



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:13 AM UTC

PDB ID : 4FDG / pdb_00004fdg
Title : Crystal Structure of an Archaeal MCM Filament
Authors : Slaymaker, I.M.; Fu, Y.; Brewster, A.B.; Chen, X.S.
Deposited on : 2012-05-28
Resolution : 4.10 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

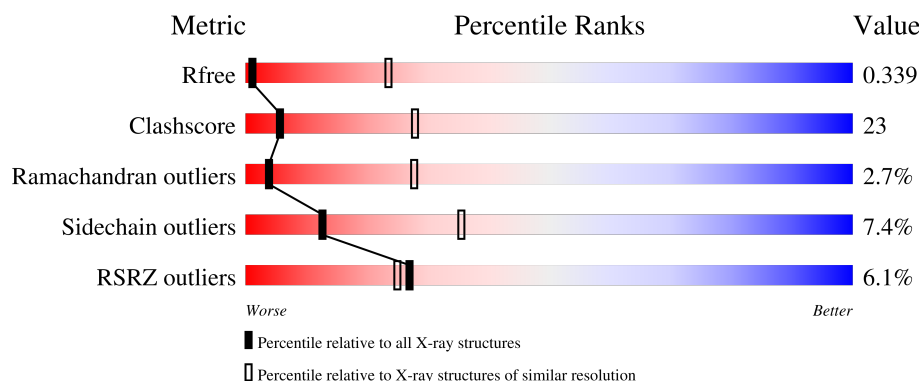
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	692	6% 50% 31% • • 14%
1	B	692	6% 49% 32% • • 14%
1	C	692	6% 49% 33% • • 14%
1	D	692	4% 49% 32% • • 14%
1	E	692	4% 49% 32% • • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23585 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 Minichromosome maintenance protein MCM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	A	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	C	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	D	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			
1	E	592	Total	C	N	O	S	0	0	0
			4716	3009	808	886	13			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q9UXG1
B	-4	HIS	-	expression tag	UNP Q9UXG1
B	-3	HIS	-	expression tag	UNP Q9UXG1
B	-2	HIS	-	expression tag	UNP Q9UXG1
B	-1	HIS	-	expression tag	UNP Q9UXG1
B	0	HIS	-	expression tag	UNP Q9UXG1
B	1	MET	-	expression tag	UNP Q9UXG1
B	2	GLU	-	expression tag	UNP Q9UXG1
B	3	ILE	-	expression tag	UNP Q9UXG1
B	4	PRO	-	expression tag	UNP Q9UXG1
B	5	SER	-	expression tag	UNP Q9UXG1
B	6	LYS	-	expression tag	UNP Q9UXG1
A	-5	HIS	-	expression tag	UNP Q9UXG1
A	-4	HIS	-	expression tag	UNP Q9UXG1
A	-3	HIS	-	expression tag	UNP Q9UXG1
A	-2	HIS	-	expression tag	UNP Q9UXG1
A	-1	HIS	-	expression tag	UNP Q9UXG1
A	0	HIS	-	expression tag	UNP Q9UXG1
A	1	MET	-	expression tag	UNP Q9UXG1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	-	expression tag	UNP Q9UXG1
A	3	ILE	-	expression tag	UNP Q9UXG1
A	4	PRO	-	expression tag	UNP Q9UXG1
A	5	SER	-	expression tag	UNP Q9UXG1
A	6	LYS	-	expression tag	UNP Q9UXG1
C	-5	HIS	-	expression tag	UNP Q9UXG1
C	-4	HIS	-	expression tag	UNP Q9UXG1
C	-3	HIS	-	expression tag	UNP Q9UXG1
C	-2	HIS	-	expression tag	UNP Q9UXG1
C	-1	HIS	-	expression tag	UNP Q9UXG1
C	0	HIS	-	expression tag	UNP Q9UXG1
C	1	MET	-	expression tag	UNP Q9UXG1
C	2	GLU	-	expression tag	UNP Q9UXG1
C	3	ILE	-	expression tag	UNP Q9UXG1
C	4	PRO	-	expression tag	UNP Q9UXG1
C	5	SER	-	expression tag	UNP Q9UXG1
C	6	LYS	-	expression tag	UNP Q9UXG1
D	-5	HIS	-	expression tag	UNP Q9UXG1
D	-4	HIS	-	expression tag	UNP Q9UXG1
D	-3	HIS	-	expression tag	UNP Q9UXG1
D	-2	HIS	-	expression tag	UNP Q9UXG1
D	-1	HIS	-	expression tag	UNP Q9UXG1
D	0	HIS	-	expression tag	UNP Q9UXG1
D	1	MET	-	expression tag	UNP Q9UXG1
D	2	GLU	-	expression tag	UNP Q9UXG1
D	3	ILE	-	expression tag	UNP Q9UXG1
D	4	PRO	-	expression tag	UNP Q9UXG1
D	5	SER	-	expression tag	UNP Q9UXG1
D	6	LYS	-	expression tag	UNP Q9UXG1
E	-5	HIS	-	expression tag	UNP Q9UXG1
E	-4	HIS	-	expression tag	UNP Q9UXG1
E	-3	HIS	-	expression tag	UNP Q9UXG1
E	-2	HIS	-	expression tag	UNP Q9UXG1
E	-1	HIS	-	expression tag	UNP Q9UXG1
E	0	HIS	-	expression tag	UNP Q9UXG1
E	1	MET	-	expression tag	UNP Q9UXG1
E	2	GLU	-	expression tag	UNP Q9UXG1
E	3	ILE	-	expression tag	UNP Q9UXG1
E	4	PRO	-	expression tag	UNP Q9UXG1
E	5	SER	-	expression tag	UNP Q9UXG1
E	6	LYS	-	expression tag	UNP Q9UXG1

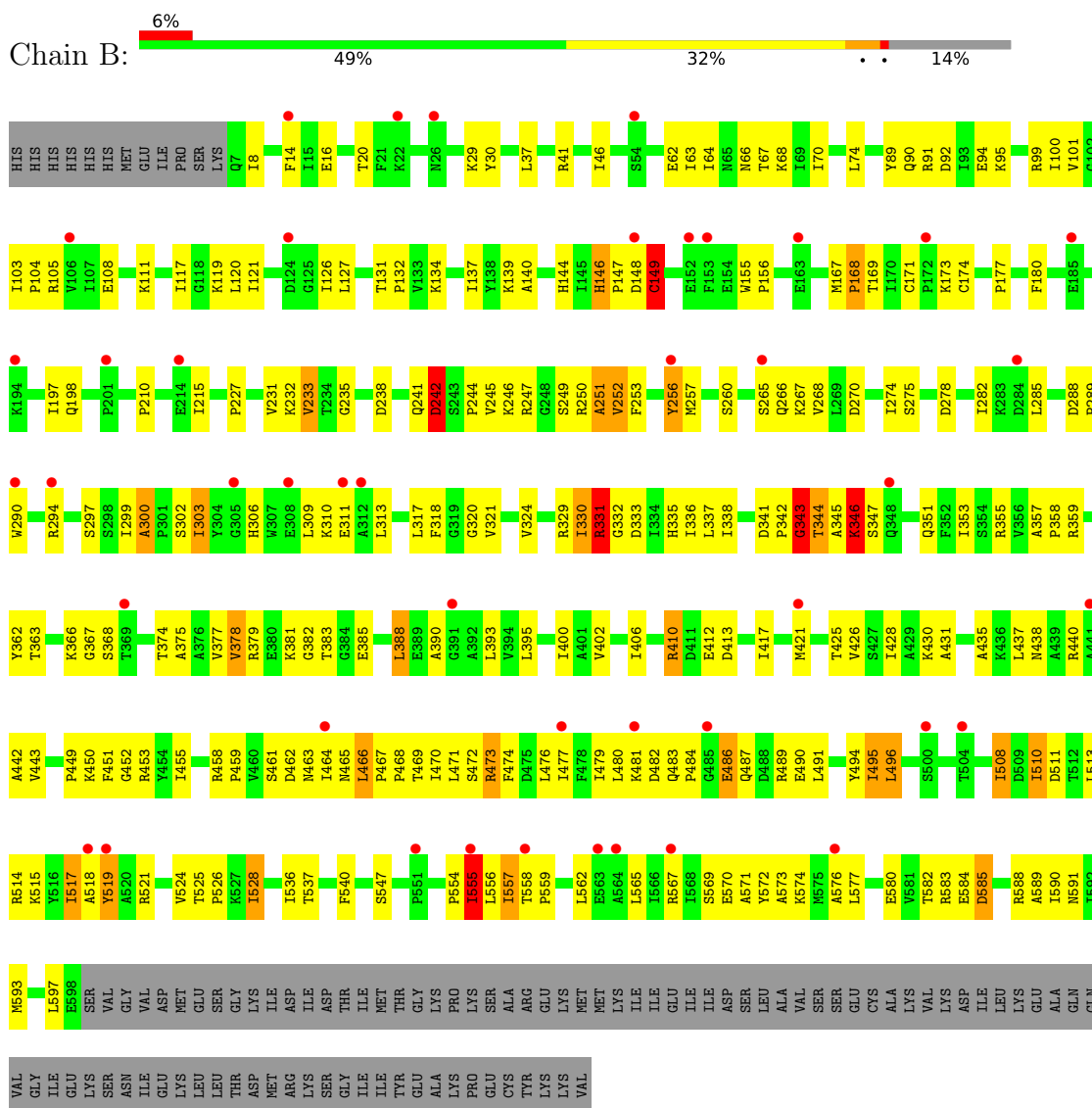
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0

3 Residue-property plots

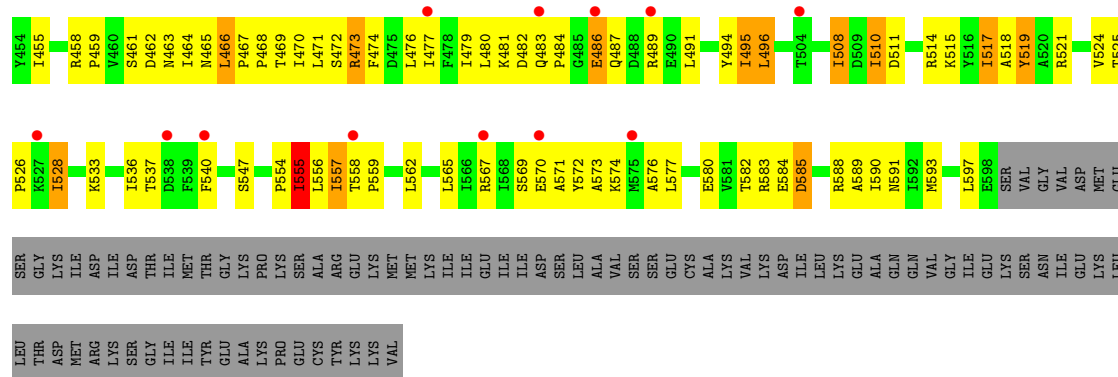
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

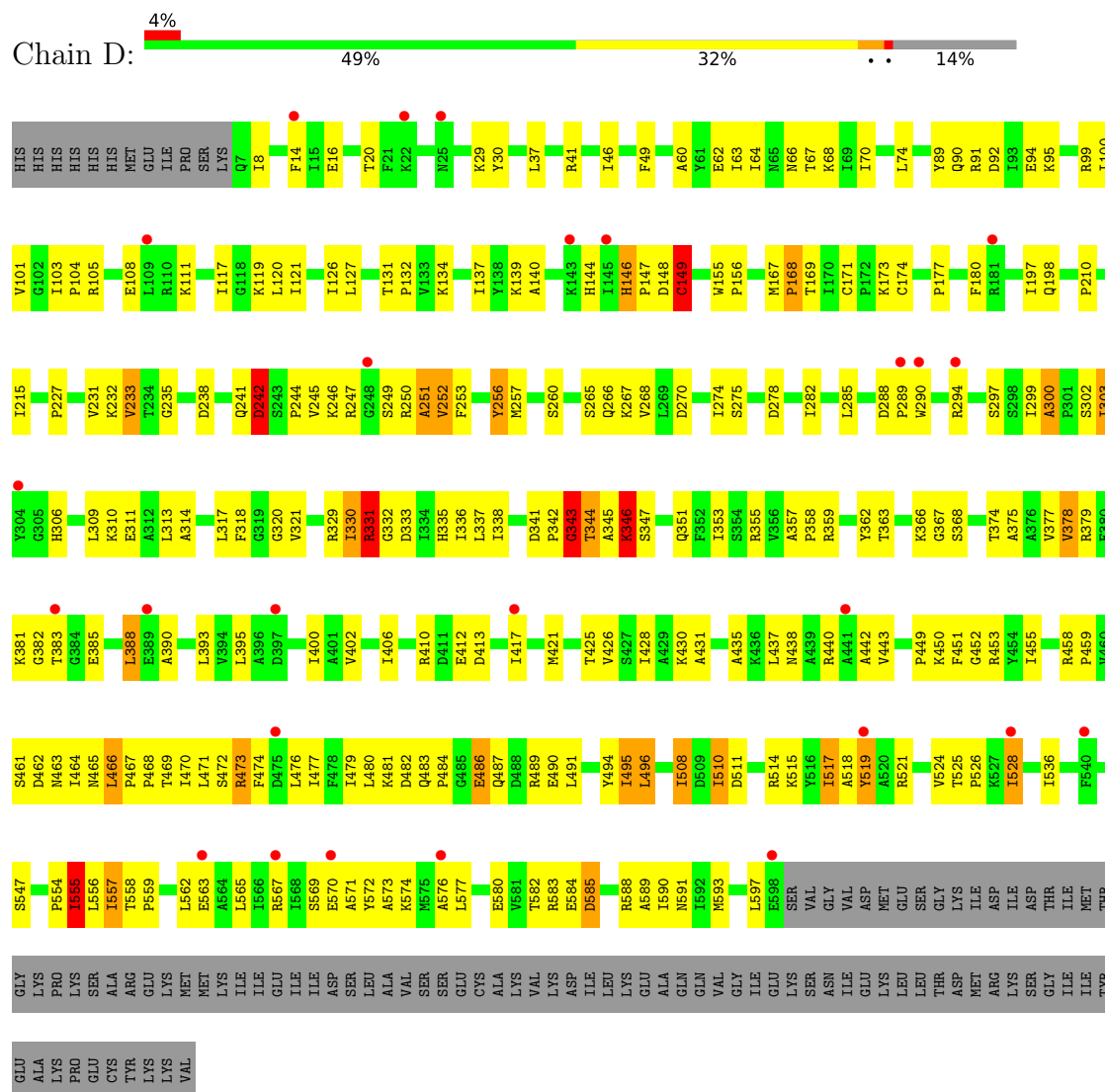


• Molecule 1: Minichromosome maintenance protein MCM





• Molecule 1: Minichromosome maintenance protein MCM



• Molecule 1: Minichromosome maintenance protein MCM



IIE	IIE	S547	D462	E380	H306	V231			HIS
MET	K381	K381	K463	K381	K306	V231		K111	HIS
TYR	I464	K382	I464	K382	L309	V233		I112	HIS
GLU	D552	D552	D465	T363	L309	V233		R113	HIS
ALA	S553	S553	L466	G384	K310	T234			HIS
LYS	P554	P554	P467	E385	E311	G235			HIS
PRO	F555	F555	P468		A312	I286		D116	HIS
LYS	F556	F556	P469		L313	L237		I117	MET
GLU	F557	F557	I470	L388	L317	D238		G118	GLU
TYR	A558	A558	I471	A390	F318	K119		L120	PRO
ARG	F559	F559	S472	L393	G319	I121		I121	SER
GLU			R473	L394	G320				SER
LYS	L562	L562	P474	L395	V321	I126		I126	LYS
MET	E563	E563	D475	V394	V245	L127		L127	Q7
MET	A564	A564	L476	L395	K246				I8
LYS	L565	L565	I477	I400	R247	T131		T131	V13
IIE	F566	F566	F478	A401	G248	P132		P132	F14
GLU	R567	R567	I479	V402	S249	V133		V133	F14
IIE	F568	F568	L480	I406	R250	K134		K134	K29
LYS	S569	S569	K481		A251				Y30
ASP	E570	E570	D482	D333	V252	F253		V252	Y29
SER	A571	A571	Q483	R410	I334			I137	L37
LEU	Y572	Y572	P484	D411	H335	Y138		Y138	L37
ALA	A573	A573	G485	E412	I336	K139		K139	R41
VAL	K574	K574	E486	D413	I337	A140		A140	R41
ASP	M575	M575	Q487	I417	I338				I46
SER	A576	A576	D488	I417	I339	H144		H144	I46
GLU	L577	L577	R489		S280	I145		I145	F49
CYS			F490	M421	D341	H146		H146	F49
ALA	E580	E580	L491		P342	S265		S265	A60
LYS	F581	F581	A492	T425	G343	Q266		D148	A60
VAL	T582	T582	M493	V426	T344	K267		G149	Y61
LYS	R583	R583	Y494	S427	N434	V268		E62	E62
ASP	E584	E584	I495	I428	A345	L269		I63	I63
ASP	L585	L585	L496	A429	K346	D270		P156	I64
IIE	D585	D585		K430	S347				N65
LEU						I274		M167	N65
LYS	R588	R588	I508	A431	Q351	S275		P168	T67
GLU	A589	A589	D609		F352	K68		K68	T67
ALA	T590	T590	I510	A435	I353	T169		I170	I69
GLN	N591	N591	D511	K436	R354	C171		C171	I70
GLN	F592	F592	L437	L437	R355	P172		P172	L74
VAL	M593	M593	R514	M438	V586	K173		C174	L74
GLY			K515	A439	A357				
IIE	L597	L597	Y516	R440	P358	D284			
GLU			I517	A441	R359				
LYS	SER	SER	A518	A442		D288		G178	Y89
SER	VAL	VAL	Y519	A442		P289		D92	R91
ASN	GLY	GLY	A520	V443	Y362	F180			I83
IIE	VAL	VAL	R521		T363			E185	E94
GLU	ASP	ASP	K450	P449	K366	R294			K95
LYS	MET	MET	F451	K450	G367	S297		T197	R99
LEU	GLU	GLU	T524	G452	S368	S296		Q198	I100
LEU	SER	SER	P526	R453		I299		P210	V101
THR	GLY	GLY	K527	Y454	L373	A300		I215	G102
LYS	I528	I528		L455	T374	I301			I103
ASP	IIE	IIE			A375	S302			G102
ARG	ASP	ASP	I536	R458	A376	I303			R105
LYS	IIE	IIE		P459	V377	I303			R105
GLY	THR	THR	F540	V460	V378	Y304		P227	F108
CYS	GLU	GLU		S461	R370	C255			F108

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	169.66Å 107.74Å 170.21Å 90.00° 107.89° 90.00°	Depositor
Resolution (Å)	47.58 – 4.10 47.58 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.58-4.10) 91.1 (47.58-4.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.7.2_863	Depositor
R, R_{free}	0.331 , 0.341 0.317 , 0.339	Depositor DCC
R_{free} test set	2009 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	142.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 158.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	23585	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7771e-03.*

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:
ZN

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	0.58	0/4796	0.62	0/6486
1	B	0.58	0/4796	0.61	0/6486
1	C	0.58	0/4796	0.62	0/6486
1	D	0.58	0/4796	0.62	0/6486
1	E	0.57	0/4796	0.62	0/6486
All	All	0.58	0/23980	0.62	0/32430

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
1	C	0	9
1	D	0	9
1	E	0	9
All	All	0	45

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	PRO	Peptide
1	A	242	ASP	Peptide
1	A	247	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	249	SER	Peptide
1	A	251	ALA	Peptide
1	A	300	ALA	Peptide
1	A	343	GLY	Peptide
1	A	381	LYS	Peptide
1	A	521	ARG	Peptide
1	B	168	PRO	Peptide
1	B	242	ASP	Peptide
1	B	247	ARG	Peptide
1	B	249	SER	Peptide
1	B	251	ALA	Peptide
1	B	300	ALA	Peptide
1	B	343	GLY	Peptide
1	B	381	LYS	Peptide
1	B	521	ARG	Peptide
1	C	168	PRO	Peptide
1	C	242	ASP	Peptide
1	C	247	ARG	Peptide
1	C	249	SER	Peptide
1	C	251	ALA	Peptide
1	C	300	ALA	Peptide
1	C	343	GLY	Peptide
1	C	381	LYS	Peptide
1	C	521	ARG	Peptide
1	D	168	PRO	Peptide
1	D	242	ASP	Peptide
1	D	247	ARG	Peptide
1	D	249	SER	Peptide
1	D	251	ALA	Peptide
1	D	300	ALA	Peptide
1	D	343	GLY	Peptide
1	D	381	LYS	Peptide
1	D	521	ARG	Peptide
1	E	168	PRO	Peptide
1	E	242	ASP	Peptide
1	E	247	ARG	Peptide
1	E	249	SER	Peptide
1	E	251	ALA	Peptide
1	E	300	ALA	Peptide
1	E	343	GLY	Peptide
1	E	381	LYS	Peptide
1	E	521	ARG	Peptide

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	4716	0	4865	227	0
1	B	4716	0	4865	228	0
1	C	4716	0	4865	228	0
1	D	4716	0	4865	228	0
1	E	4716	0	4865	227	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	23585	0	24325	1122	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 23.

All (1122) 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:547:SER:HB2	1:A:557:ILE:HD12	1.38	1.05
1:D:547:SER:HB2	1:D:557:ILE:HD12	1.38	1.04
1:C:547:SER:HB2	1:C:557:ILE:HD12	1.38	1.03
1:B:547:SER:HB2	1:B:557:ILE:HD12	1.38	1.02
1:E:547:SER:HB2	1:E:557:ILE:HD12	1.38	1.01
1:A:251:ALA:HB3	1:A:253:PHE:H	1.26	1.01
1:E:251:ALA:HB3	1:E:253:PHE:H	1.26	1.00
1:C:251:ALA:HB3	1:C:253:PHE:H	1.26	1.00
1:B:251:ALA:HB3	1:B:253:PHE:H	1.26	0.98
1:A:303:ILE:HG13	1:A:306:HIS:HE1	1.29	0.97
1:A:274:ILE:HG23	1:A:275:SER:H	1.30	0.96
1:D:251:ALA:HB3	1:D:253:PHE:H	1.26	0.96
1:D:274:ILE:HG23	1:D:275:SER:H	1.30	0.96
1:B:303:ILE:HG13	1:B:306:HIS:HE1	1.30	0.95
1:E:303:ILE:HG13	1:E:306:HIS:HE1	1.29	0.95
1:C:303:ILE:HG13	1:C:306:HIS:HE1	1.30	0.94
1:C:274:ILE:HG23	1:C:275:SER:H	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:HG23	1:B:275:SER:H	1.30	0.92
1:E:274:ILE:HG23	1:E:275:SER:H	1.30	0.92
1:D:303:ILE:HG13	1:D:306:HIS:HE1	1.30	0.92
1:D:303:ILE:HG13	1:D:306:HIS:CE1	2.05	0.92
1:C:303:ILE:HG13	1:C:306:HIS:CE1	2.05	0.92
1:B:303:ILE:HG13	1:B:306:HIS:CE1	2.05	0.91
1:E:303:ILE:HG13	1:E:306:HIS:CE1	2.05	0.91
1:A:303:ILE:HG13	1:A:306:HIS:CE1	2.05	0.91
1:A:547:SER:HB2	1:A:557:ILE:CD1	2.03	0.89
1:C:455:ILE:HG21	1:C:479:ILE:HG21	1.55	0.89
1:B:233:VAL:CG2	1:B:257:MET:HE1	2.04	0.88
1:E:455:ILE:HG21	1:E:479:ILE:HG21	1.55	0.88
1:E:233:VAL:CG2	1:E:257:MET:HE1	2.04	0.88
1:D:233:VAL:CG2	1:D:257:MET:HE1	2.04	0.88
1:E:547:SER:HB2	1:E:557:ILE:CD1	2.03	0.88
1:D:547:SER:HB2	1:D:557:ILE:CD1	2.03	0.88
1:B:547:SER:HB2	1:B:557:ILE:CD1	2.03	0.88
1:E:558:THR:HG22	1:E:558:THR:O	1.74	0.87
1:A:235:GLY:HA3	1:A:257:MET:HE3	1.56	0.87
1:C:251:ALA:HB3	1:C:253:PHE:N	1.89	0.87
1:B:235:GLY:HA3	1:B:257:MET:HE3	1.57	0.87
1:E:105:ARG:HD3	1:E:120:LEU:O	1.74	0.87
1:E:235:GLY:HA3	1:E:257:MET:HE3	1.57	0.87
1:E:251:ALA:HB3	1:E:253:PHE:N	1.88	0.87
1:A:455:ILE:HG21	1:A:479:ILE:HG21	1.55	0.87
1:B:455:ILE:HG21	1:B:479:ILE:HG21	1.55	0.87
1:C:233:VAL:CG2	1:C:257:MET:HE1	2.04	0.87
1:A:558:THR:HG22	1:A:558:THR:O	1.73	0.86
1:C:547:SER:HB2	1:C:557:ILE:CD1	2.03	0.86
1:A:233:VAL:CG2	1:A:257:MET:HE1	2.04	0.86
1:D:251:ALA:HB3	1:D:253:PHE:N	1.89	0.86
1:B:251:ALA:HB3	1:B:253:PHE:N	1.89	0.86
1:A:251:ALA:HB3	1:A:253:PHE:N	1.88	0.86
1:D:455:ILE:HG21	1:D:479:ILE:HG21	1.55	0.86
1:C:105:ARG:HD3	1:C:120:LEU:O	1.74	0.86
1:D:105:ARG:HD3	1:D:120:LEU:O	1.74	0.86
1:B:105:ARG:HD3	1:B:120:LEU:O	1.74	0.86
1:C:558:THR:HG22	1:C:558:THR:O	1.74	0.86
1:B:558:THR:O	1:B:558:THR:HG22	1.74	0.85
1:D:558:THR:O	1:D:558:THR:HG22	1.74	0.85
1:A:105:ARG:HD3	1:A:120:LEU:O	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:GLY:HA3	1:C:257:MET:HE3	1.57	0.85
1:D:235:GLY:HA3	1:D:257:MET:HE3	1.57	0.84
1:D:362:TYR:HD2	1:D:402:VAL:HG23	1.44	0.82
1:B:362:TYR:HD2	1:B:402:VAL:HG23	1.44	0.81
1:A:362:TYR:HD2	1:A:402:VAL:HG23	1.44	0.81
1:C:362:TYR:HD2	1:C:402:VAL:HG23	1.44	0.81
1:C:366:LYS:HG3	1:C:367:GLY:H	1.46	0.81
1:E:366:LYS:HG3	1:E:367:GLY:H	1.46	0.81
1:B:366:LYS:HG3	1:B:367:GLY:H	1.47	0.80
1:E:362:TYR:HD2	1:E:402:VAL:HG23	1.44	0.80
1:A:486:GLU:O	1:A:487:GLN:HG2	1.82	0.80
1:A:366:LYS:HG3	1:A:367:GLY:H	1.46	0.79
1:D:366:LYS:HG3	1:D:367:GLY:H	1.47	0.79
1:D:486:GLU:O	1:D:487:GLN:HG2	1.82	0.79
1:C:486:GLU:O	1:C:487:GLN:HG2	1.82	0.78
1:B:486:GLU:O	1:B:487:GLN:HG2	1.83	0.78
1:E:486:GLU:O	1:E:487:GLN:HG2	1.82	0.77
1:B:333:ASP:HB3	1:B:442:ALA:HB2	1.67	0.77
1:C:496:LEU:HD21	1:E:324:VAL:HG21	1.67	0.77
1:D:299:ILE:HD13	1:D:306:HIS:NE2	2.00	0.77
1:A:333:ASP:HB3	1:A:442:ALA:HB2	1.67	0.77
1:C:333:ASP:HB3	1:C:442:ALA:HB2	1.67	0.76
1:E:299:ILE:HD13	1:E:306:HIS:NE2	2.00	0.76
1:C:299:ILE:HD13	1:C:306:HIS:NE2	2.00	0.76
1:A:299:ILE:HD13	1:A:306:HIS:NE2	2.00	0.76
1:B:299:ILE:HD13	1:B:306:HIS:NE2	1.99	0.75
1:E:333:ASP:HB3	1:E:442:ALA:HB2	1.67	0.75
1:D:333:ASP:HB3	1:D:442:ALA:HB2	1.67	0.75
1:C:299:ILE:HD13	1:C:306:HIS:CD2	2.22	0.75
1:E:299:ILE:HD13	1:E:306:HIS:CD2	2.22	0.75
1:B:299:ILE:HD13	1:B:306:HIS:CD2	2.21	0.75
1:E:347:SER:HB2	1:E:351:GLN:HB2	1.69	0.75
1:B:347:SER:HB2	1:B:351:GLN:HB2	1.69	0.75
1:A:347:SER:HB2	1:A:351:GLN:HB2	1.69	0.75
1:A:537:THR:OG1	1:D:490:GLU:HG2	1.87	0.75
1:D:299:ILE:HD13	1:D:306:HIS:CD2	2.22	0.75
1:C:347:SER:HB2	1:C:351:GLN:HB2	1.69	0.74
1:D:347:SER:HB2	1:D:351:GLN:HB2	1.68	0.74
1:A:299:ILE:HD13	1:A:306:HIS:CD2	2.22	0.74
1:B:338:ILE:O	1:B:338:ILE:HG13	1.88	0.74
1:B:410:ARG:NE	1:B:412:GLU:OE2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:481:LYS:HE3	1:E:484:PRO:HD2	1.70	0.73
1:B:481:LYS:HE3	1:B:484:PRO:HD2	1.70	0.73
1:D:410:ARG:NE	1:D:412:GLU:OE2	2.21	0.73
1:A:481:LYS:HE3	1:A:484:PRO:HD2	1.70	0.73
1:C:338:ILE:O	1:C:338:ILE:HG13	1.88	0.73
1:E:410:ARG:NE	1:E:412:GLU:OE2	2.21	0.73
1:A:410:ARG:NE	1:A:412:GLU:OE2	2.21	0.73
1:C:481:LYS:HE3	1:C:484:PRO:HD2	1.70	0.73
1:D:481:LYS:HE3	1:D:484:PRO:HD2	1.70	0.73
1:B:525:THR:HG23	1:B:525:THR:O	1.90	0.72
1:E:338:ILE:HG13	1:E:338:ILE:O	1.88	0.72
1:C:525:THR:HG23	1:C:525:THR:O	1.90	0.72
1:A:338:ILE:O	1:A:338:ILE:HG13	1.88	0.72
1:D:338:ILE:HG13	1:D:338:ILE:O	1.88	0.72
1:B:233:VAL:CG2	1:B:257:MET:CE	2.68	0.72
1:C:410:ARG:NE	1:C:412:GLU:OE2	2.21	0.72
1:D:233:VAL:HG23	1:D:257:MET:HE1	1.72	0.72
1:A:525:THR:HG23	1:A:525:THR:O	1.90	0.71
1:D:233:VAL:CG2	1:D:257:MET:CE	2.68	0.71
1:D:366:LYS:HG3	1:D:367:GLY:N	2.05	0.71
1:B:366:LYS:HG3	1:B:367:GLY:N	2.05	0.71
1:D:525:THR:HG23	1:D:525:THR:O	1.90	0.71
1:E:233:VAL:CG2	1:E:257:MET:CE	2.68	0.71
1:C:366:LYS:HG3	1:C:367:GLY:N	2.04	0.71
1:B:303:ILE:CG1	1:B:306:HIS:HE1	2.03	0.71
1:E:233:VAL:HG23	1:E:257:MET:HE1	1.72	0.71
1:E:366:LYS:HG3	1:E:367:GLY:N	2.04	0.71
1:C:233:VAL:CG2	1:C:257:MET:CE	2.68	0.71
1:E:525:THR:O	1:E:525:THR:HG23	1.90	0.71
1:B:374:THR:HG21	1:B:426:VAL:HG11	1.73	0.71
1:A:366:LYS:HG3	1:A:367:GLY:N	2.04	0.71
1:C:235:GLY:HA3	1:C:257:MET:CE	2.21	0.70
1:B:233:VAL:HG23	1:B:257:MET:HE1	1.72	0.70
1:A:233:VAL:CG2	1:A:257:MET:CE	2.68	0.70
1:E:303:ILE:CG1	1:E:306:HIS:HE1	2.04	0.70
1:E:374:THR:HG21	1:E:426:VAL:HG11	1.73	0.70
1:A:235:GLY:HA3	1:A:257:MET:CE	2.21	0.70
1:C:233:VAL:HG23	1:C:257:MET:HE1	1.72	0.70
1:D:235:GLY:HA3	1:D:257:MET:CE	2.21	0.70
1:C:288:ASP:O	1:C:290:TRP:N	2.25	0.70
1:D:303:ILE:CG1	1:D:306:HIS:HE1	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLY:CA	1:A:257:MET:HE3	2.22	0.70
1:E:235:GLY:HA3	1:E:257:MET:CE	2.21	0.70
1:A:233:VAL:HG23	1:A:257:MET:HE1	1.72	0.69
1:B:235:GLY:HA3	1:B:257:MET:CE	2.21	0.69
1:D:374:THR:HG21	1:D:426:VAL:HG11	1.73	0.69
1:C:374:THR:HG21	1:C:426:VAL:HG11	1.73	0.69
1:B:288:ASP:O	1:B:290:TRP:N	2.24	0.69
1:A:303:ILE:CG1	1:A:306:HIS:HE1	2.04	0.69
1:A:374:THR:HG21	1:A:426:VAL:HG11	1.73	0.69
1:A:455:ILE:HG22	1:A:455:ILE:O	1.93	0.69
1:E:288:ASP:O	1:E:290:TRP:N	2.25	0.69
1:E:235:GLY:CA	1:E:257:MET:HE3	2.23	0.69
1:A:288:ASP:O	1:A:290:TRP:N	2.25	0.68
1:D:288:ASP:O	1:D:290:TRP:N	2.24	0.68
1:B:455:ILE:O	1:B:455:ILE:HG22	1.93	0.68
1:A:299:ILE:CD1	1:A:306:HIS:CD2	2.77	0.68
1:C:299:ILE:CD1	1:C:306:HIS:CD2	2.77	0.68
1:E:299:ILE:CD1	1:E:306:HIS:CD2	2.76	0.68
1:E:455:ILE:HG22	1:E:455:ILE:O	1.93	0.68
1:B:235:GLY:CA	1:B:257:MET:HE3	2.23	0.68
1:B:299:ILE:CD1	1:B:306:HIS:CD2	2.76	0.68
1:D:299:ILE:CD1	1:D:306:HIS:CD2	2.77	0.68
1:D:235:GLY:CA	1:D:257:MET:HE3	2.23	0.68
1:D:455:ILE:HG22	1:D:455:ILE:O	1.93	0.68
1:B:309:LEU:HG	1:B:313:LEU:HD13	1.77	0.67
1:D:105:ARG:NE	1:D:121:ILE:HG22	2.09	0.67
1:B:105:ARG:NE	1:B:121:ILE:HG22	2.10	0.67
1:B:320:GLY:HA3	1:B:572:TYR:CG	2.30	0.67
1:E:105:ARG:NE	1:E:121:ILE:HG22	2.10	0.67
1:C:388:LEU:HD21	1:C:428:ILE:HD13	1.76	0.67
1:C:105:ARG:NE	1:C:121:ILE:HG22	2.10	0.67
1:C:235:GLY:CA	1:C:257:MET:HE3	2.23	0.67
1:C:303:ILE:CG1	1:C:306:HIS:HE1	2.04	0.67
1:D:309:LEU:HG	1:D:313:LEU:HD13	1.77	0.67
1:A:388:LEU:HD21	1:A:428:ILE:HD13	1.76	0.67
1:D:343:GLY:HA2	1:D:344:THR:HB	1.77	0.67
1:D:388:LEU:HD21	1:D:428:ILE:HD13	1.77	0.67
1:E:168:PRO:HB2	1:E:169:THR:HA	1.77	0.67
1:E:343:GLY:HA2	1:E:344:THR:HB	1.77	0.67
1:A:337:LEU:HB2	1:A:474:PHE:CE1	2.31	0.66
1:C:455:ILE:HG22	1:C:455:ILE:O	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:LEU:HD21	1:E:428:ILE:HD13	1.76	0.66
1:C:320:GLY:HA3	1:C:572:TYR:CG	2.31	0.66
1:E:309:LEU:HG	1:E:313:LEU:HD13	1.77	0.66
1:B:388:LEU:HD21	1:B:428:ILE:HD13	1.76	0.66
1:A:105:ARG:NE	1:A:121:ILE:HG22	2.10	0.66
1:D:320:GLY:HA3	1:D:572:TYR:CG	2.30	0.66
1:E:320:GLY:HA3	1:E:572:TYR:CG	2.30	0.66
1:E:569:SER:O	1:E:573:ALA:N	2.29	0.66
1:A:569:SER:O	1:A:573:ALA:N	2.29	0.66
1:C:343:GLY:HA2	1:C:344:THR:HB	1.78	0.66
1:D:569:SER:O	1:D:573:ALA:N	2.28	0.66
1:C:168:PRO:HB2	1:C:169:THR:HA	1.77	0.66
1:C:337:LEU:HB2	1:C:474:PHE:CE1	2.31	0.66
1:C:331:ARG:HD2	1:C:565:LEU:HD21	1.78	0.66
1:C:309:LEU:HG	1:C:313:LEU:HD13	1.77	0.65
1:E:331:ARG:HD2	1:E:565:LEU:HD21	1.77	0.65
1:A:320:GLY:HA3	1:A:572:TYR:CG	2.31	0.65
1:C:569:SER:O	1:C:573:ALA:N	2.28	0.65
1:B:331:ARG:HD2	1:B:565:LEU:HD21	1.77	0.65
1:A:309:LEU:HG	1:A:313:LEU:HD13	1.77	0.65
1:B:267:LYS:HG3	1:B:268:VAL:H	1.62	0.65
1:B:343:GLY:HA2	1:B:344:THR:HB	1.77	0.65
1:B:569:SER:O	1:B:573:ALA:N	2.29	0.65
1:D:267:LYS:HG3	1:D:268:VAL:H	1.62	0.65
1:A:168:PRO:HB2	1:A:169:THR:HA	1.77	0.65
1:A:343:GLY:HA2	1:A:344:THR:HB	1.77	0.65
1:A:331:ARG:HD2	1:A:565:LEU:HD21	1.77	0.65
1:D:168:PRO:HB2	1:D:169:THR:HA	1.77	0.65
1:D:331:ARG:HD2	1:D:565:LEU:HD21	1.77	0.65
1:E:337:LEU:HB2	1:E:474:PHE:CE1	2.31	0.65
1:B:168:PRO:HB2	1:B:169:THR:HA	1.77	0.64
1:C:267:LYS:HG3	1:C:268:VAL:H	1.62	0.64
1:B:337:LEU:HB2	1:B:474:PHE:CE1	2.31	0.64
1:D:337:LEU:HB2	1:D:474:PHE:CE1	2.32	0.64
1:D:144:HIS:HB3	1:D:149:CYS:SG	2.37	0.64
1:E:144:HIS:HB3	1:E:149:CYS:SG	2.37	0.64
1:B:144:HIS:HB3	1:B:149:CYS:SG	2.38	0.64
1:E:267:LYS:HG3	1:E:268:VAL:H	1.62	0.64
1:A:144:HIS:HB3	1:A:149:CYS:SG	2.37	0.64
1:A:267:LYS:HG3	1:A:268:VAL:H	1.62	0.64
1:C:144:HIS:HB3	1:C:149:CYS:SG	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:558:THR:O	1:E:558:THR:CG2	2.46	0.64
1:A:570:GLU:HB3	1:A:589:ALA:CB	2.28	0.64
1:C:274:ILE:HG23	1:C:275:SER:N	2.09	0.64
1:A:274:ILE:HG23	1:A:275:SER:N	2.09	0.63
1:D:570:GLU:HB3	1:D:589:ALA:CB	2.28	0.63
1:B:570:GLU:HB3	1:B:589:ALA:CB	2.28	0.63
1:B:233:VAL:HG23	1:B:257:MET:CE	2.29	0.63
1:B:274:ILE:HG23	1:B:275:SER:N	2.09	0.63
1:C:233:VAL:HG23	1:C:257:MET:CE	2.29	0.63
1:E:274:ILE:HG23	1:E:275:SER:N	2.09	0.63
1:E:570:GLU:HB3	1:E:589:ALA:CB	2.29	0.63
1:D:517:ILE:HD11	1:D:577:LEU:HD12	1.81	0.63
1:B:366:LYS:CG	1:B:367:GLY:H	2.13	0.62
1:C:278:ASP:O	1:C:282:ILE:HG12	1.99	0.62
1:E:233:VAL:HG23	1:E:257:MET:CE	2.29	0.62
1:E:486:GLU:O	1:E:487:GLN:CG	2.47	0.62
1:C:570:GLU:HB3	1:C:589:ALA:CB	2.28	0.62
1:E:366:LYS:CG	1:E:367:GLY:H	2.12	0.62
1:C:517:ILE:HD11	1:C:577:LEU:HD12	1.81	0.62
1:D:278:ASP:O	1:D:282:ILE:HG12	1.99	0.62
1:B:486:GLU:O	1:B:487:GLN:CG	2.48	0.62
1:D:455:ILE:HG21	1:D:479:ILE:CG2	2.29	0.62
1:E:517:ILE:HD11	1:E:577:LEU:HD12	1.81	0.62
1:D:362:TYR:CD2	1:D:402:VAL:HG23	2.33	0.62
1:B:517:ILE:HD11	1:B:577:LEU:HD12	1.81	0.62
1:D:233:VAL:HG23	1:D:257:MET:CE	2.29	0.62
1:A:233:VAL:HG23	1:A:257:MET:CE	2.29	0.62
1:A:278:ASP:O	1:A:282:ILE:HG12	2.00	0.62
1:D:366:LYS:CG	1:D:367:GLY:H	2.13	0.62
1:C:486:GLU:O	1:C:487:GLN:CG	2.48	0.61
1:D:486:GLU:O	1:D:487:GLN:CG	2.47	0.61
1:B:278:ASP:O	1:B:282:ILE:HG12	2.00	0.61
1:E:278:ASP:O	1:E:282:ILE:HG12	1.99	0.61
1:A:455:ILE:HG21	1:A:479:ILE:CG2	2.29	0.61
1:A:486:GLU:O	1:A:487:GLN:CG	2.47	0.61
1:A:517:ILE:HD11	1:A:577:LEU:HD12	1.81	0.61
1:D:558:THR:O	1:D:558:THR:CG2	2.46	0.61
1:D:274:ILE:HG23	1:D:275:SER:N	2.09	0.60
1:B:362:TYR:CD2	1:B:402:VAL:HG23	2.33	0.60
1:B:455:ILE:HG21	1:B:479:ILE:CG2	2.29	0.60
1:B:558:THR:O	1:B:558:THR:CG2	2.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ILE:HG21	1:C:479:ILE:CG2	2.29	0.60
1:E:362:TYR:CD2	1:E:402:VAL:HG23	2.33	0.60
1:B:483:GLN:HB3	1:B:486:GLU:HG2	1.84	0.59
1:C:366:LYS:CG	1:C:367:GLY:H	2.12	0.59
1:E:303:ILE:O	1:E:489:ARG:NH1	2.35	0.59
1:B:282:ILE:O	1:B:285:LEU:HG	2.03	0.59
1:C:274:ILE:CG2	1:C:275:SER:H	2.11	0.59
1:D:483:GLN:HB3	1:D:486:GLU:HG2	1.85	0.59
1:B:324:VAL:HG21	1:A:496:LEU:HD21	1.84	0.59
1:A:558:THR:O	1:A:558:THR:CG2	2.46	0.59
1:E:483:GLN:HB3	1:E:486:GLU:HG2	1.85	0.59
1:A:366:LYS:CG	1:A:367:GLY:H	2.12	0.59
1:A:483:GLN:HB3	1:A:486:GLU:HG2	1.85	0.59
1:A:537:THR:OG1	1:D:490:GLU:CG	2.51	0.59
1:C:362:TYR:CD2	1:C:402:VAL:HG23	2.33	0.59
1:C:282:ILE:O	1:C:285:LEU:HG	2.03	0.59
1:D:282:ILE:O	1:D:285:LEU:HG	2.03	0.59
1:A:274:ILE:CG2	1:A:275:SER:H	2.12	0.59
1:A:215:ILE:HG22	1:A:257:MET:HB3	1.85	0.58
1:D:303:ILE:O	1:D:489:ARG:NH1	2.35	0.58
1:A:282:ILE:O	1:A:285:LEU:HG	2.03	0.58
1:E:282:ILE:O	1:E:285:LEU:HG	2.03	0.58
1:B:303:ILE:O	1:B:489:ARG:NH1	2.36	0.58
1:C:215:ILE:HG22	1:C:257:MET:HB3	1.85	0.58
1:C:486:GLU:C	1:C:487:GLN:HG2	2.29	0.58
1:D:215:ILE:HG22	1:D:257:MET:HB3	1.85	0.58
1:C:483:GLN:HB3	1:C:486:GLU:HG2	1.85	0.58
1:E:413:ASP:O	1:E:417:ILE:HD12	2.03	0.58
1:E:215:ILE:HG22	1:E:257:MET:HB3	1.85	0.58
1:A:303:ILE:O	1:A:489:ARG:NH1	2.35	0.58
1:A:486:GLU:C	1:A:487:GLN:HG2	2.29	0.58
1:C:251:ALA:CB	1:C:253:PHE:H	2.11	0.58
1:C:303:ILE:O	1:C:489:ARG:NH1	2.36	0.58
1:B:413:ASP:O	1:B:417:ILE:HD12	2.03	0.58
1:E:486:GLU:C	1:E:487:GLN:HG2	2.29	0.58
1:B:215:ILE:HG22	1:B:257:MET:HB3	1.85	0.57
1:A:362:TYR:CD2	1:A:402:VAL:HG23	2.33	0.57
1:D:486:GLU:C	1:D:487:GLN:HG2	2.29	0.57
1:D:494:TYR:O	1:D:495:ILE:C	2.47	0.57
1:B:251:ALA:HB3	1:B:252:VAL:CA	2.34	0.57
1:B:486:GLU:C	1:B:487:GLN:HG2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HH12	1:A:119:LYS:HD3	1.70	0.57
1:A:494:TYR:O	1:A:495:ILE:C	2.47	0.57
1:D:251:ALA:HB3	1:D:252:VAL:CA	2.35	0.57
1:D:413:ASP:O	1:D:417:ILE:HD12	2.03	0.57
1:E:105:ARG:HH12	1:E:119:LYS:HD3	1.70	0.57
1:A:251:ALA:HB3	1:A:252:VAL:CA	2.34	0.57
1:A:413:ASP:O	1:A:417:ILE:HD12	2.03	0.57
1:C:413:ASP:O	1:C:417:ILE:HD12	2.03	0.57
1:E:494:TYR:O	1:E:495:ILE:C	2.47	0.57
1:C:251:ALA:HB3	1:C:252:VAL:CA	2.35	0.57
1:E:251:ALA:HB3	1:E:252:VAL:CA	2.34	0.57
1:B:105:ARG:HH12	1:B:119:LYS:HD3	1.69	0.57
1:E:483:GLN:N	1:E:484:PRO:HD3	2.19	0.57
1:B:483:GLN:N	1:B:484:PRO:HD3	2.19	0.56
1:C:105:ARG:HH12	1:C:119:LYS:HD3	1.69	0.56
1:C:558:THR:N	1:C:559:PRO:HD3	2.20	0.56
1:C:574:LYS:CG	1:C:585:ASP:HB3	2.35	0.56
1:A:483:GLN:N	1:A:484:PRO:HD3	2.20	0.56
1:C:494:TYR:O	1:C:495:ILE:C	2.48	0.56
1:D:483:GLN:N	1:D:484:PRO:HD3	2.20	0.56
1:D:558:THR:N	1:D:559:PRO:HD3	2.20	0.56
1:E:455:ILE:HG21	1:E:479:ILE:CG2	2.29	0.56
1:E:558:THR:N	1:E:559:PRO:HD3	2.20	0.56
1:B:558:THR:N	1:B:559:PRO:HD3	2.20	0.56
1:A:558:THR:N	1:A:559:PRO:HD3	2.20	0.56
1:A:574:LYS:CG	1:A:585:ASP:HB3	2.36	0.56
1:D:245:VAL:HG22	1:D:246:LYS:H	1.71	0.56
1:A:455:ILE:O	1:A:455:ILE:CG2	2.54	0.56
1:C:496:LEU:HD21	1:E:324:VAL:CG2	2.35	0.56
1:E:574:LYS:CG	1:E:585:ASP:HB3	2.36	0.56
1:B:358:PRO:O	1:B:359:ARG:C	2.49	0.56
1:B:494:TYR:O	1:B:495:ILE:C	2.48	0.56
1:C:483:GLN:N	1:C:484:PRO:HD3	2.20	0.56
1:D:105:ARG:HH12	1:D:119:LYS:HD3	1.69	0.56
1:D:574:LYS:CG	1:D:585:ASP:HB3	2.36	0.56
1:A:453:ARG:HD2	1:A:482:ASP:CG	2.32	0.55
1:C:455:ILE:O	1:C:455:ILE:CG2	2.54	0.55
1:E:358:PRO:O	1:E:359:ARG:C	2.50	0.55
1:C:342:PRO:O	1:C:343:GLY:C	2.50	0.55
1:B:574:LYS:CG	1:B:585:ASP:HB3	2.36	0.55
1:A:466:LEU:HB2	1:A:467:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ARG:HD2	1:C:482:ASP:CG	2.32	0.55
1:E:342:PRO:O	1:E:343:GLY:C	2.50	0.55
1:A:245:VAL:HG22	1:A:246:LYS:H	1.71	0.55
1:D:358:PRO:O	1:D:359:ARG:C	2.48	0.55
1:C:245:VAL:HG22	1:C:246:LYS:H	1.71	0.55
1:D:466:LEU:HB2	1:D:467:PRO:HD3	1.89	0.55
1:B:342:PRO:O	1:B:343:GLY:C	2.50	0.55
1:A:469:THR:O	1:A:472:SER:N	2.40	0.55
1:D:469:THR:O	1:D:472:SER:N	2.40	0.55
1:E:274:ILE:CG2	1:E:275:SER:H	2.12	0.55
1:E:455:ILE:O	1:E:455:ILE:CG2	2.54	0.55
1:A:342:PRO:O	1:A:343:GLY:C	2.49	0.55
1:D:169:THR:HB	1:D:177:PRO:HB3	1.89	0.55
1:D:251:ALA:HB3	1:D:252:VAL:HA	1.89	0.55
1:D:342:PRO:O	1:D:343:GLY:C	2.50	0.55
1:E:169:THR:HB	1:E:177:PRO:HB3	1.89	0.55
1:B:455:ILE:O	1:B:455:ILE:CG2	2.54	0.55
1:A:245:VAL:HG22	1:A:246:LYS:N	2.22	0.55
1:B:169:THR:HB	1:B:177:PRO:HB3	1.89	0.54
1:B:90:GLN:HG3	1:B:91:ARG:N	2.23	0.54
1:B:496:LEU:HD21	1:C:324:VAL:HG21	1.89	0.54
1:C:358:PRO:O	1:C:359:ARG:C	2.50	0.54
1:D:343:GLY:CA	1:D:344:THR:HB	2.38	0.54
1:D:455:ILE:O	1:D:455:ILE:CG2	2.54	0.54
1:D:481:LYS:HG2	1:D:483:GLN:H	1.72	0.54
1:E:245:VAL:HG22	1:E:246:LYS:H	1.71	0.54
1:B:245:VAL:HG22	1:B:246:LYS:N	2.22	0.54
1:A:358:PRO:O	1:A:359:ARG:C	2.50	0.54
1:D:245:VAL:HG22	1:D:246:LYS:N	2.22	0.54
1:D:251:ALA:CB	1:D:253:PHE:H	2.11	0.54
1:D:570:GLU:HB3	1:D:589:ALA:HB3	1.89	0.54
1:E:90:GLN:HG3	1:E:91:ARG:N	2.23	0.54
1:E:245:VAL:HG22	1:E:246:LYS:N	2.23	0.54
1:E:251:ALA:CB	1:E:253:PHE:N	2.68	0.54
1:E:343:GLY:CA	1:E:344:THR:HB	2.38	0.54
1:C:251:ALA:HB3	1:C:252:VAL:HA	1.89	0.54
1:E:455:ILE:CG2	1:E:479:ILE:HG21	2.34	0.54
1:B:251:ALA:HB3	1:B:252:VAL:HA	1.88	0.54
1:B:453:ARG:HD2	1:B:482:ASP:CG	2.32	0.54
1:C:90:GLN:HG3	1:C:91:ARG:N	2.23	0.54
1:C:169:THR:HB	1:C:177:PRO:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:LEU:HB2	1:C:467:PRO:HD3	1.89	0.54
1:E:251:ALA:HB3	1:E:252:VAL:HA	1.89	0.54
1:B:245:VAL:HG22	1:B:246:LYS:H	1.71	0.54
1:B:481:LYS:HG2	1:B:483:GLN:H	1.72	0.54
1:D:90:GLN:HG3	1:D:91:ARG:N	2.23	0.54
1:E:453:ARG:HD2	1:E:482:ASP:CG	2.33	0.54
1:A:481:LYS:HG2	1:A:483:GLN:H	1.72	0.54
1:A:570:GLU:HB3	1:A:589:ALA:HB3	1.89	0.54
1:E:466:LEU:HB2	1:E:467:PRO:HD3	1.89	0.54
1:A:251:ALA:HB3	1:A:252:VAL:HA	1.89	0.54
1:E:536:ILE:HD12	1:E:567:ARG:CD	2.38	0.54
1:B:343:GLY:CA	1:B:344:THR:HB	2.38	0.53
1:B:466:LEU:HB2	1:B:467:PRO:HD3	1.89	0.53
1:C:297:SER:HA	1:C:508:ILE:CG2	2.39	0.53
1:A:343:GLY:CA	1:A:344:THR:HB	2.38	0.53
1:C:168:PRO:HG3	1:C:180:PHE:CG	2.44	0.53
1:E:297:SER:HA	1:E:508:ILE:CG2	2.39	0.53
1:B:536:ILE:HD12	1:B:567:ARG:CD	2.38	0.53
1:A:90:GLN:HG3	1:A:91:ARG:N	2.23	0.53
1:A:297:SER:HA	1:A:508:ILE:CG2	2.38	0.53
1:A:536:ILE:HD12	1:A:567:ARG:CD	2.38	0.53
1:C:245:VAL:HG22	1:C:246:LYS:N	2.23	0.53
1:D:453:ARG:HD2	1:D:482:ASP:CG	2.33	0.53
1:D:536:ILE:HD12	1:D:567:ARG:CD	2.38	0.53
1:E:168:PRO:HG3	1:E:180:PHE:CG	2.44	0.53
1:B:168:PRO:HG3	1:B:180:PHE:CG	2.44	0.53
1:B:251:ALA:CB	1:B:253:PHE:H	2.10	0.53
1:A:168:PRO:HG3	1:A:180:PHE:CG	2.44	0.53
1:A:251:ALA:CB	1:A:253:PHE:N	2.69	0.53
1:C:366:LYS:CG	1:C:367:GLY:N	2.71	0.53
1:E:481:LYS:HG2	1:E:483:GLN:H	1.72	0.53
1:C:481:LYS:HG2	1:C:483:GLN:H	1.72	0.53
1:C:536:ILE:HD12	1:C:567:ARG:CD	2.38	0.53
1:B:570:GLU:HB3	1:B:589:ALA:HB3	1.89	0.53
1:A:139:LYS:HG2	1:A:156:PRO:HG2	1.91	0.53
1:B:297:SER:HA	1:B:508:ILE:CG2	2.39	0.53
1:B:357:ALA:HA	1:B:519:TYR:CD2	2.44	0.53
1:A:536:ILE:HD12	1:A:567:ARG:HD2	1.91	0.53
1:C:469:THR:O	1:C:472:SER:N	2.40	0.53
1:B:536:ILE:HD12	1:B:567:ARG:HD2	1.91	0.53
1:A:169:THR:HB	1:A:177:PRO:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:SER:HA	1:D:508:ILE:CG2	2.39	0.53
1:E:139:LYS:HG2	1:E:156:PRO:HG2	1.91	0.53
1:B:274:ILE:CG2	1:B:275:SER:H	2.12	0.52
1:A:41:ARG:HH12	1:A:89:TYR:HA	1.74	0.52
1:C:570:GLU:HB3	1:C:589:ALA:HB3	1.89	0.52
1:D:274:ILE:CG2	1:D:275:SER:H	2.11	0.52
1:E:357:ALA:HA	1:E:519:TYR:CD2	2.44	0.52
1:E:469:THR:O	1:E:472:SER:N	2.40	0.52
1:E:536:ILE:HD12	1:E:567:ARG:HD2	1.91	0.52
1:D:168:PRO:HG3	1:D:180:PHE:CG	2.44	0.52
1:C:343:GLY:CA	1:C:344:THR:HB	2.38	0.52
1:C:574:LYS:HG3	1:C:585:ASP:HB3	1.92	0.52
1:D:241:GLN:HG3	1:D:242:ASP:N	2.25	0.52
1:B:41:ARG:HH12	1:B:89:TYR:HA	1.74	0.52
1:B:139:LYS:HG2	1:B:156:PRO:HG2	1.91	0.52
1:A:455:ILE:CG2	1:A:479:ILE:HG21	2.34	0.52
1:A:470:ILE:HA	1:A:473:ARG:HG3	1.92	0.52
1:D:536:ILE:HD12	1:D:567:ARG:HD2	1.91	0.52
1:B:168:PRO:HG3	1:B:180:PHE:CD2	2.45	0.52
1:C:41:ARG:HH12	1:C:89:TYR:HA	1.74	0.52
1:D:168:PRO:HG3	1:D:180:PHE:CD2	2.45	0.52
1:B:438:ASN:HD21	1:B:440:ARG:HG2	1.75	0.52
1:C:115:THR:HA	1:E:185:GLU:O	2.09	0.52
1:C:241:GLN:HG3	1:C:242:ASP:N	2.25	0.52
1:E:570:GLU:HB3	1:E:589:ALA:HB3	1.89	0.52
1:E:168:PRO:HG3	1:E:180:PHE:CD2	2.45	0.52
1:E:438:ASN:HD21	1:E:440:ARG:CG	2.23	0.52
1:B:241:GLN:HG3	1:B:242:ASP:N	2.25	0.51
1:B:470:ILE:HA	1:B:473:ARG:HG3	1.92	0.51
1:B:574:LYS:HG3	1:B:585:ASP:HB3	1.92	0.51
1:C:251:ALA:CB	1:C:253:PHE:N	2.69	0.51
1:B:438:ASN:HD21	1:B:440:ARG:CG	2.23	0.51
1:A:458:ARG:HD3	1:A:459:PRO:HD2	1.92	0.51
1:C:168:PRO:HG3	1:C:180:PHE:CD2	2.45	0.51
1:C:357:ALA:HA	1:C:519:TYR:CD2	2.45	0.51
1:C:438:ASN:HD21	1:C:440:ARG:HG2	1.75	0.51
1:C:536:ILE:HD12	1:C:567:ARG:HD2	1.91	0.51
1:C:558:THR:O	1:C:558:THR:CG2	2.46	0.51
1:D:438:ASN:HD21	1:D:440:ARG:HG2	1.76	0.51
1:E:41:ARG:HH12	1:E:89:TYR:HA	1.74	0.51
1:E:574:LYS:HG3	1:E:585:ASP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:ILE:CG2	1:D:479:ILE:HG21	2.34	0.51
1:B:388:LEU:CD2	1:B:428:ILE:HD13	2.40	0.51
1:A:357:ALA:HA	1:A:519:TYR:CD2	2.45	0.51
1:A:438:ASN:HD21	1:A:440:ARG:HG2	1.76	0.51
1:A:168:PRO:HG3	1:A:180:PHE:CD2	2.45	0.51
1:A:383:THR:HG22	1:A:383:THR:O	2.11	0.51
1:C:438:ASN:HD21	1:C:440:ARG:CG	2.23	0.51
1:D:357:ALA:HA	1:D:519:TYR:CD2	2.45	0.51
1:D:438:ASN:HD21	1:D:440:ARG:CG	2.24	0.51
1:B:455:ILE:CG2	1:B:479:ILE:HG21	2.34	0.51
1:E:241:GLN:HG3	1:E:242:ASP:N	2.26	0.51
1:A:417:ILE:CG2	1:A:421:MET:HE2	2.41	0.51
1:D:139:LYS:HG2	1:D:156:PRO:HG2	1.91	0.51
1:E:458:ARG:HD3	1:E:459:PRO:HD2	1.92	0.51
1:B:469:THR:O	1:B:472:SER:N	2.40	0.51
1:D:41:ARG:HH12	1:D:89:TYR:HA	1.74	0.51
1:A:134:LYS:NZ	1:A:385:GLU:OE1	2.44	0.51
1:C:139:LYS:HG2	1:C:156:PRO:HG2	1.91	0.51
1:D:297:SER:HA	1:D:508:ILE:HG23	1.93	0.51
1:E:297:SER:HA	1:E:508:ILE:HG23	1.93	0.51
1:B:458:ARG:HD3	1:B:459:PRO:HD2	1.93	0.51
1:D:517:ILE:HD11	1:D:577:LEU:CD1	2.41	0.51
1:E:388:LEU:CD2	1:E:428:ILE:HD13	2.40	0.51
1:B:417:ILE:CG2	1:B:421:MET:HE2	2.41	0.50
1:A:517:ILE:HD11	1:A:577:LEU:CD1	2.41	0.50
1:C:321:VAL:HG13	1:C:330:ILE:HG21	1.93	0.50
1:D:134:LYS:NZ	1:D:385:GLU:OE1	2.44	0.50
1:E:417:ILE:CG2	1:E:421:MET:HE2	2.41	0.50
1:B:517:ILE:HD11	1:B:577:LEU:CD1	2.42	0.50
1:A:345:ALA:O	1:A:346:LYS:C	2.54	0.50
1:C:297:SER:HA	1:C:508:ILE:HG23	1.93	0.50
1:D:470:ILE:HA	1:D:473:ARG:HG3	1.92	0.50
1:E:464:ILE:HG12	1:E:464:ILE:O	2.12	0.50
1:B:168:PRO:CB	1:B:169:THR:HA	2.42	0.50
1:A:574:LYS:HG3	1:A:585:ASP:HB3	1.92	0.50
1:C:383:THR:O	1:C:383:THR:HG22	2.11	0.50
1:E:383:THR:O	1:E:383:THR:HG22	2.11	0.50
1:E:517:ILE:HD11	1:E:577:LEU:CD1	2.41	0.50
1:C:388:LEU:CD2	1:C:428:ILE:HD13	2.40	0.50
1:E:227:PRO:HG2	1:E:437:LEU:HD11	1.94	0.50
1:E:438:ASN:HD21	1:E:440:ARG:HG2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:SER:HA	1:B:508:ILE:HG23	1.93	0.50
1:A:470:ILE:HD12	1:A:470:ILE:H	1.77	0.50
1:D:227:PRO:HG2	1:D:437:LEU:HD11	1.94	0.50
1:D:321:VAL:HG13	1:D:330:ILE:HG21	1.93	0.50
1:D:458:ARG:HD3	1:D:459:PRO:HD2	1.93	0.50
1:E:470:ILE:HA	1:E:473:ARG:HG3	1.92	0.50
1:A:241:GLN:HG3	1:A:242:ASP:N	2.26	0.50
1:C:313:LEU:HD12	1:C:336:ILE:HD12	1.94	0.50
1:C:458:ARG:HD3	1:C:459:PRO:HD2	1.93	0.50
1:C:470:ILE:HA	1:C:473:ARG:HG3	1.92	0.50
1:B:299:ILE:CD1	1:B:306:HIS:HD2	2.25	0.50
1:B:383:THR:HG22	1:B:383:THR:O	2.11	0.50
1:C:168:PRO:CB	1:C:169:THR:HA	2.42	0.50
1:D:417:ILE:CG2	1:D:421:MET:HE2	2.41	0.50
1:D:574:LYS:HG3	1:D:585:ASP:HB3	1.92	0.50
1:B:134:LYS:NZ	1:B:385:GLU:OE1	2.44	0.50
1:B:345:ALA:O	1:B:346:LYS:C	2.55	0.50
1:B:464:ILE:HG12	1:B:464:ILE:O	2.11	0.50
1:A:438:ASN:HD21	1:A:440:ARG:CG	2.24	0.50
1:C:417:ILE:CG2	1:C:421:MET:HE2	2.41	0.50
1:D:470:ILE:HD12	1:D:470:ILE:H	1.77	0.50
1:B:470:ILE:HD12	1:B:470:ILE:H	1.77	0.49
1:D:464:ILE:HG12	1:D:464:ILE:O	2.12	0.49
1:B:313:LEU:HD12	1:B:336:ILE:HD12	1.94	0.49
1:C:464:ILE:HG12	1:C:464:ILE:O	2.11	0.49
1:A:321:VAL:HG13	1:A:330:ILE:HG21	1.94	0.49
1:E:321:VAL:HG13	1:E:330:ILE:HG21	1.93	0.49
1:E:345:ALA:O	1:E:346:LYS:C	2.54	0.49
1:A:297:SER:HA	1:A:508:ILE:HG23	1.93	0.49
1:E:470:ILE:HD12	1:E:470:ILE:H	1.77	0.49
1:A:227:PRO:HG2	1:A:437:LEU:HD11	1.94	0.49
1:E:251:ALA:CB	1:E:253:PHE:H	2.11	0.49
1:E:313:LEU:HD12	1:E:336:ILE:HD12	1.94	0.49
1:B:366:LYS:CG	1:B:367:GLY:N	2.71	0.49
1:A:313:LEU:HD12	1:A:336:ILE:HD12	1.94	0.49
1:A:464:ILE:HG12	1:A:464:ILE:O	2.12	0.49
1:C:227:PRO:HG2	1:C:437:LEU:HD11	1.94	0.49
1:D:345:ALA:O	1:D:346:LYS:C	2.55	0.49
1:D:168:PRO:CB	1:D:169:THR:HA	2.41	0.49
1:D:388:LEU:CD2	1:D:428:ILE:HD13	2.40	0.49
1:A:388:LEU:CD2	1:A:428:ILE:HD13	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LYS:O	1:C:30:TYR:HB2	2.13	0.49
1:C:167:MET:CB	1:C:168:PRO:HD2	2.43	0.49
1:E:556:LEU:O	1:E:557:ILE:HB	2.13	0.49
1:B:167:MET:CB	1:B:168:PRO:HD2	2.43	0.49
1:B:251:ALA:CB	1:B:253:PHE:N	2.68	0.49
1:A:167:MET:CB	1:A:168:PRO:HD2	2.43	0.49
1:D:383:THR:HG22	1:D:383:THR:O	2.11	0.49
1:E:515:LYS:HA	1:E:519:TYR:CD2	2.48	0.49
1:B:148:ASP:O	1:B:174:CYS:CB	2.61	0.49
1:B:227:PRO:HG2	1:B:437:LEU:HD11	1.94	0.49
1:C:299:ILE:CD1	1:C:306:HIS:HD2	2.25	0.49
1:C:310:LYS:HG3	1:C:311:GLU:N	2.28	0.49
1:C:345:ALA:O	1:C:346:LYS:C	2.54	0.49
1:C:517:ILE:HD11	1:C:577:LEU:CD1	2.42	0.49
1:E:41:ARG:NH1	1:E:89:TYR:HA	2.28	0.49
1:E:168:PRO:CB	1:E:169:THR:HA	2.42	0.49
1:B:41:ARG:NH1	1:B:89:TYR:HA	2.28	0.48
1:B:556:LEU:O	1:B:557:ILE:HB	2.13	0.48
1:A:41:ARG:NH1	1:A:89:TYR:HA	2.28	0.48
1:E:134:LYS:NZ	1:E:385:GLU:OE1	2.44	0.48
1:E:148:ASP:O	1:E:174:CYS:CB	2.61	0.48
1:C:515:LYS:HA	1:C:519:TYR:CD2	2.48	0.48
1:E:167:MET:CB	1:E:168:PRO:HD2	2.43	0.48
1:E:593:MET:O	1:E:597:LEU:HG	2.13	0.48
1:B:29:LYS:O	1:B:30:TYR:HB2	2.13	0.48
1:B:321:VAL:HG13	1:B:330:ILE:HG21	1.94	0.48
1:A:593:MET:O	1:A:597:LEU:HG	2.13	0.48
1:D:41:ARG:NH1	1:D:89:TYR:HA	2.29	0.48
1:B:515:LYS:HA	1:B:519:TYR:CD2	2.48	0.48
1:A:29:LYS:O	1:A:30:TYR:HB2	2.13	0.48
1:A:515:LYS:HA	1:A:519:TYR:CD2	2.48	0.48
1:C:470:ILE:H	1:C:470:ILE:HD12	1.78	0.48
1:C:491:LEU:O	1:C:495:ILE:HG13	2.14	0.48
1:D:310:LYS:HG3	1:D:311:GLU:N	2.29	0.48
1:D:491:LEU:O	1:D:495:ILE:HG13	2.14	0.48
1:E:29:LYS:O	1:E:30:TYR:HB2	2.13	0.48
1:B:593:MET:O	1:B:597:LEU:HG	2.13	0.48
1:A:148:ASP:O	1:A:174:CYS:CB	2.61	0.48
1:A:491:LEU:O	1:A:495:ILE:HG13	2.14	0.48
1:D:100:ILE:HG22	1:D:103:ILE:HG23	1.96	0.48
1:D:515:LYS:HA	1:D:519:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LYS:HG3	1:E:311:GLU:N	2.29	0.48
1:B:310:LYS:HG3	1:B:311:GLU:N	2.29	0.48
1:C:148:ASP:O	1:C:174:CYS:CB	2.62	0.48
1:D:148:ASP:O	1:D:174:CYS:CB	2.61	0.48
1:D:167:MET:CB	1:D:168:PRO:HD2	2.43	0.48
1:D:426:VAL:HB	1:D:437:LEU:HB2	1.96	0.48
1:E:491:LEU:O	1:E:495:ILE:HG13	2.14	0.48
1:A:556:LEU:O	1:A:557:ILE:HB	2.13	0.48
1:B:63:ILE:O	1:B:67:THR:N	2.46	0.48
1:A:168:PRO:CB	1:A:169:THR:HA	2.42	0.48
1:D:131:THR:HB	1:D:132:PRO:HD2	1.96	0.48
1:D:374:THR:HG21	1:D:426:VAL:CG1	2.44	0.48
1:B:426:VAL:HB	1:B:437:LEU:HB2	1.96	0.47
1:C:574:LYS:HG3	1:C:585:ASP:OD1	2.14	0.47
1:E:63:ILE:O	1:E:67:THR:N	2.47	0.47
1:B:450:LYS:HG3	1:B:451:PHE:H	1.79	0.47
1:B:574:LYS:HG3	1:B:585:ASP:OD1	2.14	0.47
1:A:63:ILE:O	1:A:67:THR:N	2.47	0.47
1:A:310:LYS:HG3	1:A:311:GLU:N	2.29	0.47
1:C:63:ILE:O	1:C:67:THR:N	2.48	0.47
1:C:593:MET:O	1:C:597:LEU:HG	2.13	0.47
1:D:251:ALA:CB	1:D:253:PHE:N	2.69	0.47
1:B:490:GLU:OE2	1:C:533:LYS:HD2	2.14	0.47
1:B:491:LEU:O	1:B:495:ILE:HG13	2.14	0.47
1:C:134:LYS:NZ	1:C:385:GLU:OE1	2.44	0.47
1:A:574:LYS:HG3	1:A:585:ASP:OD1	2.14	0.47
1:C:450:LYS:HG3	1:C:451:PHE:H	1.79	0.47
1:C:556:LEU:O	1:C:557:ILE:HB	2.13	0.47
1:D:593:MET:O	1:D:597:LEU:HG	2.13	0.47
1:A:131:THR:HB	1:A:132:PRO:HD2	1.96	0.47
1:A:450:LYS:HG3	1:A:451:PHE:H	1.79	0.47
1:E:450:LYS:HG3	1:E:451:PHE:H	1.79	0.47
1:B:358:PRO:HD3	1:B:519:TYR:CB	2.45	0.47
1:C:355:ARG:CD	1:C:362:TYR:HB2	2.45	0.47
1:D:313:LEU:HD12	1:D:336:ILE:HD12	1.94	0.47
1:D:430:LYS:O	1:D:431:ALA:HB3	2.15	0.47
1:E:167:MET:HB3	1:E:168:PRO:HD2	1.97	0.47
1:E:355:ARG:CD	1:E:362:TYR:HB2	2.45	0.47
1:E:428:ILE:HG22	1:E:435:ALA:O	2.15	0.47
1:E:430:LYS:O	1:E:431:ALA:HB3	2.15	0.47
1:B:428:ILE:HG22	1:B:435:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ARG:NH1	1:C:89:TYR:HA	2.29	0.47
1:C:100:ILE:HG22	1:C:103:ILE:HG23	1.96	0.47
1:C:131:THR:HB	1:C:132:PRO:HD2	1.96	0.47
1:D:29:LYS:O	1:D:30:TYR:HB2	2.13	0.47
1:D:428:ILE:HG22	1:D:435:ALA:O	2.15	0.47
1:D:556:LEU:O	1:D:557:ILE:HB	2.13	0.47
1:E:299:ILE:CD1	1:E:306:HIS:HD2	2.25	0.47
1:E:426:VAL:HB	1:E:437:LEU:HB2	1.96	0.47
1:E:467:PRO:HB3	1:E:470:ILE:HB	1.97	0.47
1:C:167:MET:HB3	1:C:168:PRO:HD2	1.96	0.47
1:D:241:GLN:HG3	1:D:242:ASP:H	1.80	0.47
1:B:62:GLU:O	1:B:66:ASN:HB2	2.15	0.47
1:B:131:THR:HB	1:B:132:PRO:HD2	1.96	0.47
1:B:355:ARG:CD	1:B:362:TYR:HB2	2.44	0.47
1:A:167:MET:HB3	1:A:168:PRO:HD2	1.96	0.47
1:A:430:LYS:O	1:A:431:ALA:HB3	2.15	0.47
1:E:358:PRO:HD3	1:E:519:TYR:CB	2.45	0.47
1:A:16:GLU:O	1:A:20:THR:OG1	2.23	0.47
1:C:317:LEU:HD23	1:C:400:ILE:CD1	2.45	0.47
1:C:358:PRO:HD3	1:C:519:TYR:CB	2.45	0.47
1:D:62:GLU:O	1:D:66:ASN:HB2	2.15	0.47
1:E:241:GLN:HB2	1:E:244:PRO:HG3	1.97	0.47
1:E:317:LEU:HD23	1:E:400:ILE:CD1	2.45	0.47
1:A:355:ARG:CD	1:A:362:TYR:HB2	2.45	0.46
1:C:14:PHE:CD1	1:C:74:LEU:HD22	2.51	0.46
1:C:197:ILE:HD11	1:C:233:VAL:HG11	1.97	0.46
1:D:362:TYR:HA	1:D:402:VAL:HG23	1.98	0.46
1:B:100:ILE:HG22	1:B:103:ILE:HG23	1.96	0.46
1:B:430:LYS:O	1:B:431:ALA:HB3	2.15	0.46
1:D:167:MET:HB3	1:D:168:PRO:HD2	1.96	0.46
1:E:362:TYR:HA	1:E:402:VAL:HG23	1.98	0.46
1:E:526:PRO:HA	1:E:580:GLU:HA	1.97	0.46
1:B:241:GLN:HB2	1:B:244:PRO:HG3	1.98	0.46
1:B:362:TYR:HA	1:B:402:VAL:HG23	1.98	0.46
1:A:14:PHE:CD1	1:A:74:LEU:HD22	2.50	0.46
1:A:358:PRO:HD3	1:A:519:TYR:CB	2.46	0.46
1:A:426:VAL:HB	1:A:437:LEU:HB2	1.96	0.46
1:D:63:ILE:O	1:D:67:THR:N	2.47	0.46
1:D:363:THR:HG23	1:D:363:THR:O	2.15	0.46
1:B:167:MET:HB3	1:B:168:PRO:HD2	1.97	0.46
1:A:251:ALA:CB	1:A:253:PHE:H	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:THR:HG21	1:D:490:GLU:HB2	1.97	0.46
1:C:428:ILE:HG22	1:C:435:ALA:O	2.15	0.46
1:D:317:LEU:HD23	1:D:400:ILE:CD1	2.46	0.46
1:D:355:ARG:CD	1:D:362:TYR:HB2	2.45	0.46
1:E:330:ILE:HG22	1:E:332:GLY:H	1.81	0.46
1:B:317:LEU:HD23	1:B:400:ILE:CD1	2.45	0.46
1:A:197:ILE:HD11	1:A:233:VAL:HG11	1.97	0.46
1:A:241:GLN:HB2	1:A:244:PRO:HG3	1.97	0.46
1:A:428:ILE:HG22	1:A:435:ALA:O	2.15	0.46
1:C:430:LYS:O	1:C:431:ALA:HB3	2.15	0.46
1:D:467:PRO:HB3	1:D:470:ILE:HB	1.97	0.46
1:E:574:LYS:HG3	1:E:585:ASP:OD1	2.15	0.46
1:B:363:THR:HG23	1:B:363:THR:O	2.16	0.46
1:A:100:ILE:HG22	1:A:103:ILE:HG23	1.96	0.46
1:A:241:GLN:HG3	1:A:242:ASP:H	1.81	0.46
1:C:241:GLN:HG3	1:C:242:ASP:H	1.81	0.46
1:C:330:ILE:HG22	1:C:332:GLY:H	1.81	0.46
1:C:341:ASP:N	1:C:341:ASP:OD1	2.49	0.46
1:C:526:PRO:HA	1:C:580:GLU:HA	1.97	0.46
1:E:62:GLU:O	1:E:66:ASN:HB2	2.15	0.46
1:E:131:THR:HB	1:E:132:PRO:HD2	1.96	0.46
1:E:197:ILE:HD11	1:E:233:VAL:HG11	1.97	0.46
1:B:197:ILE:HD11	1:B:233:VAL:HG11	1.97	0.46
1:B:525:THR:O	1:B:525:THR:CG2	2.61	0.46
1:A:238:ASP:N	1:A:256:TYR:O	2.49	0.46
1:C:455:ILE:CG2	1:C:479:ILE:HG21	2.34	0.46
1:D:197:ILE:HD11	1:D:233:VAL:HG11	1.97	0.46
1:D:450:LYS:HG3	1:D:451:PHE:H	1.79	0.46
1:D:526:PRO:HA	1:D:580:GLU:HA	1.98	0.46
1:E:100:ILE:HG22	1:E:103:ILE:HG23	1.97	0.46
1:E:137:ILE:HG21	1:E:140:ALA:HB2	1.98	0.46
1:B:241:GLN:HG3	1:B:242:ASP:H	1.80	0.46
1:A:299:ILE:CD1	1:A:306:HIS:HD2	2.25	0.46
1:A:526:PRO:HA	1:A:580:GLU:HA	1.98	0.46
1:C:426:VAL:HB	1:C:437:LEU:HB2	1.97	0.46
1:C:583:ARG:HG3	1:C:584:GLU:N	2.31	0.46
1:D:14:PHE:CD1	1:D:74:LEU:HD22	2.51	0.46
1:D:461:SER:C	1:D:463:ASN:H	2.24	0.46
1:C:62:GLU:O	1:C:66:ASN:HB2	2.15	0.46
1:D:358:PRO:HD3	1:D:519:TYR:CB	2.46	0.46
1:D:574:LYS:HG3	1:D:585:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HG22	1:A:332:GLY:H	1.81	0.46
1:E:267:LYS:CG	1:E:268:VAL:H	2.29	0.46
1:B:146:HIS:CG	1:B:147:PRO:HD2	2.51	0.45
1:B:238:ASP:N	1:B:256:TYR:O	2.49	0.45
1:B:526:PRO:HA	1:B:580:GLU:HA	1.97	0.45
1:D:238:ASP:N	1:D:256:TYR:O	2.50	0.45
1:B:14:PHE:CD1	1:B:74:LEU:HD22	2.51	0.45
1:B:467:PRO:HB3	1:B:470:ILE:HB	1.97	0.45
1:A:62:GLU:O	1:A:66:ASN:HB2	2.15	0.45
1:A:341:ASP:OD1	1:A:341:ASP:N	2.48	0.45
1:A:362:TYR:HA	1:A:402:VAL:HG23	1.98	0.45
1:D:146:HIS:CG	1:D:147:PRO:HD2	2.51	0.45
1:E:363:THR:HG23	1:E:363:THR:O	2.16	0.45
1:B:374:THR:HG21	1:B:426:VAL:CG1	2.44	0.45
1:A:317:LEU:HD23	1:A:400:ILE:CD1	2.45	0.45
1:A:583:ARG:HG3	1:A:584:GLU:N	2.31	0.45
1:E:303:ILE:CG1	1:E:306:HIS:CE1	2.88	0.45
1:B:253:PHE:CE1	1:C:184:PRO:HB3	2.51	0.45
1:A:467:PRO:HB3	1:A:470:ILE:HB	1.98	0.45
1:C:241:GLN:HB2	1:C:244:PRO:HG3	1.98	0.45
1:D:241:GLN:HB2	1:D:244:PRO:HG3	1.98	0.45
1:B:90:GLN:HG3	1:B:91:ARG:H	1.82	0.45
1:B:341:ASP:OD1	1:B:341:ASP:N	2.48	0.45
1:A:363:THR:HG23	1:A:363:THR:O	2.16	0.45
1:A:574:LYS:HE2	1:A:588:ARG:CD	2.47	0.45
1:E:146:HIS:CG	1:E:147:PRO:HD2	2.51	0.45
1:E:341:ASP:OD1	1:E:341:ASP:N	2.49	0.45
1:E:574:LYS:C	1:E:576:ALA:H	2.24	0.45
1:A:146:HIS:CG	1:A:147:PRO:HD2	2.52	0.45
1:A:337:LEU:HB3	1:A:477:ILE:HG12	1.99	0.45
1:A:574:LYS:C	1:A:576:ALA:H	2.25	0.45
1:E:299:ILE:HD11	1:E:310:LYS:HD2	1.99	0.45
1:C:299:ILE:HD11	1:C:310:LYS:HD2	1.98	0.45
1:D:299:ILE:HD11	1:D:310:LYS:HD2	1.98	0.45
1:D:554:PRO:O	1:D:555:ILE:HG22	2.17	0.45
1:D:574:LYS:HE2	1:D:588:ARG:CD	2.47	0.45
1:E:14:PHE:CD1	1:E:74:LEU:HD22	2.51	0.45
1:E:574:LYS:HE2	1:E:588:ARG:CD	2.47	0.45
1:B:330:ILE:HG22	1:B:332:GLY:H	1.81	0.45
1:A:37:LEU:C	1:A:37:LEU:HD23	2.42	0.45
1:C:362:TYR:HA	1:C:402:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:THR:O	1:C:363:THR:HG23	2.16	0.45
1:C:467:PRO:HB3	1:C:470:ILE:HB	1.97	0.45
1:C:528:ILE:HG22	1:C:582:THR:OG1	2.17	0.45
1:C:574:LYS:HE2	1:C:588:ARG:CD	2.47	0.45
1:D:137:ILE:HG21	1:D:140:ALA:HB2	1.98	0.45
1:D:341:ASP:OD1	1:D:341:ASP:N	2.49	0.45
1:E:144:HIS:CB	1:E:149:CYS:SG	3.05	0.45
1:B:461:SER:C	1:B:463:ASN:H	2.24	0.45
1:B:583:ARG:HG3	1:B:584:GLU:N	2.32	0.45
1:A:554:PRO:O	1:A:555:ILE:HG22	2.17	0.45
1:C:137:ILE:HG21	1:C:140:ALA:HB2	1.98	0.45
1:C:330:ILE:C	1:C:332:GLY:N	2.75	0.45
1:D:528:ILE:HG22	1:D:582:THR:OG1	2.17	0.45
1:E:137:ILE:N	1:E:137:ILE:HD12	2.32	0.45
1:B:528:ILE:HG22	1:B:582:THR:OG1	2.17	0.45
1:A:299:ILE:HD11	1:A:310:LYS:HD2	1.98	0.45
1:C:238:ASP:N	1:C:256:TYR:O	2.49	0.45
1:D:337:LEU:HB3	1:D:477:ILE:HG12	1.99	0.45
1:B:137:ILE:HG21	1:B:140:ALA:HB2	1.98	0.44
1:B:250:ARG:O	1:B:250:ARG:HG3	2.17	0.44
1:A:461:SER:C	1:A:463:ASN:H	2.25	0.44
1:C:37:LEU:C	1:C:37:LEU:HD23	2.42	0.44
1:C:574:LYS:C	1:C:576:ALA:H	2.25	0.44
1:D:297:SER:OG	1:D:508:ILE:O	2.32	0.44
1:E:330:ILE:C	1:E:332:GLY:N	2.75	0.44
1:E:337:LEU:HB3	1:E:477:ILE:HG12	1.99	0.44
1:E:528:ILE:HG22	1:E:582:THR:OG1	2.17	0.44
1:E:557:ILE:C	1:E:559:PRO:HD3	2.43	0.44
1:E:583:ARG:HG3	1:E:584:GLU:N	2.32	0.44
1:B:299:ILE:HD11	1:B:310:LYS:HD2	1.98	0.44
1:B:574:LYS:HE2	1:B:588:ARG:CD	2.46	0.44
1:C:417:ILE:HG22	1:C:421:MET:HE2	2.00	0.44
1:C:461:SER:C	1:C:463:ASN:H	2.25	0.44
1:D:574:LYS:C	1:D:576:ALA:H	2.24	0.44
1:E:318:PHE:CE1	1:E:518:ALA:HB1	2.53	0.44
1:A:198:GLN:HE21	1:A:210:PRO:CG	2.31	0.44
1:C:137:ILE:N	1:C:137:ILE:HD12	2.32	0.44
1:C:146:HIS:CG	1:C:147:PRO:HD2	2.52	0.44
1:C:250:ARG:HG3	1:C:250:ARG:O	2.17	0.44
1:C:525:THR:O	1:C:525:THR:CG2	2.61	0.44
1:D:417:ILE:HG22	1:D:421:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:528:ILE:HG23	1:E:571:ALA:HB1	2.00	0.44
1:B:341:ASP:HB2	1:B:342:PRO:HD2	1.99	0.44
1:B:378:VAL:O	1:B:379:ARG:C	2.61	0.44
1:A:528:ILE:HG22	1:A:582:THR:OG1	2.18	0.44
1:A:567:ARG:HH22	1:D:494:TYR:HA	1.82	0.44
1:C:465:ASN:O	1:C:466:LEU:C	2.61	0.44
1:D:250:ARG:O	1:D:250:ARG:HG3	2.18	0.44
1:E:37:LEU:HD23	1:E:37:LEU:C	2.42	0.44
1:E:238:ASP:N	1:E:256:TYR:O	2.50	0.44
1:E:341:ASP:HB2	1:E:342:PRO:HD2	1.99	0.44
1:B:574:LYS:C	1:B:576:ALA:H	2.24	0.44
1:A:137:ILE:HG21	1:A:140:ALA:HB2	1.98	0.44
1:A:465:ASN:O	1:A:466:LEU:C	2.61	0.44
1:C:148:ASP:O	1:C:174:CYS:HB3	2.18	0.44
1:C:557:ILE:C	1:C:559:PRO:HD3	2.43	0.44
1:D:37:LEU:C	1:D:37:LEU:HD23	2.42	0.44
1:D:148:ASP:O	1:D:174:CYS:HB3	2.18	0.44
1:D:583:ARG:HG3	1:D:584:GLU:N	2.31	0.44
1:E:554:PRO:O	1:E:555:ILE:HG22	2.17	0.44
1:B:148:ASP:O	1:B:174:CYS:HB3	2.18	0.44
1:B:557:ILE:C	1:B:559:PRO:HD3	2.42	0.44
1:A:250:ARG:O	1:A:250:ARG:HG3	2.18	0.44
1:A:417:ILE:HG22	1:A:421:MET:HE2	1.99	0.44
1:A:528:ILE:HG23	1:A:571:ALA:HB1	2.00	0.44
1:A:557:ILE:C	1:A:559:PRO:HD3	2.43	0.44
1:C:90:GLN:HG3	1:C:91:ARG:H	1.82	0.44
1:D:198:GLN:HE21	1:D:210:PRO:CG	2.31	0.44
1:D:330:ILE:C	1:D:332:GLY:N	2.75	0.44
1:D:378:VAL:O	1:D:379:ARG:C	2.61	0.44
1:E:90:GLN:HG3	1:E:91:ARG:H	1.82	0.44
1:E:148:ASP:O	1:E:174:CYS:HB3	2.18	0.44
1:E:241:GLN:HG3	1:E:242:ASP:H	1.81	0.44
1:B:37:LEU:HD23	1:B:37:LEU:C	2.42	0.44
1:B:303:ILE:CG1	1:B:306:HIS:CE1	2.87	0.44
1:C:496:LEU:HD21	1:E:324:VAL:CB	2.47	0.44
1:B:528:ILE:HG23	1:B:571:ALA:HB1	2.00	0.44
1:A:233:VAL:HG21	1:A:257:MET:CE	2.48	0.44
1:A:330:ILE:C	1:A:332:GLY:N	2.75	0.44
1:A:341:ASP:HB2	1:A:342:PRO:HD2	1.99	0.44
1:C:318:PHE:CE1	1:C:518:ALA:HB1	2.53	0.44
1:C:337:LEU:HB3	1:C:477:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:THR:HG21	1:C:426:VAL:CG1	2.44	0.44
1:E:250:ARG:HG3	1:E:250:ARG:O	2.18	0.44
1:E:465:ASN:O	1:E:466:LEU:C	2.61	0.44
1:A:137:ILE:N	1:A:137:ILE:HD12	2.32	0.44
1:C:198:GLN:HE21	1:C:210:PRO:CG	2.31	0.44
1:E:374:THR:HG21	1:E:426:VAL:CG1	2.44	0.44
1:B:554:PRO:O	1:B:555:ILE:HG22	2.17	0.43
1:A:318:PHE:CE1	1:A:518:ALA:HB1	2.53	0.43
1:A:324:VAL:HG11	1:D:496:LEU:HD21	2.00	0.43
1:C:321:VAL:HA	1:C:330:ILE:HG23	2.00	0.43
1:D:528:ILE:HG23	1:D:571:ALA:HB1	2.00	0.43
1:D:557:ILE:C	1:D:559:PRO:HD3	2.43	0.43
1:E:198:GLN:HE21	1:E:210:PRO:CG	2.31	0.43
1:A:148:ASP:O	1:A:174:CYS:HB3	2.18	0.43
1:A:374:THR:HG21	1:A:426:VAL:CG1	2.44	0.43
1:C:554:PRO:O	1:C:555:ILE:HG22	2.17	0.43
1:D:90:GLN:HG3	1:D:91:ARG:H	1.82	0.43
1:D:233:VAL:HG21	1:D:257:MET:CE	2.48	0.43
1:D:341:ASP:HB2	1:D:342:PRO:HD2	1.99	0.43
1:E:105:ARG:CZ	1:E:121:ILE:HG22	2.48	0.43
1:B:198:GLN:HE21	1:B:210:PRO:CG	2.31	0.43
1:B:318:PHE:CE1	1:B:518:ALA:HB1	2.53	0.43
1:B:337:LEU:HB3	1:B:477:ILE:HG12	1.99	0.43
1:B:417:ILE:HG22	1:B:421:MET:HE2	2.00	0.43
1:C:321:VAL:O	1:C:321:VAL:HG12	2.19	0.43
1:C:341:ASP:HB2	1:C:342:PRO:HD2	1.99	0.43
1:D:318:PHE:CE1	1:D:518:ALA:HB1	2.52	0.43
1:D:330:ILE:HG22	1:D:332:GLY:H	1.81	0.43
1:E:378:VAL:O	1:E:379:ARG:C	2.61	0.43
1:E:590:ILE:HG13	1:E:591:ASN:N	2.34	0.43
1:B:137:ILE:HD12	1:B:137:ILE:N	2.32	0.43
1:B:344:THR:O	1:B:344:THR:HG22	2.18	0.43
1:B:590:ILE:HG13	1:B:591:ASN:N	2.33	0.43
1:A:290:TRP:HZ3	1:A:576:ALA:HB1	1.84	0.43
1:B:330:ILE:C	1:B:332:GLY:N	2.76	0.43
1:C:344:THR:HG22	1:C:344:THR:O	2.19	0.43
1:D:137:ILE:HD12	1:D:137:ILE:N	2.33	0.43
1:E:321:VAL:HA	1:E:330:ILE:HG23	2.01	0.43
1:B:290:TRP:HZ3	1:B:576:ALA:HB1	1.84	0.43
1:C:105:ARG:CZ	1:C:121:ILE:HG22	2.48	0.43
1:D:105:ARG:CZ	1:D:121:ILE:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:LYS:CG	1:D:367:GLY:N	2.71	0.43
1:E:417:ILE:HG22	1:E:421:MET:HE2	2.00	0.43
1:E:461:SER:C	1:E:463:ASN:H	2.25	0.43
1:A:321:VAL:HA	1:A:330:ILE:HG23	2.01	0.43
1:D:321:VAL:HA	1:D:330:ILE:HG23	2.00	0.43
1:D:465:ASN:O	1:D:466:LEU:C	2.61	0.43
1:E:321:VAL:HG12	1:E:321:VAL:O	2.18	0.43
1:B:450:LYS:HG3	1:B:451:PHE:N	2.34	0.43
1:A:99:ARG:HG2	1:A:260:SER:O	2.19	0.43
1:A:105:ARG:CZ	1:A:121:ILE:HG22	2.48	0.43
1:A:450:LYS:HG3	1:A:451:PHE:N	2.34	0.43
1:C:329:ARG:O	1:C:329:ARG:HG3	2.19	0.43
1:D:450:LYS:HG3	1:D:451:PHE:N	2.34	0.43
1:B:16:GLU:O	1:B:20:THR:OG1	2.23	0.43
1:B:105:ARG:CZ	1:B:121:ILE:HG22	2.48	0.43
1:B:253:PHE:CZ	1:C:184:PRO:HB3	2.54	0.43
1:A:90:GLN:HG3	1:A:91:ARG:H	1.82	0.43
1:C:103:ILE:HB	1:C:104:PRO:HD2	2.01	0.43
1:D:105:ARG:HG3	1:D:105:ARG:O	2.19	0.43
1:E:290:TRP:HZ3	1:E:576:ALA:HB1	1.83	0.43
1:B:99:ARG:HG2	1:B:260:SER:O	2.19	0.43
1:B:321:VAL:HA	1:B:330:ILE:HG23	2.01	0.43
1:A:90:GLN:C	1:A:92:ASP:H	2.27	0.43
1:A:108:GLU:OE2	1:A:111:LYS:HD2	2.19	0.43
1:A:378:VAL:O	1:A:379:ARG:C	2.61	0.43
1:C:108:GLU:OE2	1:C:111:LYS:HD2	2.19	0.43
1:D:299:ILE:CD1	1:D:306:HIS:HD2	2.25	0.43
1:D:590:ILE:HG13	1:D:591:ASN:N	2.34	0.43
1:E:105:ARG:O	1:E:105:ARG:HG3	2.19	0.43
1:E:233:VAL:HG21	1:E:257:MET:CE	2.48	0.43
1:E:450:LYS:HG3	1:E:451:PHE:N	2.34	0.43
1:B:382:GLY:O	1:B:383:THR:HB	2.19	0.42
1:A:321:VAL:HG12	1:A:321:VAL:O	2.19	0.42
1:C:450:LYS:HG3	1:C:451:PHE:N	2.34	0.42
1:C:528:ILE:HG23	1:C:571:ALA:HB1	2.00	0.42
1:C:590:ILE:HG13	1:C:591:ASN:N	2.33	0.42
1:D:126:ILE:HG21	1:D:395:LEU:HD22	2.01	0.42
1:B:103:ILE:HB	1:B:104:PRO:HD2	2.01	0.42
1:B:155:TRP:HB3	1:B:156:PRO:HD3	2.01	0.42
1:A:126:ILE:HG21	1:A:395:LEU:HD22	2.01	0.42
1:C:290:TRP:CZ2	1:C:517:ILE:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ILE:HG21	1:E:395:LEU:HD22	2.01	0.42
1:B:126:ILE:HG21	1:B:395:LEU:HD22	2.00	0.42
1:B:144:HIS:CB	1:B:149:CYS:SG	3.05	0.42
1:C:393:LEU:HD11	1:C:443:VAL:HG22	2.02	0.42
1:D:344:THR:O	1:D:344:THR:HG22	2.19	0.42
1:E:99:ARG:HG2	1:E:260:SER:O	2.19	0.42
1:E:374:THR:OG1	1:E:390:ALA:HB2	2.19	0.42
1:E:382:GLY:O	1:E:383:THR:HB	2.19	0.42
1:B:321:VAL:O	1:B:321:VAL:HG12	2.19	0.42
1:B:465:ASN:O	1:B:466:LEU:C	2.61	0.42
1:A:155:TRP:HB3	1:A:156:PRO:HD3	2.01	0.42
1:C:378:VAL:O	1:C:379:ARG:C	2.61	0.42
1:C:382:GLY:O	1:C:383:THR:HB	2.19	0.42
1:D:99:ARG:HG2	1:D:260:SER:O	2.19	0.42
1:D:103:ILE:HB	1:D:104:PRO:HD2	2.01	0.42
1:D:155:TRP:HB3	1:D:156:PRO:HD3	2.01	0.42
1:E:90:GLN:C	1:E:92:ASP:H	2.27	0.42
1:E:346:LYS:CG	1:E:347:SER:H	2.32	0.42
1:B:374:THR:OG1	1:B:390:ALA:HB2	2.19	0.42
1:A:346:LYS:HA	1:A:480:LEU:HD11	2.01	0.42
1:A:537:THR:CG2	1:D:490:GLU:HB2	2.50	0.42
1:C:99:ARG:HG2	1:C:260:SER:O	2.19	0.42
1:C:105:ARG:O	1:C:105:ARG:HG3	2.19	0.42
1:C:126:ILE:HG21	1:C:395:LEU:HD22	2.01	0.42
1:C:290:TRP:HZ3	1:C:576:ALA:HB1	1.84	0.42
1:D:238:ASP:HB3	1:D:256:TYR:HB3	2.02	0.42
1:E:329:ARG:O	1:E:329:ARG:HG3	2.20	0.42
1:E:362:TYR:HA	1:E:402:VAL:CG2	2.50	0.42
1:B:346:LYS:HA	1:B:480:LEU:HD11	2.01	0.42
1:A:393:LEU:HD11	1:A:443:VAL:HG22	2.02	0.42
1:C:265:SER:O	1:C:266:GLN:HB3	2.20	0.42
1:C:362:TYR:HA	1:C:402:VAL:CG2	2.50	0.42
1:D:290:TRP:HZ3	1:D:576:ALA:HB1	1.84	0.42
1:D:321:VAL:O	1:D:321:VAL:HG12	2.19	0.42
1:D:374:THR:OG1	1:D:390:ALA:HB2	2.20	0.42
1:D:469:THR:O	1:D:470:ILE:C	2.63	0.42
1:E:103:ILE:HB	1:E:104:PRO:HD2	2.01	0.42
1:B:267:LYS:CG	1:B:268:VAL:H	2.29	0.42
1:B:346:LYS:CG	1:B:347:SER:H	2.31	0.42
1:A:290:TRP:CZ2	1:A:517:ILE:HD13	2.55	0.42
1:A:362:TYR:HA	1:A:402:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LYS:CG	1:D:268:VAL:H	2.29	0.42
1:D:362:TYR:HA	1:D:402:VAL:CG2	2.50	0.42
1:D:393:LEU:HD11	1:D:443:VAL:HG22	2.02	0.42
1:B:329:ARG:HG3	1:B:329:ARG:O	2.19	0.42
1:B:469:THR:O	1:B:470:ILE:C	2.63	0.42
1:B:510:ILE:HG22	1:B:511:ASP:H	1.85	0.42
1:A:103:ILE:HB	1:A:104:PRO:HD2	2.01	0.42
1:E:108:GLU:OE2	1:E:111:LYS:HD2	2.19	0.42
1:E:344:THR:HG22	1:E:344:THR:O	2.19	0.42
1:E:496:LEU:HG	1:E:496:LEU:O	2.20	0.42
1:A:66:ASN:O	1:A:67:THR:C	2.63	0.42
1:A:105:ARG:O	1:A:105:ARG:HG3	2.19	0.42
1:A:267:LYS:CG	1:A:268:VAL:H	2.29	0.42
1:A:382:GLY:O	1:A:383:THR:HB	2.20	0.42
1:A:464:ILE:HG23	1:A:467:PRO:HD2	2.02	0.42
1:C:100:ILE:CG2	1:C:103:ILE:HG23	2.50	0.42
1:C:238:ASP:HB3	1:C:256:TYR:HB3	2.01	0.42
1:D:290:TRP:CZ2	1:D:517:ILE:HD13	2.55	0.42
1:D:346:LYS:CG	1:D:347:SER:H	2.32	0.42
1:E:346:LYS:HA	1:E:480:LEU:HD11	2.02	0.42
1:B:105:ARG:O	1:B:105:ARG:HG3	2.19	0.42
1:A:329:ARG:O	1:A:329:ARG:HG3	2.20	0.42
1:C:90:GLN:C	1:C:92:ASP:H	2.27	0.42
1:C:144:HIS:CB	1:C:149:CYS:SG	3.05	0.42
1:C:374:THR:OG1	1:C:390:ALA:HB2	2.20	0.42
1:C:496:LEU:HG	1:C:496:LEU:O	2.20	0.42
1:D:90:GLN:C	1:D:92:ASP:H	2.27	0.42
1:D:100:ILE:CG2	1:D:103:ILE:HG23	2.50	0.42
1:D:108:GLU:OE2	1:D:111:LYS:HD2	2.19	0.42
1:D:329:ARG:O	1:D:329:ARG:HG3	2.19	0.42
1:E:290:TRP:CZ2	1:E:517:ILE:HD13	2.55	0.42
1:B:265:SER:O	1:B:266:GLN:HB3	2.20	0.41
1:B:290:TRP:CZ2	1:B:517:ILE:HD13	2.55	0.41
1:A:100:ILE:CG2	1:A:103:ILE:HG23	2.50	0.41
1:A:469:THR:O	1:A:471:LEU:N	2.53	0.41
1:C:469:THR:O	1:C:471:LEU:N	2.53	0.41
1:D:16:GLU:O	1:D:20:THR:OG1	2.23	0.41
1:D:265:SER:O	1:D:266:GLN:HB3	2.20	0.41
1:D:559:PRO:O	1:D:562:LEU:N	2.53	0.41
1:E:265:SER:O	1:E:266:GLN:HB3	2.20	0.41
1:E:469:THR:O	1:E:470:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLN:C	1:B:92:ASP:H	2.27	0.41
1:D:67:THR:O	1:D:68:LYS:C	2.64	0.41
1:D:469:THR:O	1:D:471:LEU:N	2.53	0.41
1:E:393:LEU:HD11	1:E:443:VAL:HG22	2.01	0.41
1:E:464:ILE:HG23	1:E:467:PRO:HD2	2.02	0.41
1:E:556:LEU:C	1:E:558:THR:H	2.28	0.41
1:B:100:ILE:CG2	1:B:103:ILE:HG23	2.51	0.41
1:B:148:ASP:O	1:B:149:CYS:HB2	2.20	0.41
1:B:362:TYR:HA	1:B:402:VAL:CG2	2.50	0.41
1:B:496:LEU:O	1:B:496:LEU:HG	2.20	0.41
1:A:265:SER:O	1:A:266:GLN:HB3	2.20	0.41
1:A:374:THR:OG1	1:A:390:ALA:HB2	2.20	0.41
1:A:510:ILE:HG22	1:A:511:ASP:H	1.85	0.41
1:C:346:LYS:CG	1:C:347:SER:H	2.32	0.41
1:C:346:LYS:HA	1:C:480:LEU:HD11	2.01	0.41
1:D:559:PRO:O	1:D:563:GLU:N	2.44	0.41
1:E:66:ASN:O	1:E:67:THR:C	2.63	0.41
1:E:100:ILE:CG2	1:E:103:ILE:HG23	2.51	0.41
1:E:299:ILE:HG23	1:E:302:SER:O	2.21	0.41
1:E:469:THR:O	1:E:471:LEU:N	2.54	0.41
1:B:108:GLU:OE2	1:B:111:LYS:HD2	2.19	0.41
1:B:469:THR:O	1:B:471:LEU:N	2.53	0.41
1:A:346:LYS:CG	1:A:347:SER:H	2.32	0.41
1:A:590:ILE:HG13	1:A:591:ASN:N	2.34	0.41
1:D:510:ILE:HG22	1:D:511:ASP:H	1.85	0.41
1:E:127:LEU:HD23	1:E:227:PRO:HA	2.02	0.41
1:E:155:TRP:HB3	1:E:156:PRO:HD3	2.01	0.41
1:B:67:THR:O	1:B:68:LYS:C	2.63	0.41
1:A:238:ASP:HB3	1:A:256:TYR:HB3	2.01	0.41
1:A:449:PRO:HG2	1:A:452:GLY:O	2.20	0.41
1:A:469:THR:O	1:A:470:ILE:C	2.63	0.41
1:C:233:VAL:HG21	1:C:257:MET:CE	2.48	0.41
1:C:267:LYS:CG	1:C:268:VAL:H	2.29	0.41
1:D:496:LEU:O	1:D:496:LEU:HG	2.20	0.41
1:E:559:PRO:O	1:E:562:LEU:N	2.53	0.41
1:B:393:LEU:HD11	1:B:443:VAL:HG22	2.02	0.41
1:B:513:LEU:HD23	1:B:513:LEU:HA	1.97	0.41
1:B:559:PRO:O	1:B:562:LEU:N	2.54	0.41
1:A:198:GLN:HE21	1:A:210:PRO:HG2	1.85	0.41
1:A:483:GLN:HB3	1:A:486:GLU:CG	2.50	0.41
1:D:66:ASN:O	1:D:67:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:THR:O	1:D:375:ALA:HB2	2.21	0.41
1:E:198:GLN:HE21	1:E:210:PRO:HG2	1.85	0.41
1:B:299:ILE:HG23	1:B:302:SER:O	2.21	0.41
1:B:374:THR:O	1:B:375:ALA:HB2	2.21	0.41
1:A:344:THR:HG22	1:A:344:THR:O	2.18	0.41
1:A:556:LEU:C	1:A:558:THR:H	2.28	0.41
1:A:559:PRO:O	1:A:562:LEU:N	2.54	0.41
1:C:299:ILE:HG23	1:C:302:SER:O	2.21	0.41
1:D:148:ASP:O	1:D:149:CYS:HB2	2.20	0.41
1:D:336:ILE:HG22	1:D:476:LEU:HB2	2.02	0.41
1:D:556:LEU:C	1:D:558:THR:H	2.28	0.41
1:E:374:THR:O	1:E:375:ALA:HB2	2.21	0.41
1:E:483:GLN:HB3	1:E:486:GLU:CG	2.49	0.41
1:B:66:ASN:O	1:B:67:THR:C	2.63	0.41
1:B:127:LEU:HD23	1:B:227:PRO:HA	2.02	0.41
1:B:285:LEU:HB3	1:B:577:LEU:HD13	2.03	0.41
1:B:556:LEU:C	1:B:558:THR:H	2.28	0.41
1:A:148:ASP:O	1:A:149:CYS:HB2	2.21	0.41
1:C:148:ASP:O	1:C:149:CYS:HB2	2.21	0.41
1:D:127:LEU:HD23	1:D:227:PRO:HA	2.03	0.41
1:A:49:PHE:CZ	1:A:60:ALA:HB1	2.56	0.41
1:A:63:ILE:HA	1:A:70:ILE:HG21	2.03	0.41
1:A:144:HIS:CB	1:A:149:CYS:SG	3.05	0.41
1:A:374:THR:O	1:A:375:ALA:HB2	2.21	0.41
1:A:496:LEU:HG	1:A:496:LEU:O	2.20	0.41
1:A:555:ILE:O	1:A:556:LEU:HB3	2.21	0.41
1:A:567:ARG:NH1	1:D:494:TYR:HB2	2.36	0.41
1:C:155:TRP:HB3	1:C:156:PRO:HD3	2.01	0.41
1:C:309:LEU:HG	1:C:313:LEU:CD1	2.49	0.41
1:C:374:THR:O	1:C:375:ALA:HB2	2.21	0.41
1:C:559:PRO:O	1:C:562:LEU:N	2.53	0.41
1:D:49:PHE:CZ	1:D:60:ALA:HB1	2.56	0.41
1:D:63:ILE:HA	1:D:70:ILE:HG21	2.03	0.41
1:D:299:ILE:HG23	1:D:302:SER:O	2.21	0.41
1:D:309:LEU:HG	1:D:313:LEU:CD1	2.48	0.41
1:D:382:GLY:O	1:D:383:THR:HB	2.19	0.41
1:E:148:ASP:O	1:E:149:CYS:HB2	2.21	0.41
1:E:294:ARG:NH2	1:E:514:ARG:HG3	2.36	0.41
1:A:366:LYS:CG	1:A:367:GLY:N	2.71	0.41
1:C:336:ILE:HG22	1:C:476:LEU:HB2	2.02	0.41
1:C:510:ILE:HG22	1:C:511:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ARG:NH2	1:D:514:ARG:HG3	2.36	0.41
1:D:346:LYS:HA	1:D:480:LEU:HD11	2.02	0.41
1:E:510:ILE:HG22	1:E:511:ASP:H	1.86	0.41
1:B:238:ASP:HB3	1:B:256:TYR:HB3	2.01	0.40
1:B:464:ILE:HG23	1:B:467:PRO:HD2	2.02	0.40
1:B:537:THR:HA	1:B:540:PHE:CD2	2.56	0.40
1:A:336:ILE:HG22	1:A:476:LEU:HB2	2.02	0.40
1:C:49:PHE:CZ	1:C:60:ALA:HB1	2.56	0.40
1:C:449:PRO:HG2	1:C:452:GLY:O	2.21	0.40
1:C:469:THR:O	1:C:470:ILE:C	2.63	0.40
1:E:49:PHE:CZ	1:E:60:ALA:HB1	2.56	0.40
1:E:312:ALA:HB2	1:E:478:PHE:CZ	2.57	0.40
1:B:294:ARG:NH2	1:B:514:ARG:HG3	2.36	0.40
1:B:449:PRO:HG2	1:B:452:GLY:O	2.21	0.40
1:C:66:ASN:O	1:C:67:THR:C	2.63	0.40
1:E:437:LEU:HD13	1:E:437:LEU:HA	1.98	0.40
1:B:63:ILE:HA	1:B:70:ILE:HG21	2.03	0.40
1:B:198:GLN:HE21	1:B:210:PRO:HG2	1.85	0.40
1:B:388:LEU:HD21	1:B:428:ILE:CD1	2.49	0.40
1:A:127:LEU:HD23	1:A:227:PRO:HA	2.02	0.40
1:C:67:THR:O	1:C:68:LYS:C	2.64	0.40
1:C:464:ILE:HG23	1:C:467:PRO:HD2	2.02	0.40
1:E:63:ILE:HA	1:E:70:ILE:HG21	2.04	0.40
1:E:67:THR:O	1:E:68:LYS:C	2.64	0.40
1:E:336:ILE:HG22	1:E:476:LEU:HB2	2.02	0.40
1:E:340:GLY:O	1:E:346:LYS:NZ	2.49	0.40
1:E:553:SER:N	1:E:554:PRO:HD3	2.37	0.40
1:A:285:LEU:HB3	1:A:577:LEU:HD13	2.03	0.40
1:C:285:LEU:HB3	1:C:577:LEU:HD13	2.03	0.40
1:C:537:THR:HA	1:C:540:PHE:CD2	2.57	0.40
1:D:311:GLU:O	1:D:314:ALA:N	2.55	0.40
1:D:555:ILE:O	1:D:556:LEU:HB3	2.21	0.40
1:E:251:ALA:CB	1:E:252:VAL:CA	2.99	0.40
1:E:449:PRO:HG2	1:E:452:GLY:O	2.21	0.40
1:B:336:ILE:HG22	1:B:476:LEU:HB2	2.02	0.40
1:C:63:ILE:HA	1:C:70:ILE:HG21	2.03	0.40
1:C:294:ARG:NH2	1:C:514:ARG:HG3	2.37	0.40
1:C:409:MET:HG2	1:C:410:ARG:N	2.37	0.40
1:D:449:PRO:HG2	1:D:452:GLY:O	2.21	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	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	4	28
1	B	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	4	28
1	C	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	4	28
1	D	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	4	28
1	E	590/692 (85%)	495 (84%)	79 (13%)	16 (3%)	4	28
All	All	2950/3460 (85%)	2475 (84%)	395 (13%)	80 (3%)	4	28

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	CYS
1	B	557	ILE
1	A	149	CYS
1	A	557	ILE
1	C	149	CYS
1	C	557	ILE
1	D	149	CYS
1	D	557	ILE
1	E	149	CYS
1	E	557	ILE
1	B	173	LYS
1	B	331	ARG
1	B	495	ILE
1	B	555	ILE
1	A	331	ARG
1	A	343	GLY
1	A	495	ILE
1	A	555	ILE
1	C	331	ARG
1	C	495	ILE
1	C	555	ILE

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Mol	Chain	Res	Type
1	D	173	LYS
1	D	331	ARG
1	D	495	ILE
1	D	555	ILE
1	E	173	LYS
1	E	331	ARG
1	E	495	ILE
1	E	555	ILE
1	B	343	GLY
1	B	346	LYS
1	B	486	GLU
1	B	510	ILE
1	A	173	LYS
1	A	346	LYS
1	A	486	GLU
1	A	510	ILE
1	C	173	LYS
1	C	343	GLY
1	C	486	GLU
1	C	510	ILE
1	D	343	GLY
1	D	346	LYS
1	D	486	GLU
1	D	510	ILE
1	E	343	GLY
1	E	346	LYS
1	E	486	GLU
1	E	510	ILE
1	A	242	ASP
1	C	346	LYS
1	D	242	ASP
1	B	242	ASP
1	B	289	PRO
1	B	344	THR
1	A	289	PRO
1	A	344	THR
1	C	242	ASP
1	C	289	PRO
1	C	344	THR
1	D	289	PRO
1	D	344	THR
1	E	242	ASP

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Mol	Chain	Res	Type
1	E	289	PRO
1	E	344	THR
1	B	300	ALA
1	B	468	PRO
1	B	508	ILE
1	A	468	PRO
1	A	508	ILE
1	C	300	ALA
1	C	468	PRO
1	C	508	ILE
1	D	468	PRO
1	D	508	ILE
1	E	300	ALA
1	E	468	PRO
1	E	508	ILE
1	A	300	ALA
1	D	300	ALA

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	518/608 (85%)	480 (93%)	38 (7%)	13	36
1	B	518/608 (85%)	479 (92%)	39 (8%)	12	35
1	C	518/608 (85%)	480 (93%)	38 (7%)	13	36
1	D	518/608 (85%)	480 (93%)	38 (7%)	13	36
1	E	518/608 (85%)	479 (92%)	39 (8%)	12	35
All	All	2590/3040 (85%)	2398 (93%)	192 (7%)	13	35

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	ILE
1	B	46	ILE

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Mol	Chain	Res	Type
1	B	64	ILE
1	B	94	GLU
1	B	95	LYS
1	B	101	VAL
1	B	117	ILE
1	B	146	HIS
1	B	149	CYS
1	B	171	CYS
1	B	231	VAL
1	B	232	LYS
1	B	233	VAL
1	B	252	VAL
1	B	256	TYR
1	B	270	ASP
1	B	303	ILE
1	B	330	ILE
1	B	331	ARG
1	B	335	HIS
1	B	346	LYS
1	B	353	ILE
1	B	368	SER
1	B	377	VAL
1	B	378	VAL
1	B	388	LEU
1	B	406	ILE
1	B	410	ARG
1	B	425	THR
1	B	462	ASP
1	B	466	LEU
1	B	473	ARG
1	B	496	LEU
1	B	517	ILE
1	B	519	TYR
1	B	524	VAL
1	B	528	ILE
1	B	555	ILE
1	B	585	ASP
1	A	8	ILE
1	A	46	ILE
1	A	64	ILE
1	A	94	GLU
1	A	95	LYS

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Mol	Chain	Res	Type
1	A	101	VAL
1	A	146	HIS
1	A	149	CYS
1	A	171	CYS
1	A	231	VAL
1	A	232	LYS
1	A	233	VAL
1	A	252	VAL
1	A	256	TYR
1	A	270	ASP
1	A	303	ILE
1	A	330	ILE
1	A	331	ARG
1	A	335	HIS
1	A	346	LYS
1	A	353	ILE
1	A	368	SER
1	A	377	VAL
1	A	378	VAL
1	A	388	LEU
1	A	406	ILE
1	A	410	ARG
1	A	425	THR
1	A	462	ASP
1	A	466	LEU
1	A	473	ARG
1	A	496	LEU
1	A	517	ILE
1	A	519	TYR
1	A	524	VAL
1	A	528	ILE
1	A	555	ILE
1	A	585	ASP
1	C	8	ILE
1	C	46	ILE
1	C	64	ILE
1	C	94	GLU
1	C	95	LYS
1	C	101	VAL
1	C	117	ILE
1	C	146	HIS
1	C	149	CYS

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Mol	Chain	Res	Type
1	C	171	CYS
1	C	231	VAL
1	C	232	LYS
1	C	233	VAL
1	C	252	VAL
1	C	256	TYR
1	C	270	ASP
1	C	303	ILE
1	C	330	ILE
1	C	331	ARG
1	C	335	HIS
1	C	346	LYS
1	C	353	ILE
1	C	368	SER
1	C	377	VAL
1	C	378	VAL
1	C	388	LEU
1	C	406	ILE
1	C	425	THR
1	C	462	ASP
1	C	466	LEU
1	C	473	ARG
1	C	496	LEU
1	C	517	ILE
1	C	519	TYR
1	C	524	VAL
1	C	528	ILE
1	C	555	ILE
1	C	585	ASP
1	D	8	ILE
1	D	46	ILE
1	D	64	ILE
1	D	94	GLU
1	D	95	LYS
1	D	101	VAL
1	D	117	ILE
1	D	146	HIS
1	D	149	CYS
1	D	171	CYS
1	D	231	VAL
1	D	232	LYS
1	D	233	VAL

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Mol	Chain	Res	Type
1	D	252	VAL
1	D	256	TYR
1	D	270	ASP
1	D	303	ILE
1	D	330	ILE
1	D	331	ARG
1	D	335	HIS
1	D	346	LYS
1	D	353	ILE
1	D	368	SER
1	D	377	VAL
1	D	378	VAL
1	D	388	LEU
1	D	406	ILE
1	D	425	THR
1	D	462	ASP
1	D	466	LEU
1	D	473	ARG
1	D	496	LEU
1	D	517	ILE
1	D	519	TYR
1	D	524	VAL
1	D	528	ILE
1	D	555	ILE
1	D	585	ASP
1	E	8	ILE
1	E	46	ILE
1	E	64	ILE
1	E	94	GLU
1	E	95	LYS
1	E	101	VAL
1	E	117	ILE
1	E	146	HIS
1	E	149	CYS
1	E	171	CYS
1	E	231	VAL
1	E	232	LYS
1	E	233	VAL
1	E	252	VAL
1	E	256	TYR
1	E	270	ASP
1	E	303	ILE

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Mol	Chain	Res	Type
1	E	330	ILE
1	E	331	ARG
1	E	335	HIS
1	E	346	LYS
1	E	353	ILE
1	E	368	SER
1	E	377	VAL
1	E	378	VAL
1	E	388	LEU
1	E	406	ILE
1	E	410	ARG
1	E	425	THR
1	E	462	ASP
1	E	466	LEU
1	E	473	ARG
1	E	496	LEU
1	E	517	ILE
1	E	519	TYR
1	E	524	VAL
1	E	528	ILE
1	E	555	ILE
1	E	585	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	ASN
1	B	81	HIS
1	B	90	GLN
1	B	306	HIS
1	B	335	HIS
1	B	438	ASN
1	B	487	GLN
1	B	534	ASN
1	A	56	ASN
1	A	81	HIS
1	A	90	GLN
1	A	306	HIS
1	A	335	HIS
1	A	438	ASN
1	C	56	ASN
1	C	81	HIS

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Mol	Chain	Res	Type
1	C	90	GLN
1	C	306	HIS
1	C	335	HIS
1	C	438	ASN
1	D	56	ASN
1	D	81	HIS
1	D	90	GLN
1	D	306	HIS
1	D	335	HIS
1	D	438	ASN
1	D	487	GLN
1	E	56	ASN
1	E	81	HIS
1	E	90	GLN
1	E	306	HIS
1	E	335	HIS
1	E	438	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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	592/692 (85%)	0.62	44 (7%)	20	20	126, 198, 269, 306	0
1	B	592/692 (85%)	0.57	44 (7%)	20	20	116, 188, 259, 300	0
1	C	592/692 (85%)	0.58	39 (6%)	24	23	114, 192, 273, 324	0
1	D	592/692 (85%)	0.57	26 (4%)	39	31	129, 201, 270, 375	0
1	E	592/692 (85%)	0.51	29 (4%)	35	29	118, 181, 253, 349	0
All	All	2960/3460 (85%)	0.57	182 (6%)	27	25	114, 193, 267, 375	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	ARG	7.5
1	C	489	ARG	4.8
1	B	563	GLU	4.7
1	E	116	ASP	4.4
1	E	294	ARG	4.3
1	B	391	GLY	4.1
1	A	78	LEU	4.1
1	E	551	PRO	4.0
1	D	25	ASN	4.0
1	C	486	GLU	3.9
1	C	333	ASP	3.9
1	A	325	LEU	3.9
1	D	598	GLU	3.9
1	C	334	ILE	3.8
1	D	294	ARG	3.8
1	D	14	PHE	3.7
1	A	82	ILE	3.7
1	B	558	THR	3.6
1	A	549	GLU	3.6
1	C	14	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	312	ALA	3.5
1	B	555	ILE	3.5
1	D	417	ILE	3.5
1	D	567	ARG	3.3
1	C	223	ASP	3.3
1	A	117	ILE	3.3
1	B	265	SER	3.3
1	B	369	THR	3.3
1	C	477	ILE	3.2
1	B	477	ILE	3.2
1	B	311	GLU	3.2
1	C	375	ALA	3.2
1	E	576	ALA	3.2
1	A	342	PRO	3.1
1	E	509	ASP	3.1
1	A	575	MET	3.1
1	B	284	ASP	3.1
1	C	314	ALA	3.1
1	C	319	GLY	3.1
1	E	519	TYR	3.0
1	C	25	ASN	3.0
1	B	163	GLU	3.0
1	E	540	PHE	3.0
1	B	106	VAL	3.0
1	B	348	GLN	3.0
1	A	576	ALA	3.0
1	D	519	TYR	3.0
1	B	26	ASN	2.9
1	B	567	ARG	2.9
1	B	153	PHE	2.9
1	C	116	ASP	2.9
1	D	248	GLY	2.9
1	B	14	PHE	2.9
1	A	14	PHE	2.9
1	C	294	ARG	2.8
1	C	483	GLN	2.8
1	B	564	ALA	2.8
1	D	22	LYS	2.8
1	B	54	SER	2.8
1	C	538	ASP	2.8
1	A	519	TYR	2.8
1	D	181	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	2.8
1	B	152	GLU	2.7
1	B	214	GLU	2.7
1	A	328	THR	2.7
1	A	374	THR	2.7
1	D	570	GLU	2.7
1	D	528	ILE	2.7
1	A	489	ARG	2.7
1	E	13	VAL	2.7
1	D	540	PHE	2.7
1	D	143	LYS	2.7
1	A	217	LEU	2.7
1	B	124	ASP	2.7
1	A	290	TRP	2.7
1	A	329	ARG	2.7
1	A	118	GLY	2.6
1	E	68	LYS	2.6
1	C	84	GLN	2.6
1	E	563	GLU	2.6
1	E	570	GLU	2.6
1	C	373	LEU	2.6
1	D	289	PRO	2.6
1	A	509	ASP	2.6
1	C	75	GLU	2.6
1	E	179	GLN	2.6
1	B	485	GLY	2.6
1	B	441	ALA	2.6
1	B	519	TYR	2.6
1	B	308	GLU	2.6
1	E	528	ILE	2.6
1	A	138	TYR	2.6
1	D	397	ASP	2.5
1	B	464	ILE	2.5
1	E	484	PRO	2.5
1	A	364	THR	2.5
1	A	518	ALA	2.5
1	B	201	PRO	2.5
1	A	311	GLU	2.4
1	A	65	ASN	2.4
1	E	304	TYR	2.4
1	C	527	LYS	2.4
1	E	237	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	81	HIS	2.4
1	B	194	LYS	2.4
1	A	551	PRO	2.4
1	D	389	GLU	2.4
1	B	305	GLY	2.4
1	A	485	GLY	2.4
1	D	576	ALA	2.4
1	A	540	PHE	2.4
1	D	383	THR	2.3
1	E	555	ILE	2.3
1	E	117	ILE	2.3
1	A	383	THR	2.3
1	B	185	GLU	2.3
1	C	570	GLU	2.3
1	B	22	LYS	2.3
1	B	294	ARG	2.3
1	B	290	TRP	2.3
1	E	481	LYS	2.3
1	C	78	LEU	2.3
1	C	347	SER	2.3
1	C	575	MET	2.3
1	D	290	TRP	2.3
1	D	145	ILE	2.3
1	A	84	GLN	2.3
1	E	421	MET	2.3
1	C	290	TRP	2.3
1	C	558	THR	2.3
1	B	518	ALA	2.3
1	B	256	TYR	2.2
1	E	373	LEU	2.2
1	E	493	ASN	2.2
1	C	504	THR	2.2
1	A	360	ALA	2.2
1	C	286	ALA	2.2
1	C	328	THR	2.2
1	C	374	THR	2.2
1	E	284	ASP	2.2
1	C	237	LEU	2.2
1	A	486	GLU	2.2
1	C	305	GLY	2.2
1	C	320	GLY	2.2
1	C	540	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	182	LEU	2.1
1	A	493	ASN	2.1
1	D	304	TYR	2.1
1	B	504	THR	2.1
1	D	563	GLU	2.1
1	C	389	GLU	2.1
1	D	441	ALA	2.1
1	B	172	PRO	2.1
1	B	576	ALA	2.1
1	A	372	GLY	2.1
1	C	74	LEU	2.1
1	E	305	GLY	2.1
1	C	567	ARG	2.1
1	E	558	THR	2.1
1	A	46	ILE	2.1
1	B	500	SER	2.1
1	A	570	GLU	2.1
1	B	421	MET	2.1
1	D	109	LEU	2.1
1	E	312	ALA	2.1
1	B	551	PRO	2.1
1	C	168	PRO	2.1
1	C	427	SER	2.1
1	B	481	LYS	2.0
1	A	98	VAL	2.0
1	A	281	LYS	2.0
1	A	388	LEU	2.0
1	B	148	ASP	2.0
1	D	475	ASP	2.0
1	E	148	ASP	2.0
1	C	356	VAL	2.0
1	E	113	ARG	2.0
1	E	489	ARG	2.0
1	A	390	ALA	2.0
1	A	452	GLY	2.0
1	A	44	SER	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	ZN	E	701	1/1	0.94	0.07	283,283,283,283	0
2	ZN	A	701	1/1	0.96	0.09	260,260,260,260	0
2	ZN	C	701	1/1	0.97	0.08	281,281,281,281	0
2	ZN	D	701	1/1	0.98	0.03	255,255,255,255	0
2	ZN	B	701	1/1	0.99	0.04	200,200,200,200	0

6.5 Other polymers [i](#)

There are no such residues in this entry.