



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:28 AM UTC

PDB ID : 4BLA / pdb_00004bla
Title : Crystal structure of full-length human Suppressor of fused (SUFU) mutant lacking a regulatory subdomain (crystal form II)
Authors : Cherry, A.L.; Finta, C.; Karlstrom, M.; Toftgard, R.; Jovine, L.
Deposited on : 2013-05-02
Resolution : 3.50 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

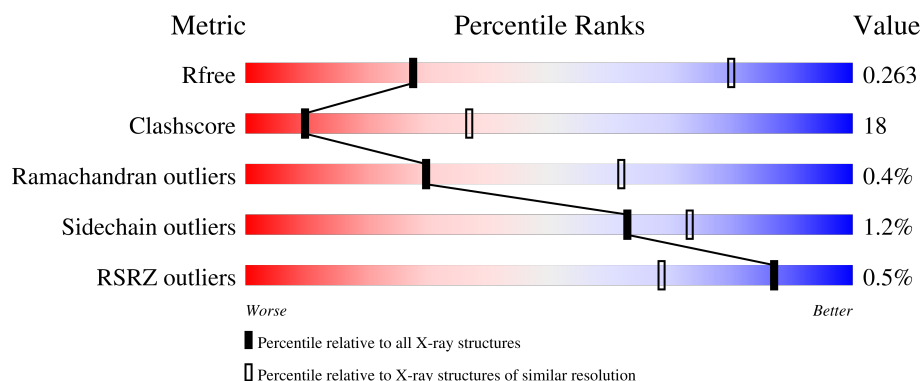
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	756	% 73% 22% ..
1	B	756	77% 18% ..
1	C	756	% 78% 17% ..
1	D	756	% 68% 28% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22889 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 MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total	C	N	O	S	0	0	0
			5718	3668	949	1083	18			
1	B	733	Total	C	N	O	S	0	0	0
			5734	3673	954	1089	18			
1	C	724	Total	C	N	O	S	0	0	0
			5665	3632	942	1073	18			
1	D	738	Total	C	N	O	S	0	0	0
			5772	3696	960	1098	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P0AEX9
A	3	THR	ILE	engineered mutation	UNP P0AEX9
A	360	ALA	GLU	engineered mutation	UNP P0AEX9
A	363	ALA	LYS	engineered mutation	UNP P0AEX9
A	364	ALA	ASP	engineered mutation	UNP P0AEX9
A	368	ASN	ARG	engineered mutation	UNP P0AEX9
A	369	ALA	-	linker	UNP P0AEX9
A	370	ALA	-	linker	UNP P0AEX9
A	371	ALA	-	linker	UNP P0AEX9
A	619	PRO	-	linker	UNP Q9UMX1
A	620	SER	-	linker	UNP Q9UMX1
A	621	ARG	-	linker	UNP Q9UMX1
A	622	GLY	-	linker	UNP Q9UMX1
A	623	GLU	-	linker	UNP Q9UMX1
A	624	ASP	-	linker	UNP Q9UMX1
A	625	PRO	-	linker	UNP Q9UMX1
A	749	VAL	-	expression tag	UNP Q9UMX1
A	750	GLU	-	expression tag	UNP Q9UMX1
A	751	HIS	-	expression tag	UNP Q9UMX1
A	752	HIS	-	expression tag	UNP Q9UMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	753	HIS	-	expression tag	UNP Q9UMX1
A	754	HIS	-	expression tag	UNP Q9UMX1
A	755	HIS	-	expression tag	UNP Q9UMX1
A	756	HIS	-	expression tag	UNP Q9UMX1
B	1	MET	-	expression tag	UNP P0AEX9
B	3	THR	ILE	engineered mutation	UNP P0AEX9
B	360	ALA	GLU	engineered mutation	UNP P0AEX9
B	363	ALA	LYS	engineered mutation	UNP P0AEX9
B	364	ALA	ASP	engineered mutation	UNP P0AEX9
B	368	ASN	ARG	engineered mutation	UNP P0AEX9
B	369	ALA	-	linker	UNP P0AEX9
B	370	ALA	-	linker	UNP P0AEX9
B	371	ALA	-	linker	UNP P0AEX9
B	619	PRO	-	linker	UNP Q9UMX1
B	620	SER	-	linker	UNP Q9UMX1
B	621	ARG	-	linker	UNP Q9UMX1
B	622	GLY	-	linker	UNP Q9UMX1
B	623	GLU	-	linker	UNP Q9UMX1
B	624	ASP	-	linker	UNP Q9UMX1
B	625	PRO	-	linker	UNP Q9UMX1
B	749	VAL	-	expression tag	UNP Q9UMX1
B	750	GLU	-	expression tag	UNP Q9UMX1
B	751	HIS	-	expression tag	UNP Q9UMX1
B	752	HIS	-	expression tag	UNP Q9UMX1
B	753	HIS	-	expression tag	UNP Q9UMX1
B	754	HIS	-	expression tag	UNP Q9UMX1
B	755	HIS	-	expression tag	UNP Q9UMX1
B	756	HIS	-	expression tag	UNP Q9UMX1
C	1	MET	-	expression tag	UNP P0AEX9
C	3	THR	ILE	engineered mutation	UNP P0AEX9
C	360	ALA	GLU	engineered mutation	UNP P0AEX9
C	363	ALA	LYS	engineered mutation	UNP P0AEX9
C	364	ALA	ASP	engineered mutation	UNP P0AEX9
C	368	ASN	ARG	engineered mutation	UNP P0AEX9
C	369	ALA	-	linker	UNP P0AEX9
C	370	ALA	-	linker	UNP P0AEX9
C	371	ALA	-	linker	UNP P0AEX9
C	619	PRO	-	linker	UNP Q9UMX1
C	620	SER	-	linker	UNP Q9UMX1
C	621	ARG	-	linker	UNP Q9UMX1
C	622	GLY	-	linker	UNP Q9UMX1
C	623	GLU	-	linker	UNP Q9UMX1

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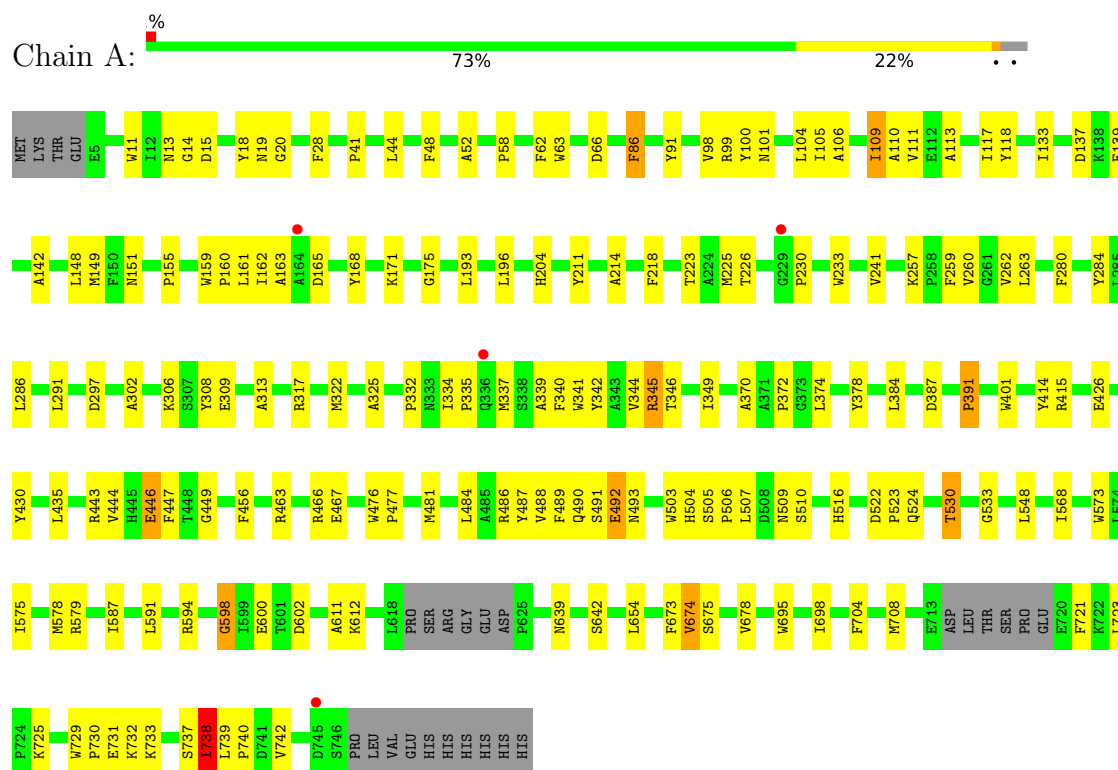
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Chain	Residue	Modelled	Actual	Comment	Reference
C	624	ASP	-	linker	UNP Q9UMX1
C	625	PRO	-	linker	UNP Q9UMX1
C	749	VAL	-	expression tag	UNP Q9UMX1
C	750	GLU	-	expression tag	UNP Q9UMX1
C	751	HIS	-	expression tag	UNP Q9UMX1
C	752	HIS	-	expression tag	UNP Q9UMX1
C	753	HIS	-	expression tag	UNP Q9UMX1
C	754	HIS	-	expression tag	UNP Q9UMX1
C	755	HIS	-	expression tag	UNP Q9UMX1
C	756	HIS	-	expression tag	UNP Q9UMX1
D	1	MET	-	expression tag	UNP P0AEX9
D	3	THR	ILE	engineered mutation	UNP P0AEX9
D	360	ALA	GLU	engineered mutation	UNP P0AEX9
D	363	ALA	LYS	engineered mutation	UNP P0AEX9
D	364	ALA	ASP	engineered mutation	UNP P0AEX9
D	368	ASN	ARG	engineered mutation	UNP P0AEX9
D	369	ALA	-	linker	UNP P0AEX9
D	370	ALA	-	linker	UNP P0AEX9
D	371	ALA	-	linker	UNP P0AEX9
D	619	PRO	-	linker	UNP Q9UMX1
D	620	SER	-	linker	UNP Q9UMX1
D	621	ARG	-	linker	UNP Q9UMX1
D	622	GLY	-	linker	UNP Q9UMX1
D	623	GLU	-	linker	UNP Q9UMX1
D	624	ASP	-	linker	UNP Q9UMX1
D	625	PRO	-	linker	UNP Q9UMX1
D	749	VAL	-	expression tag	UNP Q9UMX1
D	750	GLU	-	expression tag	UNP Q9UMX1
D	751	HIS	-	expression tag	UNP Q9UMX1
D	752	HIS	-	expression tag	UNP Q9UMX1
D	753	HIS	-	expression tag	UNP Q9UMX1
D	754	HIS	-	expression tag	UNP Q9UMX1
D	755	HIS	-	expression tag	UNP Q9UMX1
D	756	HIS	-	expression tag	UNP Q9UMX1

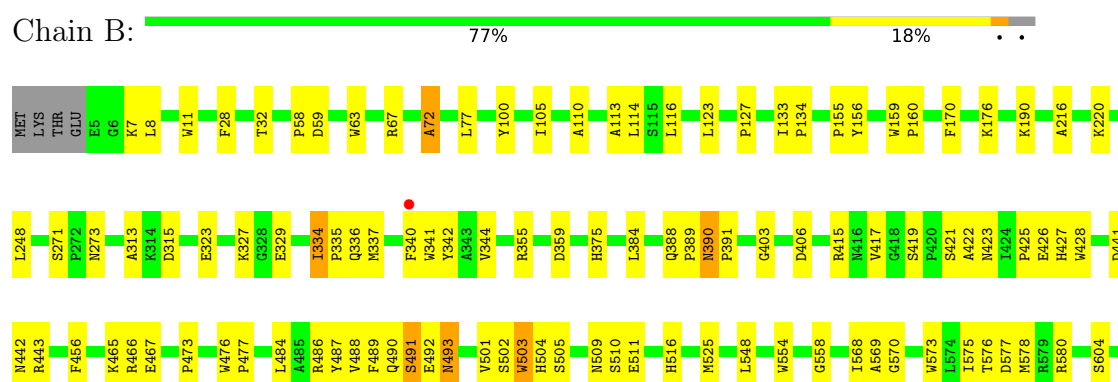
3 Residue-property plots

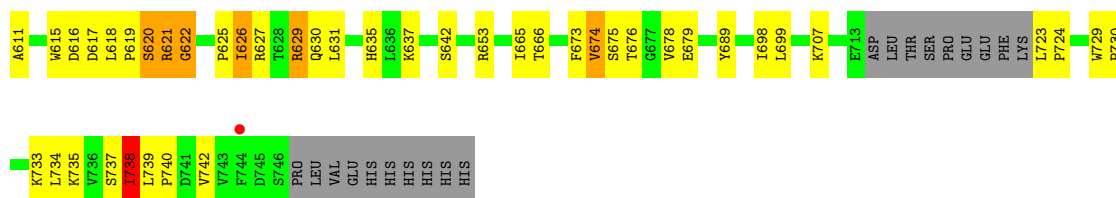
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

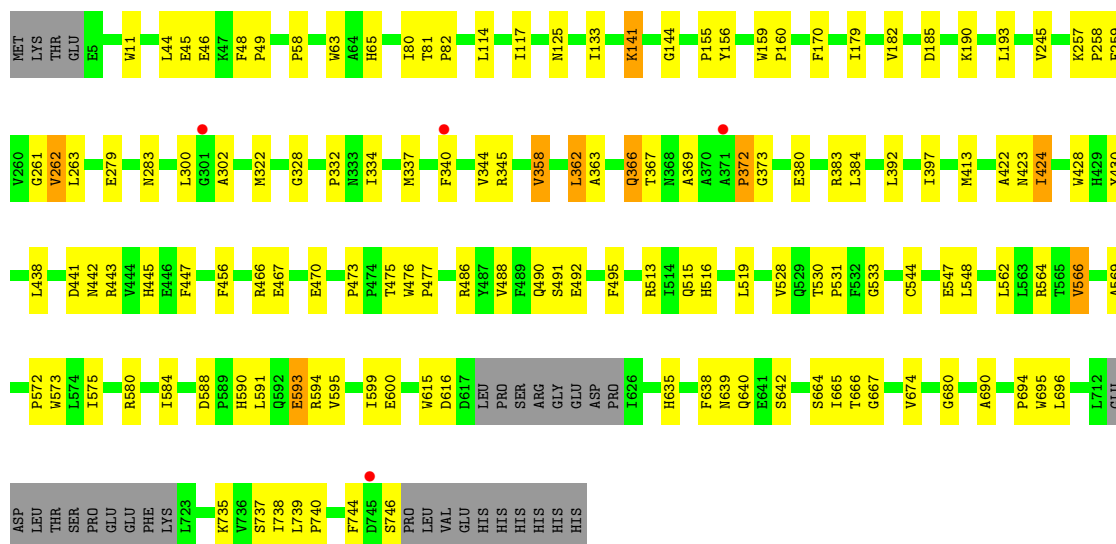
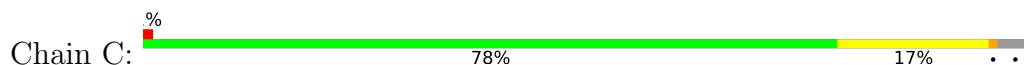


• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG

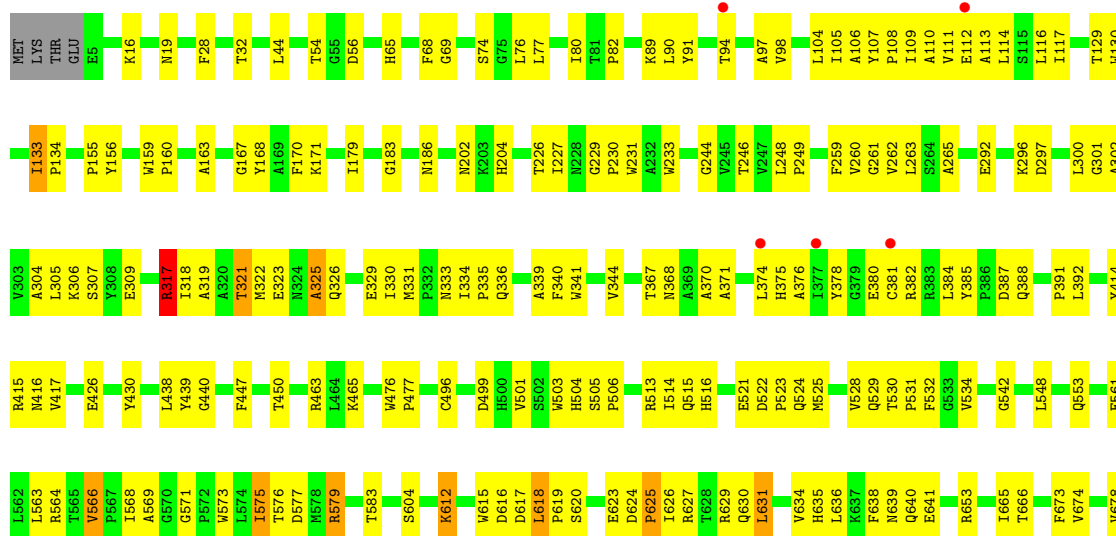




• Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN, SUPPRESSOR OF FUSED HOMOLOG



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E679		P688		H692		I698		F704	V705	E706	K707	M708	L709	E710		L715	T716	S717	PRO	GLU	GLU	PHE	K722	L723	P724	K725		K732	K733	L734	K735	V736	S737	I738	L739	P740	D741	V742	V743	F744	D745	S746	PRO	LEU	VAL	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.92Å 372.57Å 86.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.58 – 3.50 39.58 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.58-3.50) 99.5 (39.58-3.50)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.293 (Not available) , 0.263	Depositor DCC
R_{free} test set	2462 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 93.4	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	0.92	EDS
Total number of atoms	22889	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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	0.62	0/5871	0.94	11/7984 (0.1%)
1	B	0.64	1/5888 (0.0%)	0.91	13/8011 (0.2%)
1	C	0.62	2/5816 (0.0%)	0.91	8/7911 (0.1%)
1	D	0.64	4/5926 (0.1%)	0.93	10/8062 (0.1%)
All	All	0.63	7/23501 (0.0%)	0.92	42/31968 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	739	LEU	C-N	8.57	1.40	1.33
1	D	325	ALA	CA-CB	-5.90	1.44	1.53
1	B	72	ALA	CA-CB	-5.72	1.43	1.53
1	C	358	VAL	C-O	-5.46	1.18	1.24
1	D	740	PRO	N-CD	5.23	1.55	1.47
1	C	366	GLN	CD-NE2	-5.16	1.22	1.33
1	D	133	ILE	CA-CB	5.15	1.57	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	N-CA-C	8.32	121.47	111.82
1	D	301	GLY	N-CA-C	-7.32	105.62	115.36
1	B	113	ALA	N-CA-C	6.74	119.42	109.24
1	D	317	ARG	N-CA-C	6.34	118.19	111.28
1	D	739	LEU	CA-C-N	-6.25	113.48	121.04
1	D	739	LEU	C-N-CA	-6.25	113.48	121.04
1	C	141	LYS	N-CA-C	6.18	118.81	111.71
1	D	326	GLN	N-CA-C	-6.10	104.54	111.07
1	B	738	ILE	N-CA-C	6.09	116.80	111.56
1	B	738	ILE	CB-CA-C	-5.98	105.76	111.44
1	B	620	SER	CA-C-O	-5.96	114.24	120.55
1	C	600	GLU	N-CA-C	5.95	117.77	111.28
1	A	600	GLU	CB-CA-C	-5.93	100.77	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	THR	N-CA-C	-5.84	104.91	111.28
1	A	14	GLY	N-CA-C	5.83	121.46	113.99
1	C	125	ASN	CA-C-N	5.73	123.84	119.66
1	C	125	ASN	C-N-CA	5.73	123.84	119.66
1	B	110	ALA	N-CA-C	5.67	117.68	109.07
1	D	300	LEU	N-CA-C	-5.49	105.38	111.36
1	D	370	ALA	N-CA-C	5.47	117.33	111.36
1	C	300	LEU	N-CA-C	-5.39	106.66	113.18
1	A	86	PHE	N-CA-C	5.38	117.23	111.36
1	B	334	ILE	CA-C-N	5.33	124.84	119.19
1	B	334	ILE	C-N-CA	5.33	124.84	119.19
1	C	424	ILE	N-CA-C	-5.32	102.72	107.56
1	C	133	ILE	CB-CA-C	-5.30	108.73	114.35
1	A	598	GLY	N-CA-C	-5.29	106.37	112.50
1	A	738	ILE	N-CA-C	5.28	120.33	109.34
1	B	313	ALA	N-CA-C	5.25	119.31	113.01
1	B	421	SER	N-CA-C	-5.25	105.56	111.28
1	B	388	GLN	CA-C-N	5.24	124.56	118.85
1	B	388	GLN	C-N-CA	5.24	124.56	118.85
1	A	175	GLY	N-CA-C	-5.19	108.46	115.36
1	C	566	VAL	N-CA-C	5.15	112.96	107.76
1	A	133	ILE	CB-CA-C	-5.10	108.94	114.35
1	B	620	SER	O-C-N	5.10	127.52	122.12
1	B	176	LYS	N-CA-C	5.09	116.04	108.86
1	D	392	LEU	N-CA-C	-5.06	102.56	110.10
1	A	241	VAL	CA-C-N	-5.05	115.70	122.42
1	A	241	VAL	C-N-CA	-5.05	115.70	122.42
1	D	566	VAL	N-CA-C	5.02	113.39	107.77
1	A	530	THR	N-CA-C	-5.01	103.24	110.40

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	5718	0	5580	195	0
1	B	5734	0	5590	171	0
1	C	5665	0	5527	134	0
1	D	5772	0	5630	328	0
All	All	22889	0	22327	794	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 18.

All (794) 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:D:168:TYR:CE2	1:D:171:LYS:HB2	1.54	1.40
1:A:507:LEU:HB2	1:A:578:MET:CE	1.56	1.33
1:D:112:GLU:CG	1:D:262:VAL:HB	1.59	1.30
1:D:111:VAL:HB	1:D:322:MET:SD	1.79	1.22
1:A:723:LEU:HD13	1:A:738:ILE:HD11	1.24	1.12
1:D:722:LYS:O	1:D:725:LYS:HG3	1.49	1.09
1:D:80:ILE:HD12	1:D:107:TYR:CE1	1.88	1.08
1:B:674:VAL:HG13	1:B:678:VAL:HG21	1.28	1.08
1:A:507:LEU:HB2	1:A:578:MET:HE2	1.34	1.07
1:D:168:TYR:HE2	1:D:171:LYS:CB	1.66	1.07
1:A:507:LEU:HB2	1:A:578:MET:HE1	1.24	1.06
1:D:112:GLU:HG3	1:D:262:VAL:CB	1.86	1.05
1:D:112:GLU:HG3	1:D:262:VAL:HB	1.35	1.01
1:B:355:ARG:NH1	1:B:389:PRO:HG3	1.74	1.00
1:D:111:VAL:CB	1:D:322:MET:SD	2.49	1.00
1:D:113:ALA:HA	1:D:260:VAL:HG11	1.46	0.98
1:D:112:GLU:CG	1:D:262:VAL:CB	2.43	0.96
1:D:579:ARG:CZ	1:D:579:ARG:HA	1.94	0.96
1:B:733:LYS:HE2	1:B:735:LYS:HE3	1.45	0.96
1:B:456:PHE:HE2	1:B:489:PHE:CE1	1.83	0.96
1:A:738:ILE:N	1:A:738:ILE:HD12	1.78	0.96
1:C:193:LEU:HD23	1:C:362:LEU:HD21	1.48	0.94
1:D:112:GLU:HG2	1:D:262:VAL:HB	1.46	0.94
1:D:612:LYS:NZ	1:D:739:LEU:HD13	1.81	0.94
1:D:111:VAL:HG21	1:D:322:MET:HA	1.48	0.94
1:D:715:LEU:O	1:D:716:THR:OG1	1.86	0.94
1:C:182:VAL:HB	1:C:366:GLN:NE2	1.82	0.93
1:D:440:GLY:HA3	1:D:532:PHE:CE1	2.04	0.93
1:D:80:ILE:HB	1:D:107:TYR:OH	1.69	0.92
1:B:72:ALA:CB	1:B:105:ILE:HD13	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:VAL:HG13	1:B:678:VAL:CG2	1.98	0.92
1:B:72:ALA:HB2	1:B:105:ILE:HD13	1.53	0.90
1:D:159:TRP:CE2	1:D:259:PHE:CE2	2.60	0.90
1:C:182:VAL:HB	1:C:366:GLN:HE21	1.35	0.90
1:A:374:LEU:HD21	1:A:378:TYR:CZ	2.07	0.90
1:D:168:TYR:CE2	1:D:171:LYS:CB	2.47	0.89
1:A:704:PHE:CZ	1:A:708:MET:HE3	2.08	0.89
1:D:168:TYR:HE2	1:D:171:LYS:HB2	0.80	0.89
1:A:507:LEU:CB	1:A:578:MET:HE1	2.03	0.88
1:B:390:ASN:O	1:B:390:ASN:ND2	2.05	0.88
1:A:723:LEU:CD1	1:A:738:ILE:HD11	2.02	0.88
1:D:259:PHE:CD1	1:D:329:GLU:HB2	2.08	0.88
1:C:358:VAL:O	1:C:362:LEU:HG	1.74	0.88
1:B:620:SER:O	1:B:621:ARG:HG2	1.73	0.87
1:A:446:GLU:OE1	1:A:446:GLU:N	2.06	0.87
1:D:80:ILE:HB	1:D:107:TYR:CZ	2.09	0.86
1:D:113:ALA:HA	1:D:260:VAL:CG1	2.05	0.86
1:D:629:ARG:NH1	1:D:631:LEU:HD23	1.89	0.86
1:D:524:GLN:NE2	1:D:573:TRP:CZ2	2.44	0.86
1:A:729:TRP:HB3	1:A:730:PRO:HD2	1.56	0.85
1:D:114:LEU:HG	1:D:230:PRO:HD3	1.59	0.85
1:B:617:ASP:HB3	1:B:619:PRO:HD2	1.59	0.84
1:A:374:LEU:HD21	1:A:378:TYR:CE2	2.11	0.84
1:D:82:PRO:HG3	1:D:107:TYR:HE1	1.41	0.84
1:A:674:VAL:HG13	1:A:678:VAL:HG21	1.59	0.84
1:B:155:PRO:HG2	1:B:341:TRP:CE3	2.13	0.84
1:D:740:PRO:HD2	1:D:741:ASP:OD1	1.75	0.84
1:B:503:TRP:CE2	1:D:738:ILE:HG21	2.12	0.83
1:D:617:ASP:O	1:D:618:LEU:HG	1.79	0.83
1:C:441:ASP:OD2	1:C:443:ARG:NE	2.12	0.83
1:D:465:LYS:HG3	1:D:575:ILE:HG22	1.60	0.82
1:D:167:GLY:HA2	1:D:186:ASN:HD21	1.41	0.82
1:D:159:TRP:CE2	1:D:259:PHE:CZ	2.68	0.82
1:B:441:ASP:OD2	1:B:443:ARG:NH2	2.12	0.82
1:D:465:LYS:HG3	1:D:575:ILE:CG2	2.09	0.82
1:D:80:ILE:CD1	1:D:107:TYR:CE1	2.63	0.82
1:D:465:LYS:HD2	1:D:577:ASP:HB2	1.60	0.82
1:B:504:HIS:O	1:B:504:HIS:ND1	2.13	0.81
1:B:733:LYS:HE2	1:B:735:LYS:CE	2.10	0.81
1:D:722:LYS:O	1:D:725:LYS:CG	2.27	0.81
1:D:624:ASP:OD2	1:D:627:ARG:NH2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:TRP:CZ2	1:D:259:PHE:CZ	2.68	0.81
1:A:507:LEU:CB	1:A:578:MET:CE	2.52	0.80
1:B:738:ILE:HG21	1:D:503:TRP:C	2.07	0.80
1:C:190:LYS:HG2	1:C:362:LEU:HD12	1.62	0.79
1:D:111:VAL:CG1	1:D:322:MET:SD	2.71	0.79
1:C:738:ILE:HG23	1:C:739:LEU:N	1.98	0.79
1:D:259:PHE:CE1	1:D:329:GLU:HB2	2.18	0.79
1:A:704:PHE:CE2	1:A:708:MET:HE3	2.18	0.78
1:D:612:LYS:HZ2	1:D:739:LEU:HD13	1.47	0.78
1:A:467:GLU:HG3	1:A:579:ARG:NH2	1.99	0.78
1:D:564:ARG:HG3	1:D:564:ARG:HH11	1.48	0.78
1:D:110:ALA:HB1	1:D:302:ALA:CB	2.14	0.77
1:D:415:ARG:NH1	1:D:426:GLU:OE2	2.17	0.77
1:B:456:PHE:CE2	1:B:489:PHE:CE1	2.73	0.77
1:A:505:SER:OG	1:A:506:PRO:HD2	1.84	0.77
1:A:522:ASP:OD1	1:A:523:PRO:HD2	1.85	0.76
1:C:665:ILE:HG13	1:C:666:THR:N	2.00	0.76
1:A:506:PRO:HG2	1:A:509:ASN:HA	1.66	0.76
1:A:487:TYR:O	1:A:491:SER:HB3	1.85	0.76
1:B:674:VAL:CG1	1:B:678:VAL:HG21	2.12	0.76
1:D:715:LEU:C	1:D:716:THR:HG1	1.93	0.75
1:D:170:PHE:HE1	1:D:179:ILE:HA	1.51	0.75
1:D:566:VAL:HB	1:D:569:ALA:CB	2.15	0.75
1:D:112:GLU:HG3	1:D:262:VAL:CA	2.14	0.75
1:D:116:LEU:HD23	1:D:248:LEU:HD23	1.69	0.75
1:A:654:LEU:HA	1:A:675:SER:OG	1.86	0.75
1:D:110:ALA:HB1	1:D:302:ALA:HB3	1.67	0.75
1:D:159:TRP:NE1	1:D:259:PHE:CZ	2.55	0.75
1:D:566:VAL:HB	1:D:569:ALA:HB3	1.69	0.74
1:A:260:VAL:HG21	1:A:325:ALA:HA	1.69	0.74
1:B:615:TRP:O	1:B:621:ARG:NH1	2.21	0.74
1:B:626:ILE:HG12	1:B:627:ARG:H	1.53	0.74
1:D:739:LEU:HD23	1:D:739:LEU:N	2.03	0.74
1:D:639:ASN:OD1	1:D:640:GLN:N	2.19	0.74
1:A:159:TRP:CD1	1:A:259:PHE:CZ	2.75	0.74
1:C:363:ALA:O	1:C:367:THR:HG23	1.88	0.73
1:D:530:THR:HG23	1:D:531:PRO:HD2	1.71	0.73
1:D:116:LEU:HD11	1:D:246:THR:HG23	1.69	0.73
1:B:28:PHE:CE2	1:B:32:THR:HG21	2.23	0.73
1:B:734:LEU:C	1:B:734:LEU:HD12	2.14	0.73
1:C:738:ILE:HG23	1:C:739:LEU:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:ILE:O	1:D:740:PRO:HD3	1.88	0.72
1:D:69:GLY:HA3	1:D:333:ASN:HB3	1.71	0.72
1:C:615:TRP:CE3	1:C:696:LEU:HD22	2.25	0.71
1:D:440:GLY:HA3	1:D:532:PHE:CZ	2.25	0.71
1:B:390:ASN:HD22	1:B:390:ASN:C	1.95	0.71
1:C:190:LYS:HG2	1:C:362:LEU:CD1	2.19	0.71
1:C:665:ILE:HG13	1:C:666:THR:HG23	1.74	0.70
1:C:182:VAL:C	1:C:366:GLN:HE22	1.99	0.70
1:D:738:ILE:HD12	1:D:738:ILE:C	2.16	0.70
1:A:415:ARG:NH1	1:A:426:GLU:OE2	2.25	0.70
1:A:730:PRO:HG2	1:A:731:GLU:OE1	1.92	0.70
1:B:406:ASP:OD1	1:B:486:ARG:NH2	2.25	0.70
1:D:94:THR:HB	1:D:108:PRO:HB3	1.73	0.70
1:D:617:ASP:OD1	1:D:620:SER:N	2.25	0.70
1:B:630:GLN:O	1:B:631:LEU:HD23	1.92	0.69
1:D:387:ASP:OD2	1:D:388:GLN:NE2	2.25	0.69
1:D:722:LYS:N	1:D:725:LYS:HE2	2.07	0.69
1:A:456:PHE:CE2	1:A:488:VAL:HG12	2.26	0.69
1:A:739:LEU:N	1:A:740:PRO:CD	2.56	0.69
1:D:112:GLU:CD	1:D:262:VAL:HB	2.17	0.69
1:B:487:TYR:HE2	1:D:740:PRO:HB2	1.57	0.69
1:D:259:PHE:HD1	1:D:329:GLU:HB2	1.58	0.69
1:A:374:LEU:C	1:A:374:LEU:HD23	2.18	0.69
1:C:185:ASP:HB2	1:C:366:GLN:OE1	1.92	0.69
1:D:113:ALA:HB2	1:D:325:ALA:HA	1.74	0.69
1:D:387:ASP:OD2	1:D:388:GLN:CD	2.35	0.68
1:B:723:LEU:HB2	1:B:724:PRO:HA	1.76	0.68
1:D:111:VAL:HG11	1:D:322:MET:SD	2.33	0.68
1:D:94:THR:HB	1:D:108:PRO:CB	2.23	0.68
1:A:492:GLU:HA	1:A:492:GLU:OE1	1.92	0.68
1:B:618:LEU:HD21	1:C:665:ILE:CG2	2.23	0.68
1:C:635:HIS:CE1	1:C:735:LYS:HD3	2.28	0.68
1:B:422:ALA:O	1:B:423:ASN:ND2	2.27	0.68
1:C:513:ARG:HD2	1:C:544:CYS:SG	2.34	0.68
1:C:392:LEU:HD21	1:C:473:PRO:HD2	1.75	0.68
1:B:492:GLU:OE2	1:D:745:ASP:OD1	2.13	0.67
1:A:487:TYR:CE1	1:A:491:SER:HB2	2.30	0.67
1:B:28:PHE:O	1:B:32:THR:HG22	1.93	0.67
1:A:137:ASP:OD2	1:A:204:HIS:ND1	2.26	0.67
1:C:443:ARG:NH2	1:D:679:GLU:OE1	2.28	0.67
1:D:116:LEU:HB3	1:D:227:ILE:HG12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:MET:CE	1:A:732:LYS:NZ	2.58	0.67
1:D:440:GLY:HA3	1:D:532:PHE:CD1	2.29	0.67
1:C:495:PHE:CD2	1:C:519:LEU:HD11	2.30	0.67
1:D:524:GLN:NE2	1:D:573:TRP:CE2	2.63	0.67
1:A:477:PRO:O	1:A:481:MET:HG3	1.95	0.66
1:B:72:ALA:HB1	1:B:105:ILE:HD13	1.74	0.66
1:D:113:ALA:CA	1:D:260:VAL:HG11	2.23	0.66
1:B:155:PRO:HG2	1:B:341:TRP:CZ3	2.30	0.66
1:D:465:LYS:CG	1:D:575:ILE:CG2	2.73	0.66
1:D:380:GLU:HG2	1:D:525:MET:HE3	1.76	0.66
1:A:486:ARG:O	1:A:490:GLN:HG3	1.95	0.66
1:B:616:ASP:OD2	1:B:637:LYS:NZ	2.25	0.66
1:A:708:MET:CE	1:A:732:LYS:HZ1	2.08	0.66
1:B:504:HIS:NE2	1:D:641:GLU:OE2	2.29	0.66
1:B:155:PRO:HG2	1:B:341:TRP:HE3	1.59	0.65
1:B:487:TYR:HE2	1:D:740:PRO:CB	2.09	0.65
1:A:522:ASP:CG	1:A:523:PRO:HD2	2.21	0.65
1:A:374:LEU:CD2	1:A:378:TYR:CE2	2.79	0.65
1:A:524:GLN:NE2	1:A:573:TRP:CH2	2.65	0.65
1:D:636:LEU:HD12	1:D:734:LEU:HD12	1.78	0.65
1:A:491:SER:OG	1:A:493:ASN:HB2	1.96	0.65
1:A:487:TYR:CD1	1:A:491:SER:HB2	2.31	0.65
1:A:737:SER:C	1:A:738:ILE:HD12	2.22	0.65
1:A:62:PHE:CE2	1:A:109:ILE:HD12	2.31	0.65
1:B:505:SER:HB2	1:D:723:LEU:HD12	1.78	0.65
1:C:566:VAL:HB	1:C:569:ALA:CB	2.26	0.65
1:A:345:ARG:NH1	1:A:345:ARG:HG2	2.12	0.65
1:D:82:PRO:HG3	1:D:107:TYR:CE1	2.30	0.65
1:D:465:LYS:HG2	1:D:575:ILE:HG21	1.79	0.64
1:D:522:ASP:OD1	1:D:523:PRO:HD2	1.97	0.64
1:B:28:PHE:CZ	1:B:32:THR:HG21	2.33	0.64
1:D:378:TYR:HB3	1:D:382:ARG:HH12	1.62	0.64
1:A:20:GLY:N	1:A:297:ASP:OD2	2.31	0.64
1:A:506:PRO:CG	1:A:509:ASN:HA	2.28	0.64
1:C:588:ASP:HB3	1:C:591:LEU:HD13	1.78	0.64
1:B:72:ALA:CB	1:B:105:ILE:CD1	2.76	0.64
1:D:113:ALA:HB2	1:D:325:ALA:CA	2.27	0.63
1:A:111:VAL:HG23	1:A:262:VAL:HG22	1.79	0.63
1:D:159:TRP:NE1	1:D:259:PHE:CE1	2.65	0.63
1:A:100:TYR:CE1	1:A:101:ASN:HB2	2.34	0.63
1:B:105:ILE:HG22	1:B:105:ILE:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:ASP:OD2	1:D:388:GLN:OE1	2.17	0.63
1:A:729:TRP:HB3	1:A:730:PRO:CD	2.29	0.63
1:C:279:GLU:OE1	1:C:283:ASN:ND2	2.31	0.63
1:C:513:ARG:O	1:C:515:GLN:HG3	1.98	0.63
1:D:167:GLY:HA2	1:D:186:ASN:ND2	2.12	0.63
1:A:168:TYR:CE2	1:A:171:LYS:HE3	2.34	0.63
1:A:507:LEU:CB	1:A:578:MET:HE2	2.21	0.63
1:A:218:PHE:CZ	1:A:226:THR:HB	2.33	0.63
1:C:590:HIS:HA	1:C:593:GLU:HG3	1.80	0.63
1:A:704:PHE:CE2	1:A:708:MET:CE	2.82	0.63
1:C:185:ASP:O	1:C:190:LYS:NZ	2.32	0.62
1:C:566:VAL:HB	1:C:569:ALA:HB3	1.81	0.62
1:D:116:LEU:HD11	1:D:246:THR:CG2	2.28	0.62
1:A:723:LEU:HD13	1:A:738:ILE:CD1	2.14	0.62
1:B:492:GLU:CD	1:B:492:GLU:O	2.42	0.62
1:A:345:ARG:CG	1:A:345:ARG:HH11	2.12	0.62
1:A:99:ARG:HG3	1:A:104:LEU:HD23	1.82	0.62
1:D:159:TRP:CZ2	1:D:259:PHE:CE2	2.87	0.62
1:A:467:GLU:HA	1:A:467:GLU:OE1	1.99	0.62
1:C:193:LEU:CD2	1:C:362:LEU:HD21	2.27	0.62
1:C:340:PHE:CZ	1:C:369:ALA:HB1	2.36	0.61
1:A:18:TYR:CE1	1:A:19:ASN:OD1	2.52	0.61
1:A:708:MET:HE1	1:A:732:LYS:HE2	1.81	0.61
1:C:486:ARG:O	1:C:490:GLN:HG3	2.01	0.61
1:C:495:PHE:CD2	1:C:519:LEU:CD1	2.84	0.61
1:D:113:ALA:C	1:D:114:LEU:HD12	2.24	0.61
1:C:456:PHE:CE2	1:C:488:VAL:HG12	2.35	0.61
1:B:604:SER:O	1:B:653:ARG:NH1	2.34	0.61
1:B:630:GLN:C	1:B:631:LEU:HD23	2.26	0.61
1:D:723:LEU:CD2	1:D:736:VAL:HG12	2.30	0.61
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.64	0.61
1:B:738:ILE:HG21	1:D:503:TRP:O	2.01	0.61
1:D:91:TYR:CZ	1:D:306:LYS:HG2	2.36	0.61
1:B:355:ARG:NH1	1:B:389:PRO:CG	2.59	0.61
1:B:734:LEU:HD12	1:B:734:LEU:O	2.01	0.60
1:D:465:LYS:CG	1:D:575:ILE:HG21	2.29	0.60
1:A:426:GLU:CD	1:A:466:ARG:HD3	2.26	0.60
1:B:487:TYR:CE2	1:D:740:PRO:CB	2.84	0.60
1:A:110:ALA:O	1:A:263:LEU:N	2.34	0.60
1:B:675:SER:O	1:B:678:VAL:HG22	2.01	0.60
1:C:114:LEU:HD11	1:C:156:TYR:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD23	1:A:374:LEU:O	2.02	0.60
1:D:577:ASP:OD1	1:D:579:ARG:N	2.32	0.60
1:B:355:ARG:CZ	1:B:389:PRO:HG3	2.32	0.60
1:B:389:PRO:HG2	1:B:390:ASN:H	1.66	0.60
1:A:86:PHE:HZ	1:A:286:LEU:CD1	2.15	0.60
1:C:595:VAL:O	1:C:599:ILE:HG13	2.01	0.60
1:D:629:ARG:HH11	1:D:631:LEU:HD23	1.65	0.60
1:B:739:LEU:N	1:B:740:PRO:CD	2.66	0.59
1:C:182:VAL:CB	1:C:366:GLN:NE2	2.62	0.59
1:D:109:ILE:HA	1:D:304:ALA:HB2	1.84	0.59
1:C:690:ALA:O	1:C:696:LEU:HD12	2.01	0.59
1:A:486:ARG:NH1	1:D:623:GLU:CD	2.60	0.59
1:B:337:MET:HE3	1:B:341:TRP:CD1	2.37	0.59
1:B:676:THR:HG22	1:B:699:LEU:HD21	1.84	0.59
1:A:738:ILE:N	1:A:738:ILE:CD1	2.57	0.59
1:D:447:PHE:CE1	1:D:532:PHE:CD1	2.91	0.59
1:D:579:ARG:HA	1:D:579:ARG:NE	2.17	0.59
1:A:654:LEU:CA	1:A:675:SER:OG	2.51	0.59
1:A:675:SER:O	1:A:678:VAL:HG22	2.02	0.59
1:D:89:LYS:HB3	1:D:305:LEU:CD1	2.32	0.59
1:B:7:LYS:O	1:B:273:ASN:ND2	2.35	0.59
1:A:486:ARG:HH12	1:D:623:GLU:CD	2.11	0.58
1:B:72:ALA:HB1	1:B:105:ILE:CD1	2.33	0.58
1:D:391:PRO:HG2	1:D:414:TYR:CZ	2.38	0.58
1:D:723:LEU:HD22	1:D:736:VAL:HG12	1.85	0.58
1:A:612:LYS:HE2	1:A:742:VAL:HG22	1.84	0.58
1:D:168:TYR:CD1	1:D:183:GLY:HA3	2.38	0.58
1:A:334:ILE:CG2	1:A:335:PRO:HD2	2.34	0.58
1:D:114:LEU:HD23	1:D:229:GLY:CA	2.34	0.58
1:B:77:LEU:HD13	1:B:105:ILE:HG22	1.86	0.58
1:A:99:ARG:HE	1:A:104:LEU:HD21	1.68	0.58
1:B:487:TYR:CE2	1:D:740:PRO:HB2	2.38	0.58
1:D:112:GLU:HB2	1:D:260:VAL:HG23	1.86	0.58
1:D:233:TRP:CZ3	1:D:317:ARG:HB3	2.39	0.58
1:D:65:HIS:HE1	1:D:261:GLY:HA2	1.69	0.58
1:C:739:LEU:N	1:C:740:PRO:CD	2.67	0.57
1:D:168:TYR:HD2	1:D:170:PHE:O	1.87	0.57
1:B:573:TRP:HB2	1:B:575:ILE:HD11	1.85	0.57
1:D:378:TYR:HB3	1:D:382:ARG:NH1	2.19	0.57
1:B:490:GLN:O	1:B:491:SER:HB2	2.04	0.57
1:B:739:LEU:HD22	1:D:501:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLU:CD	1:A:579:ARG:CZ	2.77	0.57
1:A:739:LEU:N	1:A:740:PRO:HD3	2.20	0.57
1:B:618:LEU:HD21	1:C:665:ILE:HG21	1.85	0.57
1:C:262:VAL:HG12	1:C:263:LEU:N	2.19	0.57
1:C:358:VAL:CG1	1:C:362:LEU:HD11	2.35	0.57
1:B:575:ILE:N	1:B:575:ILE:HD12	2.20	0.56
1:C:738:ILE:CG2	1:C:739:LEU:H	2.18	0.56
1:D:625:PRO:O	1:D:626:ILE:HB	2.05	0.56
1:D:116:LEU:CD1	1:D:246:THR:CG2	2.83	0.56
1:D:463:ARG:HH22	1:D:524:GLN:HB2	1.69	0.56
1:C:738:ILE:HG23	1:C:739:LEU:HG	1.87	0.56
1:B:618:LEU:HB3	1:B:619:PRO:HD3	1.88	0.56
1:B:77:LEU:HD12	1:B:105:ILE:HG21	1.87	0.56
1:B:629:ARG:HD2	1:B:631:LEU:HD21	1.88	0.56
1:D:259:PHE:CE1	1:D:329:GLU:CB	2.88	0.56
1:D:380:GLU:CG	1:D:525:MET:HE3	2.35	0.56
1:C:392:LEU:HD21	1:C:473:PRO:CG	2.36	0.56
1:D:105:ILE:C	1:D:105:ILE:HD12	2.31	0.56
1:B:77:LEU:CD1	1:B:105:ILE:CG2	2.84	0.56
1:C:513:ARG:CD	1:C:544:CYS:SG	2.94	0.56
1:D:80:ILE:CD1	1:D:107:TYR:CD1	2.89	0.56
1:D:159:TRP:NE1	1:D:259:PHE:CE2	2.73	0.56
1:D:110:ALA:HB1	1:D:302:ALA:HB1	1.86	0.56
1:D:114:LEU:CD2	1:D:231:TRP:CH2	2.89	0.56
1:C:392:LEU:HD12	1:C:392:LEU:O	2.06	0.56
1:A:111:VAL:HG11	1:A:322:MET:SD	2.46	0.55
1:B:456:PHE:HE2	1:B:489:PHE:CD1	2.23	0.55
1:D:112:GLU:HB2	1:D:260:VAL:CG2	2.36	0.55
1:A:163:ALA:HB1	1:A:257:LYS:HD2	1.88	0.55
1:D:688:PRO:HB2	1:D:689:TYR:CE1	2.42	0.55
1:B:476:TRP:CG	1:B:477:PRO:HD3	2.42	0.55
1:D:65:HIS:HE2	1:D:331:MET:HB2	1.72	0.55
1:A:708:MET:HG2	1:A:729:TRP:CZ2	2.42	0.55
1:C:584:ILE:HD12	1:C:591:LEU:HD23	1.88	0.55
1:C:413:MET:HE1	1:C:475:THR:HA	1.88	0.55
1:C:516:HIS:ND1	1:C:548:LEU:HD22	2.20	0.55
1:D:114:LEU:HD21	1:D:231:TRP:CH2	2.42	0.55
1:A:443:ARG:HG3	1:A:444:VAL:HG23	1.88	0.55
1:C:362:LEU:HD23	1:C:362:LEU:N	2.21	0.55
1:C:392:LEU:HD21	1:C:473:PRO:CD	2.37	0.55
1:D:68:PHE:HB3	1:D:105:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:THR:CG2	1:D:531:PRO:HD2	2.37	0.55
1:A:487:TYR:O	1:A:491:SER:N	2.36	0.55
1:A:165:ASP:OD1	1:A:165:ASP:O	2.25	0.55
1:C:392:LEU:HD21	1:C:473:PRO:HG2	1.89	0.55
1:A:507:LEU:CG	1:A:578:MET:HE1	2.36	0.54
1:C:159:TRP:N	1:C:160:PRO:CD	2.70	0.54
1:D:112:GLU:HG3	1:D:262:VAL:CG2	2.37	0.54
1:D:114:LEU:HD21	1:D:231:TRP:CZ3	2.42	0.54
1:D:627:ARG:HB3	1:D:627:ARG:NH1	2.22	0.54
1:A:111:VAL:HG12	1:A:302:ALA:O	2.07	0.54
1:B:389:PRO:CG	1:B:390:ASN:H	2.20	0.54
1:D:116:LEU:CD1	1:D:246:THR:HG23	2.37	0.54
1:D:722:LYS:N	1:D:725:LYS:CE	2.69	0.54
1:D:617:ASP:CG	1:D:619:PRO:HG2	2.32	0.54
1:C:495:PHE:HD2	1:C:519:LEU:HD11	1.73	0.54
1:D:112:GLU:O	1:D:114:LEU:CD1	2.55	0.54
1:D:114:LEU:HD23	1:D:229:GLY:HA3	1.90	0.54
1:D:612:LYS:NZ	1:D:739:LEU:CD1	2.64	0.54
1:C:744:PHE:CD1	1:C:746:SER:C	2.86	0.54
1:D:68:PHE:HB3	1:D:105:ILE:CD1	2.38	0.54
1:C:495:PHE:HD2	1:C:519:LEU:CD1	2.22	0.53
1:D:440:GLY:CA	1:D:532:PHE:CE1	2.85	0.53
1:D:564:ARG:HG3	1:D:564:ARG:NH1	2.19	0.53
1:B:456:PHE:CE2	1:B:489:PHE:CD1	2.96	0.53
1:D:334:ILE:CG1	1:D:335:PRO:HD2	2.38	0.53
1:A:100:TYR:CD1	1:A:100:TYR:C	2.84	0.53
1:C:170:PHE:CZ	1:C:340:PHE:CE1	2.97	0.53
1:D:116:LEU:HD21	1:D:249:PRO:HD3	1.89	0.53
1:C:441:ASP:O	1:C:442:ASN:HB2	2.08	0.53
1:C:564:ARG:NH1	1:C:572:PRO:O	2.42	0.53
1:C:694:PRO:HG2	1:C:695:TRP:CE3	2.43	0.53
1:A:334:ILE:HG23	1:A:335:PRO:HD2	1.91	0.53
1:C:491:SER:O	1:C:492:GLU:HB3	2.09	0.53
1:D:524:GLN:NE2	1:D:573:TRP:CH2	2.76	0.53
1:D:674:VAL:CG1	1:D:678:VAL:HG21	2.39	0.53
1:A:401:TRP:NE1	1:B:679:GLU:O	2.33	0.53
1:D:447:PHE:CD1	1:D:532:PHE:CD1	2.97	0.53
1:D:629:ARG:NH1	1:D:631:LEU:CD2	2.69	0.53
1:A:160:PRO:HA	1:A:257:LYS:O	2.09	0.53
1:A:467:GLU:HG3	1:A:579:ARG:CZ	2.38	0.53
1:B:487:TYR:C	1:B:487:TYR:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:LEU:HD12	1:C:392:LEU:C	2.34	0.53
1:A:113:ALA:HB2	1:A:260:VAL:HG22	1.91	0.53
1:A:28:PHE:CE1	1:A:284:TYR:HB2	2.44	0.52
1:A:291:LEU:HB3	1:A:308:TYR:CE2	2.44	0.52
1:D:566:VAL:HB	1:D:569:ALA:HB2	1.90	0.52
1:B:337:MET:CE	1:B:341:TRP:NE1	2.72	0.52
1:C:372:PRO:HB2	1:C:531:PRO:HG2	1.91	0.52
1:C:422:ALA:O	1:C:423:ASN:HB2	2.09	0.52
1:B:315:ASP:N	1:B:315:ASP:OD1	2.42	0.52
1:D:65:HIS:NE2	1:D:331:MET:HB2	2.24	0.52
1:C:615:TRP:CZ2	1:C:694:PRO:O	2.63	0.52
1:C:738:ILE:CG2	1:C:739:LEU:N	2.68	0.52
1:D:112:GLU:HG3	1:D:262:VAL:HA	1.89	0.52
1:B:77:LEU:HD12	1:B:105:ILE:CG2	2.40	0.52
1:B:505:SER:CB	1:D:723:LEU:HD12	2.39	0.52
1:B:573:TRP:HB2	1:B:575:ILE:CD1	2.39	0.52
1:D:80:ILE:CB	1:D:107:TYR:CZ	2.88	0.52
1:D:516:HIS:ND1	1:D:548:LEU:HD22	2.24	0.52
1:D:159:TRP:CE2	1:D:163:ALA:HB2	2.45	0.52
1:D:615:TRP:CE3	1:D:616:ASP:HA	2.45	0.52
1:D:155:PRO:HG2	1:D:341:TRP:CE3	2.45	0.52
1:D:334:ILE:HG12	1:D:335:PRO:HD2	1.92	0.52
1:A:260:VAL:CG2	1:A:325:ALA:HA	2.37	0.52
1:B:509:ASN:ND2	1:D:722:LYS:HB2	2.24	0.52
1:C:372:PRO:CB	1:C:531:PRO:HG2	2.39	0.52
1:C:547:GLU:OE2	1:C:580:ARG:NH2	2.43	0.52
1:D:375:HIS:HA	1:D:378:TYR:HB2	1.91	0.52
1:A:335:PRO:HB3	1:A:447:PHE:CE1	2.45	0.52
1:B:426:GLU:OE2	1:B:466:ARG:HD3	2.10	0.52
1:D:80:ILE:HG21	1:D:107:TYR:CE2	2.45	0.52
1:A:309:GLU:O	1:A:313:ALA:N	2.42	0.52
1:A:218:PHE:CE2	1:A:226:THR:HB	2.45	0.51
1:B:738:ILE:HD12	1:B:738:ILE:N	2.25	0.51
1:D:339:ALA:HA	1:D:375:HIS:NE2	2.25	0.51
1:D:19:ASN:HB2	1:D:297:ASP:OD2	2.10	0.51
1:D:674:VAL:HG13	1:D:678:VAL:HG21	1.92	0.51
1:A:674:VAL:HG13	1:A:678:VAL:CG2	2.37	0.51
1:C:615:TRP:HZ2	1:C:694:PRO:O	1.94	0.51
1:D:109:ILE:C	1:D:304:ALA:HB2	2.36	0.51
1:D:673:PHE:CE2	1:D:698:ILE:HD11	2.45	0.51
1:D:89:LYS:HB3	1:D:305:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ALA:HB1	1:C:322:MET:SD	2.51	0.51
1:A:374:LEU:C	1:A:374:LEU:CD2	2.84	0.51
1:A:530:THR:HG22	1:A:533:GLY:O	2.11	0.51
1:A:230:PRO:HA	1:A:233:TRP:CD1	2.46	0.51
1:A:673:PHE:CE2	1:A:698:ILE:HD11	2.46	0.51
1:B:422:ALA:C	1:B:423:ASN:ND2	2.69	0.51
1:B:665:ILE:HG13	1:B:666:THR:HG23	1.91	0.51
1:B:723:LEU:HA	1:B:724:PRO:C	2.35	0.51
1:D:339:ALA:HB1	1:D:375:HIS:CE1	2.45	0.51
1:A:335:PRO:HB3	1:A:447:PHE:CZ	2.46	0.51
1:C:65:HIS:ND1	1:C:262:VAL:HB	2.26	0.50
1:C:262:VAL:CG1	1:C:263:LEU:N	2.74	0.50
1:C:665:ILE:HG13	1:C:666:THR:CG2	2.40	0.50
1:D:159:TRP:N	1:D:160:PRO:CD	2.74	0.50
1:D:732:LYS:HG2	1:D:733:LYS:N	2.24	0.50
1:A:28:PHE:CE1	1:A:280:PHE:CG	2.99	0.50
1:A:391:PRO:HG3	1:A:414:TYR:CZ	2.46	0.50
1:D:522:ASP:OD2	1:D:525:MET:HG2	2.11	0.50
1:A:41:PRO:C	1:A:44:LEU:HD21	2.37	0.50
1:C:358:VAL:HG12	1:C:362:LEU:HD11	1.94	0.50
1:A:708:MET:HE1	1:A:732:LYS:CE	2.42	0.50
1:B:426:GLU:CD	1:B:466:ARG:HD3	2.37	0.50
1:D:447:PHE:HE1	1:D:532:PHE:CD1	2.30	0.50
1:A:168:TYR:CD2	1:A:171:LYS:HE3	2.46	0.50
1:A:516:HIS:ND1	1:A:548:LEU:HD22	2.27	0.50
1:A:738:ILE:C	1:A:740:PRO:HD2	2.37	0.50
1:B:11:TRP:CD2	1:B:58:PRO:HG2	2.47	0.50
1:D:529:GLN:OE1	1:D:534:VAL:HG22	2.12	0.50
1:A:161:LEU:HD23	1:A:196:LEU:HG	1.94	0.50
1:A:704:PHE:HZ	1:A:708:MET:HE3	1.72	0.50
1:D:618:LEU:N	1:D:619:PRO:HD2	2.27	0.50
1:B:487:TYR:CD2	1:D:740:PRO:HB3	2.47	0.50
1:C:476:TRP:CG	1:C:477:PRO:HD3	2.47	0.50
1:D:80:ILE:HD12	1:D:107:TYR:CD1	2.42	0.50
1:D:447:PHE:CD1	1:D:532:PHE:HD1	2.30	0.49
1:A:111:VAL:HG23	1:A:262:VAL:CG2	2.41	0.49
1:D:112:GLU:CB	1:D:260:VAL:HG23	2.41	0.49
1:D:688:PRO:HB2	1:D:689:TYR:CD1	2.47	0.49
1:B:427:HIS:HB3	1:B:465:LYS:HA	1.93	0.49
1:D:381:CYS:HB3	1:D:414:TYR:CZ	2.47	0.49
1:D:496:CYS:N	1:D:499:ASP:OD2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:LYS:O	1:D:305:LEU:HD12	2.13	0.49
1:D:635:HIS:CE1	1:D:735:LYS:HE2	2.48	0.49
1:A:345:ARG:CD	1:A:349:ILE:HD12	2.42	0.49
1:D:98:VAL:HG21	1:D:106:ALA:HB3	1.95	0.49
1:A:332:PRO:HG2	1:A:337:MET:SD	2.53	0.49
1:A:435:LEU:HD23	1:A:489:PHE:HE1	1.78	0.49
1:B:487:TYR:CE2	1:D:740:PRO:HB3	2.47	0.49
1:A:723:LEU:HD23	1:A:725:LYS:HG3	1.94	0.48
1:D:80:ILE:HB	1:D:107:TYR:HH	1.76	0.48
1:D:168:TYR:O	1:D:183:GLY:CA	2.61	0.48
1:B:738:ILE:HD12	1:B:738:ILE:H	1.79	0.48
1:C:141:LYS:C	1:C:144:GLY:H	2.21	0.48
1:A:41:PRO:HG2	1:A:44:LEU:CD2	2.43	0.48
1:D:97:ALA:HA	1:D:330:ILE:HG12	1.95	0.48
1:A:111:VAL:CG2	1:A:260:VAL:CG1	2.91	0.48
1:A:111:VAL:CG2	1:A:262:VAL:HG22	2.44	0.48
1:A:611:ALA:HB1	1:A:642:SER:HB3	1.96	0.48
1:D:114:LEU:HD22	1:D:156:TYR:OH	2.13	0.48
1:D:732:LYS:CG	1:D:733:LYS:N	2.76	0.48
1:C:591:LEU:O	1:C:595:VAL:HG23	2.12	0.48
1:D:74:SER:HB2	1:D:76:LEU:HG	1.96	0.48
1:D:330:ILE:N	1:D:330:ILE:HD12	2.29	0.48
1:D:387:ASP:CG	1:D:388:GLN:OE1	2.57	0.48
1:B:159:TRP:N	1:B:160:PRO:CD	2.76	0.48
1:B:484:LEU:HD21	1:B:501:VAL:HG11	1.95	0.48
1:A:105:ILE:HG22	1:A:105:ILE:O	2.14	0.48
1:B:334:ILE:HG23	1:B:335:PRO:HD2	1.96	0.48
1:B:734:LEU:C	1:B:734:LEU:CD1	2.83	0.48
1:D:109:ILE:HG22	1:D:109:ILE:O	2.13	0.48
1:D:376:ALA:HB1	1:D:528:VAL:HG11	1.96	0.48
1:A:345:ARG:CD	1:A:345:ARG:C	2.85	0.47
1:B:739:LEU:N	1:B:740:PRO:HD3	2.28	0.47
1:D:65:HIS:HB3	1:D:262:VAL:HG13	1.96	0.47
1:D:689:TYR:CD1	1:D:689:TYR:N	2.78	0.47
1:A:695:TRP:HH2	1:B:403:GLY:O	1.97	0.47
1:B:504:HIS:HB3	1:D:739:LEU:HD21	1.96	0.47
1:B:729:TRP:HB3	1:B:730:PRO:HD2	1.96	0.47
1:C:397:ILE:HD13	1:D:692:HIS:CE1	2.49	0.47
1:D:615:TRP:HE3	1:D:616:ASP:CA	2.27	0.47
1:A:447:PHE:C	1:A:447:PHE:CD1	2.91	0.47
1:B:342:TYR:HD2	1:B:375:HIS:CD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ASP:CB	1:B:619:PRO:HD2	2.38	0.47
1:D:129:THR:C	1:D:249:PRO:HB3	2.39	0.47
1:A:11:TRP:CG	1:A:58:PRO:HG3	2.50	0.47
1:A:98:VAL:CG2	1:A:106:ALA:HB3	2.45	0.47
1:A:117:ILE:HB	1:A:226:THR:HG23	1.95	0.47
1:D:65:HIS:CE1	1:D:261:GLY:HA2	2.47	0.47
1:B:423:ASN:O	1:B:425:PRO:HD3	2.14	0.47
1:A:44:LEU:HB3	1:A:48:PHE:CZ	2.49	0.47
1:A:476:TRP:N	1:A:477:PRO:CD	2.77	0.47
1:A:486:ARG:NH1	1:D:623:GLU:OE2	2.48	0.47
1:B:105:ILE:O	1:B:105:ILE:CG2	2.62	0.47
1:C:413:MET:HG2	1:C:430:TYR:CD2	2.49	0.47
1:C:441:ASP:OD2	1:C:443:ARG:NH2	2.47	0.47
1:D:69:GLY:CA	1:D:333:ASN:HB3	2.42	0.47
1:B:59:ASP:OD1	1:B:271:SER:OG	2.22	0.47
1:B:389:PRO:HG2	1:B:390:ASN:N	2.30	0.47
1:B:570:GLY:HA2	1:B:575:ILE:O	2.15	0.47
1:D:629:ARG:HH12	1:D:631:LEU:HD23	1.75	0.47
1:A:233:TRP:CD1	1:A:233:TRP:H	2.33	0.47
1:B:569:ALA:HB1	1:B:580:ARG:NH1	2.30	0.47
1:D:112:GLU:CG	1:D:262:VAL:CA	2.89	0.47
1:C:615:TRP:CE3	1:C:616:ASP:O	2.67	0.47
1:D:318:ILE:O	1:D:322:MET:HG2	2.15	0.47
1:A:149:MET:HG3	1:A:223:THR:HG21	1.97	0.46
1:A:159:TRP:N	1:A:160:PRO:CD	2.78	0.46
1:C:44:LEU:HD11	1:C:63:TRP:CE3	2.50	0.46
1:D:506:PRO:HA	1:D:514:ILE:O	2.15	0.46
1:D:665:ILE:HG13	1:D:666:THR:HG23	1.97	0.46
1:D:113:ALA:HB3	1:D:321:THR:O	2.15	0.46
1:D:335:PRO:C	1:D:336:GLN:HG3	2.40	0.46
1:D:371:ALA:CB	1:D:439:TYR:HA	2.45	0.46
1:D:447:PHE:CE1	1:D:532:PHE:CE1	3.04	0.46
1:B:415:ARG:NH1	1:B:417:VAL:HG12	2.29	0.46
1:C:155:PRO:HD3	1:C:345:ARG:HG2	1.97	0.46
1:C:392:LEU:HD11	1:C:413:MET:SD	2.56	0.46
1:A:233:TRP:CZ3	1:A:317:ARG:HB3	2.51	0.46
1:A:374:LEU:CD2	1:A:378:TYR:CD2	2.99	0.46
1:A:476:TRP:CG	1:A:477:PRO:HD3	2.50	0.46
1:D:262:VAL:HG22	1:D:263:LEU:O	2.15	0.46
1:D:309:GLU:HG2	1:D:318:ILE:CG2	2.46	0.46
1:D:553:GLN:O	1:D:604:SER:OG	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ASP:OD2	1:B:580:ARG:HB2	2.14	0.46
1:C:441:ASP:OD2	1:C:443:ARG:CZ	2.64	0.46
1:B:155:PRO:HB3	1:B:344:VAL:HG12	1.98	0.46
1:B:576:THR:HG22	1:B:578:MET:HE2	1.98	0.46
1:C:392:LEU:CD2	1:C:473:PRO:HD2	2.46	0.46
1:D:16:LYS:HE2	1:D:263:LEU:HD22	1.97	0.46
1:D:168:TYR:CE1	1:D:183:GLY:HA3	2.50	0.46
1:B:441:ASP:CG	1:B:443:ARG:HE	2.24	0.46
1:A:148:LEU:HD23	1:A:225:MET:HB2	1.97	0.46
1:A:233:TRP:CD1	1:A:233:TRP:N	2.82	0.46
1:B:389:PRO:CG	1:B:390:ASN:N	2.76	0.46
1:B:617:ASP:OD1	1:B:631:LEU:HD13	2.15	0.46
1:C:476:TRP:N	1:C:477:PRO:CD	2.79	0.46
1:B:133:ILE:N	1:B:134:PRO:CD	2.79	0.46
1:B:334:ILE:HG22	1:B:336:GLN:H	1.81	0.46
1:B:503:TRP:CD2	1:D:738:ILE:HG21	2.51	0.46
1:C:65:HIS:HD1	1:C:262:VAL:HB	1.81	0.46
1:D:504:HIS:N	1:D:515:GLN:O	2.48	0.46
1:A:345:ARG:HD2	1:A:349:ILE:HD12	1.98	0.46
1:A:467:GLU:CD	1:A:579:ARG:NH1	2.74	0.46
1:B:611:ALA:HB1	1:B:642:SER:HB3	1.98	0.46
1:D:113:ALA:CB	1:D:325:ALA:N	2.79	0.46
1:D:639:ASN:ND2	1:D:641:GLU:HB2	2.30	0.46
1:D:743:VAL:HG23	1:D:743:VAL:O	2.16	0.46
1:A:704:PHE:CE2	1:A:708:MET:SD	3.09	0.45
1:D:463:ARG:HH22	1:D:524:GLN:CG	2.29	0.45
1:D:618:LEU:HB2	1:D:619:PRO:CD	2.46	0.45
1:B:77:LEU:CD1	1:B:105:ILE:HG22	2.45	0.45
1:B:575:ILE:N	1:B:575:ILE:CD1	2.79	0.45
1:C:44:LEU:HD12	1:C:45:GLU:N	2.31	0.45
1:D:77:LEU:HD13	1:D:105:ILE:HD13	1.98	0.45
1:D:476:TRP:CG	1:D:477:PRO:HD3	2.51	0.45
1:B:7:LYS:HG2	1:B:8:LEU:N	2.31	0.45
1:B:738:ILE:HG12	1:D:503:TRP:O	2.15	0.45
1:C:373:GLY:HA3	1:C:438:LEU:HA	1.97	0.45
1:D:259:PHE:HE1	1:D:329:GLU:CB	2.28	0.45
1:A:591:LEU:CD2	1:A:594:ARG:NH1	2.79	0.45
1:C:45:GLU:HG2	1:C:46:GLU:N	2.30	0.45
1:D:706:GLU:O	1:D:710:GLU:HG3	2.16	0.45
1:A:111:VAL:CB	1:A:262:VAL:HG22	2.47	0.45
1:B:441:ASP:O	1:B:442:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:PRO:C	1:B:626:ILE:HG22	2.42	0.45
1:D:476:TRP:N	1:D:477:PRO:CD	2.79	0.45
1:A:98:VAL:HG21	1:A:106:ALA:HB3	1.97	0.45
1:B:504:HIS:O	1:D:640:GLN:OE1	2.35	0.45
1:B:621:ARG:O	1:B:622:GLY:C	2.58	0.45
1:C:467:GLU:OE1	1:C:467:GLU:HA	2.15	0.45
1:D:615:TRP:CE3	1:D:616:ASP:CA	3.00	0.45
1:A:721:PHE:O	1:A:725:LYS:CE	2.65	0.45
1:B:190:LYS:HE2	1:B:359:ASP:HA	1.98	0.45
1:C:392:LEU:HD11	1:C:413:MET:HB2	1.98	0.45
1:C:562:LEU:HD21	1:C:594:ARG:HD2	1.98	0.45
1:D:117:ILE:HA	1:D:244:GLY:O	2.17	0.45
1:D:612:LYS:HZ3	1:D:739:LEU:HD13	1.72	0.45
1:A:342:TYR:O	1:A:346:THR:HG23	2.16	0.45
1:B:504:HIS:HB2	1:D:739:LEU:HD11	1.98	0.45
1:C:466:ARG:NH2	1:C:470:GLU:O	2.50	0.45
1:C:566:VAL:HB	1:C:569:ALA:HB2	1.97	0.45
1:D:450:THR:HG22	1:D:531:PRO:HA	1.99	0.45
1:D:638:PHE:HE2	1:D:734:LEU:HD11	1.82	0.45
1:C:48:PHE:N	1:C:49:PRO:HD2	2.32	0.45
1:D:105:ILE:HD12	1:D:106:ALA:CB	2.46	0.45
1:D:112:GLU:HB3	1:D:261:GLY:O	2.17	0.45
1:D:130:TRP:CD1	1:D:249:PRO:HB2	2.52	0.45
1:D:259:PHE:HB3	1:D:331:MET:SD	2.57	0.45
1:D:513:ARG:HH11	1:D:583:THR:HG23	1.82	0.45
1:A:387:ASP:OD1	1:A:387:ASP:N	2.49	0.44
1:A:739:LEU:HD12	1:A:739:LEU:C	2.43	0.44
1:B:337:MET:HE2	1:B:341:TRP:HE1	1.81	0.44
1:C:332:PRO:HB2	1:C:337:MET:SD	2.57	0.44
1:D:440:GLY:O	1:D:532:PHE:CE1	2.71	0.44
1:A:86:PHE:HZ	1:A:286:LEU:HD12	1.81	0.44
1:A:506:PRO:HB3	1:A:510:SER:O	2.17	0.44
1:C:81:THR:N	1:C:82:PRO:HD3	2.32	0.44
1:C:562:LEU:HB3	1:C:591:LEU:HD23	1.99	0.44
1:D:168:TYR:CD2	1:D:170:PHE:C	2.96	0.44
1:B:337:MET:CE	1:B:341:TRP:HE1	2.30	0.44
1:B:635:HIS:HA	1:B:733:LYS:O	2.17	0.44
1:C:430:TYR:CZ	1:C:477:PRO:HG2	2.53	0.44
1:D:111:VAL:H	1:D:302:ALA:HB1	1.82	0.44
1:B:114:LEU:HD11	1:B:156:TYR:CE2	2.53	0.44
1:B:502:SER:HB3	1:B:548:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:TRP:NE1	1:D:163:ALA:HB2	2.33	0.44
1:D:604:SER:O	1:D:653:ARG:NH1	2.50	0.44
1:B:11:TRP:CG	1:B:58:PRO:HG2	2.53	0.44
1:B:389:PRO:CD	1:B:390:ASN:H	2.30	0.44
1:B:737:SER:HB3	1:B:740:PRO:HG2	1.99	0.44
1:D:80:ILE:CD1	1:D:107:TYR:CZ	3.00	0.44
1:B:425:PRO:HG3	1:B:465:LYS:HD2	1.99	0.44
1:D:305:LEU:HD23	1:D:307:SER:OG	2.17	0.44
1:A:48:PHE:O	1:A:52:ALA:HB2	2.18	0.44
1:A:463:ARG:NH2	1:A:524:GLN:HG2	2.32	0.44
1:A:575:ILE:HD12	1:A:575:ILE:N	2.33	0.44
1:D:463:ARG:NH2	1:D:524:GLN:HB2	2.32	0.44
1:D:564:ARG:O	1:D:571:GLY:HA2	2.18	0.44
1:D:741:ASP:OD1	1:D:741:ASP:N	2.50	0.44
1:A:487:TYR:O	1:A:491:SER:CB	2.62	0.44
1:C:664:SER:OG	1:C:667:GLY:N	2.51	0.44
1:D:111:VAL:HG23	1:D:325:ALA:CB	2.47	0.44
1:D:133:ILE:N	1:D:134:PRO:CD	2.81	0.44
1:D:522:ASP:OD1	1:D:523:PRO:CD	2.66	0.44
1:D:542:GLY:HA3	1:D:576:THR:HG21	1.98	0.44
1:D:738:ILE:C	1:D:738:ILE:CD1	2.86	0.44
1:D:54:THR:HG23	1:D:56:ASP:CG	2.43	0.44
1:D:368:ASN:HA	1:D:374:LEU:HD13	1.99	0.44
1:A:430:TYR:CZ	1:A:477:PRO:HG2	2.53	0.43
1:B:63:TRP:CD1	1:B:67:ARG:HG3	2.52	0.43
1:B:476:TRP:CD2	1:B:477:PRO:HD3	2.53	0.43
1:D:112:GLU:OE2	1:D:262:VAL:HB	2.17	0.43
1:A:568:ILE:HD11	1:A:587:ILE:HD13	1.99	0.43
1:B:576:THR:HG22	1:B:578:MET:CE	2.48	0.43
1:B:737:SER:CB	1:B:740:PRO:HG2	2.48	0.43
1:C:80:ILE:C	1:C:82:PRO:HD3	2.42	0.43
1:C:193:LEU:CD2	1:C:362:LEU:CD2	2.95	0.43
1:D:116:LEU:HB2	1:D:226:THR:O	2.17	0.43
1:D:564:ARG:HH11	1:D:564:ARG:CG	2.24	0.43
1:A:334:ILE:CG2	1:A:335:PRO:CD	2.96	0.43
1:B:569:ALA:CB	1:B:580:ARG:HH11	2.31	0.43
1:D:391:PRO:HG3	1:D:414:TYR:CE2	2.53	0.43
1:A:505:SER:OG	1:A:506:PRO:CD	2.63	0.43
1:C:179:ILE:HG22	1:C:334:ILE:HD13	2.01	0.43
1:D:114:LEU:HD23	1:D:229:GLY:HA2	2.01	0.43
1:D:170:PHE:CE1	1:D:179:ILE:HA	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:615:TRP:CE3	1:D:615:TRP:C	2.97	0.43
1:A:111:VAL:CG1	1:A:322:MET:SD	3.06	0.43
1:A:151:ASN:OD1	1:A:211:TYR:N	2.51	0.43
1:C:635:HIS:CE1	1:C:735:LYS:CD	3.00	0.43
1:A:639:ASN:HA	1:A:737:SER:O	2.18	0.43
1:B:170:PHE:CE1	1:B:340:PHE:CZ	3.07	0.43
1:B:384:LEU:CD1	1:B:525:MET:HG2	2.49	0.43
1:C:65:HIS:ND1	1:C:261:GLY:O	2.51	0.43
1:A:118:TYR:CB	1:A:225:MET:SD	3.07	0.43
1:A:148:LEU:O	1:A:149:MET:HG2	2.19	0.43
1:D:98:VAL:HG13	1:D:104:LEU:HD22	2.00	0.43
1:D:109:ILE:O	1:D:304:ALA:HB2	2.19	0.43
1:B:673:PHE:CE2	1:B:698:ILE:HD11	2.54	0.43
1:C:441:ASP:CG	1:C:443:ARG:HE	2.21	0.43
1:D:105:ILE:HD12	1:D:106:ALA:HB2	2.01	0.43
1:A:729:TRP:CB	1:A:730:PRO:HD2	2.39	0.43
1:B:116:LEU:HB2	1:B:248:LEU:HD23	2.00	0.43
1:C:575:ILE:HD12	1:C:575:ILE:N	2.34	0.43
1:A:110:ALA:O	1:A:262:VAL:HG13	2.19	0.43
1:C:665:ILE:HG13	1:C:666:THR:H	1.82	0.43
1:D:116:LEU:HD21	1:D:248:LEU:HA	2.01	0.43
1:A:41:PRO:HG2	1:A:44:LEU:HD21	2.00	0.42
1:A:340:PHE:O	1:A:344:VAL:HG23	2.19	0.42
1:A:598:GLY:O	1:A:602:ASP:HB2	2.18	0.42
1:C:193:LEU:HD23	1:C:362:LEU:CD2	2.32	0.42
1:D:563:LEU:HD23	1:D:569:ALA:HB1	2.01	0.42
1:B:323:GLU:O	1:B:327:LYS:HG3	2.19	0.42
1:C:380:GLU:HG3	1:C:528:VAL:CG2	2.49	0.42
1:D:90:LEU:HD22	1:D:304:ALA:O	2.19	0.42
1:A:384:LEU:HD21	1:A:524:GLN:HG3	2.01	0.42
1:B:216:ALA:O	1:B:220:LYS:HB2	2.20	0.42
1:B:415:ARG:CZ	1:B:417:VAL:HG12	2.50	0.42
1:D:292:GLU:OE2	1:D:296:LYS:NZ	2.38	0.42
1:D:384:LEU:HD23	1:D:385:TYR:CE2	2.53	0.42
1:D:505:SER:N	1:D:515:GLN:HB3	2.34	0.42
1:C:442:ASN:OD1	1:C:447:PHE:N	2.52	0.42
1:D:109:ILE:CA	1:D:304:ALA:HB2	2.48	0.42
1:D:417:VAL:O	1:D:426:GLU:HA	2.20	0.42
1:B:77:LEU:CB	1:B:105:ILE:HG23	2.49	0.42
1:B:492:GLU:O	1:B:493:ASN:HB2	2.18	0.42
1:D:80:ILE:CG2	1:D:107:TYR:CE2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:LEU:HD12	1:D:116:LEU:C	2.44	0.42
1:D:430:TYR:CZ	1:D:477:PRO:HG2	2.55	0.42
1:A:28:PHE:CE1	1:A:284:TYR:CB	3.02	0.42
1:A:214:ALA:O	1:A:218:PHE:CD2	2.72	0.42
1:A:415:ARG:HH12	1:A:466:ARG:NE	2.17	0.42
1:B:428:TRP:CE3	1:B:473:PRO:HB3	2.54	0.42
1:C:170:PHE:CZ	1:C:340:PHE:CZ	3.08	0.42
1:D:371:ALA:HB1	1:D:438:LEU:O	2.19	0.42
1:D:385:TYR:OH	1:D:416:ASN:ND2	2.48	0.42
1:A:13:ASN:HB2	1:A:63:TRP:CZ2	2.55	0.42
1:C:117:ILE:HG12	1:C:245:VAL:HG22	2.02	0.42
1:C:141:LYS:O	1:C:144:GLY:N	2.51	0.42
1:D:68:PHE:CD2	1:D:105:ILE:HD13	2.55	0.42
1:D:741:ASP:O	1:D:743:VAL:HG13	2.20	0.42
1:A:155:PRO:HG2	1:A:341:TRP:CE3	2.55	0.42
1:C:428:TRP:CH2	1:C:466:ARG:NH1	2.88	0.42
1:C:639:ASN:HA	1:C:737:SER:O	2.20	0.42
1:C:680:GLY:HA2	1:D:367:THR:HG21	2.01	0.42
1:D:309:GLU:CG	1:D:322:MET:HG3	2.50	0.42
1:D:465:LYS:NZ	1:D:568:ILE:HA	2.35	0.42
1:D:704:PHE:CE2	1:D:708:MET:CE	3.03	0.42
1:B:426:GLU:OE2	1:B:466:ARG:CD	2.68	0.42
1:B:689:TYR:CD1	1:B:689:TYR:N	2.84	0.42
1:D:334:ILE:HA	1:D:335:PRO:HD3	1.92	0.42
1:A:708:MET:HE1	1:A:732:LYS:NZ	2.35	0.41
1:C:11:TRP:CE2	1:C:58:PRO:HG3	2.54	0.41
1:C:155:PRO:HB3	1:C:344:VAL:HG12	2.02	0.41
1:D:113:ALA:CB	1:D:325:ALA:HB2	2.50	0.41
1:D:159:TRP:CD1	1:D:259:PHE:CG	3.08	0.41
1:D:380:GLU:CG	1:D:525:MET:CE	2.98	0.41
1:A:370:ALA:C	1:A:372:PRO:HD3	2.44	0.41
1:A:612:LYS:HB2	1:A:639:ASN:HB2	2.02	0.41
1:C:185:ASP:CB	1:C:366:GLN:OE1	2.64	0.41
1:D:639:ASN:HD21	1:D:641:GLU:HB2	1.85	0.41
1:D:738:ILE:O	1:D:738:ILE:HD12	2.20	0.41
1:A:503:TRP:O	1:A:504:HIS:HB2	2.19	0.41
1:A:708:MET:HE2	1:A:732:LYS:NZ	2.33	0.41
1:A:732:LYS:HG2	1:A:733:LYS:N	2.35	0.41
1:B:510:SER:O	1:B:511:GLU:C	2.62	0.41
1:B:554:TRP:CH2	1:B:558:GLY:HA3	2.56	0.41
1:C:372:PRO:CB	1:C:531:PRO:CG	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ASN:HA	1:C:445:HIS:O	2.21	0.41
1:C:635:HIS:HE1	1:C:735:LYS:HD3	1.82	0.41
1:D:91:TYR:CE2	1:D:322:MET:HE2	2.55	0.41
1:D:97:ALA:HA	1:D:330:ILE:CG2	2.50	0.41
1:D:319:ALA:O	1:D:323:GLU:HG3	2.20	0.41
1:D:615:TRP:HE3	1:D:616:ASP:N	2.18	0.41
1:A:118:TYR:HB3	1:A:225:MET:SD	2.60	0.41
1:A:334:ILE:HG22	1:A:335:PRO:HD2	2.01	0.41
1:B:123:LEU:HD21	1:B:127:PRO:HD3	2.01	0.41
1:C:694:PRO:HG2	1:C:695:TRP:HE3	1.83	0.41
1:D:617:ASP:C	1:D:619:PRO:HD2	2.45	0.41
1:A:66:ASP:OD1	1:A:66:ASP:N	2.51	0.41
1:A:111:VAL:HA	1:A:262:VAL:HA	2.01	0.41
1:B:415:ARG:NH1	1:B:415:ARG:HG2	2.36	0.41
1:B:734:LEU:C	1:B:735:LYS:HG3	2.45	0.41
1:D:617:ASP:OD2	1:D:619:PRO:HG2	2.20	0.41
1:D:629:ARG:HG2	1:D:630:GLN:N	2.34	0.41
1:A:41:PRO:CB	1:A:44:LEU:HD21	2.49	0.41
1:A:484:LEU:O	1:A:488:VAL:HG23	2.21	0.41
1:B:516:HIS:ND1	1:B:548:LEU:HD22	2.36	0.41
1:B:625:PRO:O	1:B:626:ILE:HG22	2.21	0.41
1:C:383:ARG:NH2	1:C:384:LEU:HD11	2.35	0.41
1:A:447:PHE:CE1	1:A:449:GLY:N	2.89	0.41
1:A:486:ARG:NH1	1:D:623:GLU:OE1	2.48	0.41
1:B:170:PHE:CZ	1:B:340:PHE:CZ	3.09	0.41
1:B:509:ASN:OD1	1:D:722:LYS:HD3	2.21	0.41
1:B:516:HIS:CG	1:B:548:LEU:HD22	2.56	0.41
1:C:160:PRO:HG3	1:C:258:PRO:HA	2.03	0.41
1:D:371:ALA:HB2	1:D:439:TYR:HA	2.01	0.41
1:A:332:PRO:HB2	1:A:337:MET:SD	2.60	0.41
1:B:476:TRP:N	1:B:477:PRO:CD	2.83	0.41
1:A:110:ALA:C	1:A:262:VAL:HG13	2.46	0.41
1:A:704:PHE:HE2	1:A:708:MET:CE	2.29	0.41
1:B:100:TYR:HB3	1:B:105:ILE:HD12	2.02	0.41
1:C:302:ALA:HB1	1:C:322:MET:CG	2.51	0.41
1:C:530:THR:HG22	1:C:533:GLY:O	2.20	0.41
1:B:419:SER:O	1:B:419:SER:OG	2.32	0.41
1:B:422:ALA:C	1:B:423:ASN:CG	2.89	0.41
1:B:484:LEU:O	1:B:488:VAL:HG23	2.20	0.41
1:C:638:PHE:HB3	1:C:642:SER:OG	2.21	0.41
1:D:463:ARG:NH2	1:D:524:GLN:CG	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:VAL:HG21	1:D:689:TYR:HB3	2.03	0.41
1:A:28:PHE:CZ	1:A:284:TYR:HB2	2.55	0.40
1:A:91:TYR:CZ	1:A:306:LYS:HG2	2.56	0.40
1:A:139:GLU:O	1:A:142:ALA:HB3	2.21	0.40
1:A:161:LEU:HD23	1:A:196:LEU:CD2	2.50	0.40
1:B:505:SER:HB2	1:D:640:GLN:OE1	2.21	0.40
1:C:261:GLY:O	1:C:262:VAL:HB	2.20	0.40
1:D:44:LEU:C	1:D:44:LEU:HD12	2.46	0.40
1:D:202:ASN:HB2	1:D:204:HIS:CD2	2.57	0.40
1:D:465:LYS:CG	1:D:575:ILE:HG22	2.39	0.40
1:C:424:ILE:HD13	1:C:573:TRP:CD2	2.57	0.40
1:D:340:PHE:CZ	1:D:344:VAL:HG21	2.56	0.40
1:D:561:GLU:O	1:D:564:ARG:HB2	2.22	0.40
1:D:618:LEU:HB2	1:D:619:PRO:HD3	2.03	0.40
1:A:162:ILE:HD11	1:A:193:LEU:HD21	2.03	0.40
1:B:739:LEU:HD12	1:B:742:VAL:CG2	2.51	0.40
1:D:106:ALA:HB1	1:D:265:ALA:O	2.21	0.40
1:D:638:PHE:CE2	1:D:734:LEU:HD11	2.56	0.40
1:A:168:TYR:CZ	1:A:171:LYS:HE3	2.55	0.40
1:D:114:LEU:CD1	1:D:114:LEU:N	2.85	0.40
1:D:292:GLU:HG2	1:D:296:LYS:HE3	2.02	0.40
1:A:339:ALA:HB1	1:A:372:PRO:HG2	2.02	0.40
1:B:503:TRP:CZ2	1:D:738:ILE:HG21	2.53	0.40
1:C:257:LYS:HA	1:C:328:GLY:HA2	2.03	0.40
1:D:28:PHE:O	1:D:32:THR:HB	2.21	0.40
1:D:112:GLU:C	1:D:260:VAL:HB	2.46	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	724/756 (96%)	709 (98%)	14 (2%)	1 (0%)	48	79
1	B	729/756 (96%)	707 (97%)	16 (2%)	6 (1%)	16	49
1	C	718/756 (95%)	701 (98%)	15 (2%)	2 (0%)	36	67
1	D	734/756 (97%)	713 (97%)	19 (3%)	2 (0%)	36	67
All	All	2905/3024 (96%)	2830 (97%)	64 (2%)	11 (0%)	30	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	262	VAL
1	D	618	LEU
1	B	491	SER
1	B	626	ILE
1	B	621	ARG
1	B	622	GLY
1	B	391	PRO
1	B	493	ASN
1	C	372	PRO
1	D	625	PRO
1	A	391	PRO

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	604/629 (96%)	598 (99%)	6 (1%)	68	75
1	B	606/629 (96%)	597 (98%)	9 (2%)	57	71
1	C	598/629 (95%)	593 (99%)	5 (1%)	73	77
1	D	611/629 (97%)	602 (98%)	9 (2%)	57	71
All	All	2419/2516 (96%)	2390 (99%)	29 (1%)	63	73

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ILE
1	A	345	ARG
1	A	446	GLU
1	A	492	GLU
1	A	674	VAL
1	A	738	ILE
1	B	329	GLU
1	B	390	ASN
1	B	467	GLU
1	B	503	TRP
1	B	568	ILE
1	B	629	ARG
1	B	674	VAL
1	B	707	LYS
1	B	738	ILE
1	C	259	PHE
1	C	362	LEU
1	C	593	GLU
1	C	640	GLN
1	C	674	VAL
1	D	317	ARG
1	D	521	GLU
1	D	575	ILE
1	D	579	ARG
1	D	612	LYS
1	D	631	LEU
1	D	717	SER
1	D	739	LEU
1	D	741	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	500	HIS
1	A	526	GLN
1	B	393	GLN
1	C	202	ASN
1	C	493	ASN
1	C	592	GLN
1	D	153	GLN
1	D	174	ASN
1	D	202	ASN
1	D	204	HIS

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Mol	Chain	Res	Type
1	D	295	ASN
1	D	592	GLN

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	730/756 (96%)	-0.22	4 (0%) 87 68	62, 133, 202, 298	0
1	B	733/756 (96%)	-0.23	2 (0%) 90 76	60, 158, 353, 503	0
1	C	724/756 (95%)	-0.28	4 (0%) 85 65	56, 171, 346, 474	0
1	D	738/756 (97%)	-0.23	5 (0%) 84 63	57, 184, 398, 518	0
All	All	2925/3024 (96%)	-0.24	15 (0%) 87 68	56, 152, 360, 518	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	377	ILE	4.3
1	A	745	ASP	3.7
1	D	112	GLU	3.1
1	C	340	PHE	2.9
1	C	301	GLY	2.7
1	D	374	LEU	2.7
1	D	94	THR	2.6
1	A	229	GLY	2.6
1	D	381	CYS	2.5
1	B	340	PHE	2.3
1	A	336	GLN	2.3
1	C	371	ALA	2.2
1	B	744	PHE	2.1
1	C	745	ASP	2.1
1	A	164	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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.