
1	E	356	ASP	3.6
1	D	626	GLY	3.5
1	E	303	PRO	3.5
1	A	303	PRO	3.5
1	E	304	GLY	3.4
1	B	303	PRO	3.4
1	A	304	GLY	3.3
2	F	151	ILE	3.3
1	E	615	ALA	3.2
2	F	243	TYR	3.2
1	A	642	TYR	3.1
1	E	675	PHE	3.1
1	E	539	ASN	3.1
1	E	667	SER	3.1
2	C	32	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	624	THR	3.0
1	D	465	GLU	3.0
1	D	627	LEU	2.9
1	E	678	PHE	2.9
1	B	338	LEU	2.9
1	D	303	PRO	2.9
1	A	339	SER	2.9
2	C	240	ALA	2.9
2	F	94	LEU	2.8
1	A	402	SER	2.8
1	D	437	ASN	2.8
2	C	199	THR	2.8
1	E	669	ARG	2.7
1	B	676	ILE	2.7
1	D	643	ILE	2.7
1	D	656	ILE	2.7
1	B	402	SER	2.7
1	B	617	ARG	2.6
2	F	170	PHE	2.6
1	E	697	ASN	2.6
1	D	644	VAL	2.6
1	B	731	GLY	2.6
1	B	614	GLU	2.6
1	B	689	ILE	2.6
1	D	419	ILE	2.6
2	C	97	LEU	2.6
1	B	345	THR	2.6
1	B	471	VAL	2.5
1	D	354	THR	2.5
1	B	339	SER	2.5
1	E	182	GLY	2.5
1	E	301	SER	2.5
1	E	668	LEU	2.5
1	D	678	PHE	2.5
1	B	352	LEU	2.5
1	B	423	ALA	2.4
1	B	631	ILE	2.4
1	A	357	THR	2.4
2	F	213	VAL	2.4
2	F	247	PHE	2.4
1	D	339	SER	2.4
1	D	628	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	631	ILE	2.4
1	E	705	ASN	2.4
2	C	248	ASN	2.4
1	E	425	ASP	2.4
1	D	526	ALA	2.4
1	E	689	ILE	2.4
1	D	304	GLY	2.3
1	D	271	LEU	2.3
1	E	692	PRO	2.3
1	D	421	LEU	2.3
2	F	71	LEU	2.3
2	C	205	PHE	2.3
2	F	221	PHE	2.3
1	D	362	ALA	2.3
1	A	345	THR	2.3
1	E	673	LYS	2.3
1	A	689	ILE	2.3
1	D	687	LEU	2.3
1	B	622	SER	2.3
1	D	631	ILE	2.2
1	D	333	ALA	2.2
1	E	628	LEU	2.2
2	C	241	PHE	2.2
1	D	272	SER	2.2
2	F	211	ASN	2.2
2	F	217	PHE	2.2
1	E	706	THR	2.2
1	D	642	TYR	2.2
2	F	154	ILE	2.2
1	D	530	ALA	2.2
1	D	604	ALA	2.2
1	B	195	ASP	2.2
1	E	202	PHE	2.2
2	F	120	TYR	2.1
1	D	248	SER	2.1
1	B	727	PHE	2.1
1	B	425	ASP	2.1
1	D	646	ILE	2.1
1	B	634	ASP	2.1
1	E	352	LEU	2.1
2	C	167	TYR	2.1
2	F	96	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	375	TYR	2.1
1	A	627	LEU	2.1
2	F	138	VAL	2.0
1	A	391	LEU	2.0
1	A	423	ALA	2.0
1	D	355	ALA	2.0
2	F	203	VAL	2.0
2	F	81	ILE	2.0
1	E	713	ASN	2.0
1	A	727	PHE	2.0
1	E	271	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	D	737	1/1	0.99	0.03	55,55,55,55	0
3	CA	A	737	1/1	1.00	0.03	45,45,45,45	0
3	CA	B	736	1/1	1.00	0.04	57,57,57,57	0
3	CA	B	737	1/1	1.00	0.01	48,48,48,48	0
3	CA	D	736	1/1	1.00	0.02	65,65,65,65	0
3	CA	A	736	1/1	1.00	0.04	52,52,52,52	0
3	CA	E	736	1/1	1.00	0.02	52,52,52,52	0
3	CA	E	737	1/1	1.00	0.04	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.