Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 11:51 PM EDT

PDB ID	:	5ERB
Title	:	Ketosynthase from module 5 of the bacillaene synthase from Bacillus amyloliquefaciens FZB42
Authors	:	Wagner, D.T.; Gay, D.C.; Keatinge-Clay, A.T.; Meinke, J.
Deposited on	:	2015-11-13
Resolution	:	4.20 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:

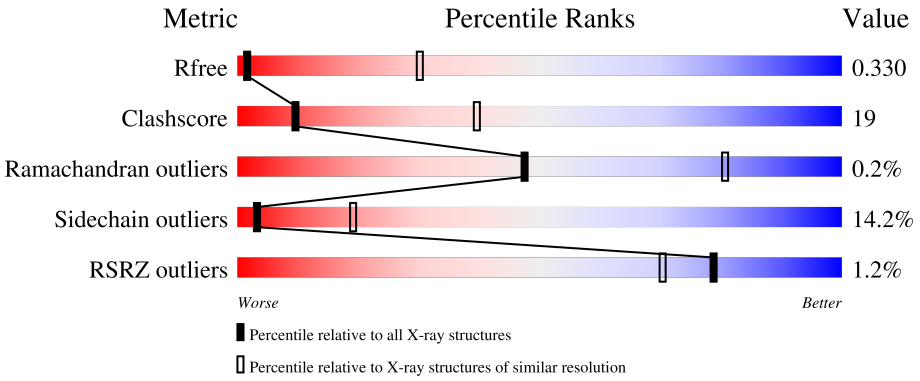
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 <=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	640	61% 24% 5% • 9%
1	B	640	60% 25% 7% • 7%
1	C	640	60% 23% 7% • 8%
1	D	640	61% 24% 7% • 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18315 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 Polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4543	2859	790	873	21			
1	B	593	Total	C	N	O	S	0	0	0
			4618	2907	798	892	21			
1	C	586	Total	C	N	O	S	0	0	0
			4562	2872	792	878	20			
1	D	590	Total	C	N	O	S	0	0	0
			4592	2886	797	888	21			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1RS72
A	-18	GLY	-	expression tag	UNP Q1RS72
A	-17	SER	-	expression tag	UNP Q1RS72
A	-16	SER	-	expression tag	UNP Q1RS72
A	-15	HIS	-	expression tag	UNP Q1RS72
A	-14	HIS	-	expression tag	UNP Q1RS72
A	-13	HIS	-	expression tag	UNP Q1RS72
A	-12	HIS	-	expression tag	UNP Q1RS72
A	-11	HIS	-	expression tag	UNP Q1RS72
A	-10	HIS	-	expression tag	UNP Q1RS72
A	-9	SER	-	expression tag	UNP Q1RS72
A	-8	SER	-	expression tag	UNP Q1RS72
A	-7	GLY	-	expression tag	UNP Q1RS72
A	-6	LEU	-	expression tag	UNP Q1RS72
A	-5	VAL	-	expression tag	UNP Q1RS72
A	-4	PRO	-	expression tag	UNP Q1RS72
A	-3	ARG	-	expression tag	UNP Q1RS72
A	-2	GLY	-	expression tag	UNP Q1RS72
A	-1	SER	-	expression tag	UNP Q1RS72
A	0	SER	-	expression tag	UNP Q1RS72
B	-19	MET	-	initiating methionine	UNP Q1RS72

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q1RS72
B	-17	SER	-	expression tag	UNP Q1RS72
B	-16	SER	-	expression tag	UNP Q1RS72
B	-15	HIS	-	expression tag	UNP Q1RS72
B	-14	HIS	-	expression tag	UNP Q1RS72
B	-13	HIS	-	expression tag	UNP Q1RS72
B	-12	HIS	-	expression tag	UNP Q1RS72
B	-11	HIS	-	expression tag	UNP Q1RS72
B	-10	HIS	-	expression tag	UNP Q1RS72
B	-9	SER	-	expression tag	UNP Q1RS72
B	-8	SER	-	expression tag	UNP Q1RS72
B	-7	GLY	-	expression tag	UNP Q1RS72
B	-6	LEU	-	expression tag	UNP Q1RS72
B	-5	VAL	-	expression tag	UNP Q1RS72
B	-4	PRO	-	expression tag	UNP Q1RS72
B	-3	ARG	-	expression tag	UNP Q1RS72
B	-2	GLY	-	expression tag	UNP Q1RS72
B	-1	SER	-	expression tag	UNP Q1RS72
B	0	SER	-	expression tag	UNP Q1RS72
C	-19	MET	-	initiating methionine	UNP Q1RS72
C	-18	GLY	-	expression tag	UNP Q1RS72
C	-17	SER	-	expression tag	UNP Q1RS72
C	-16	SER	-	expression tag	UNP Q1RS72
C	-15	HIS	-	expression tag	UNP Q1RS72
C	-14	HIS	-	expression tag	UNP Q1RS72
C	-13	HIS	-	expression tag	UNP Q1RS72
C	-12	HIS	-	expression tag	UNP Q1RS72
C	-11	HIS	-	expression tag	UNP Q1RS72
C	-10	HIS	-	expression tag	UNP Q1RS72
C	-9	SER	-	expression tag	UNP Q1RS72
C	-8	SER	-	expression tag	UNP Q1RS72
C	-7	GLY	-	expression tag	UNP Q1RS72
C	-6	LEU	-	expression tag	UNP Q1RS72
C	-5	VAL	-	expression tag	UNP Q1RS72
C	-4	PRO	-	expression tag	UNP Q1RS72
C	-3	ARG	-	expression tag	UNP Q1RS72
C	-2	GLY	-	expression tag	UNP Q1RS72
C	-1	SER	-	expression tag	UNP Q1RS72
C	0	SER	-	expression tag	UNP Q1RS72
D	-19	MET	-	initiating methionine	UNP Q1RS72
D	-18	GLY	-	expression tag	UNP Q1RS72
D	-17	SER	-	expression tag	UNP Q1RS72

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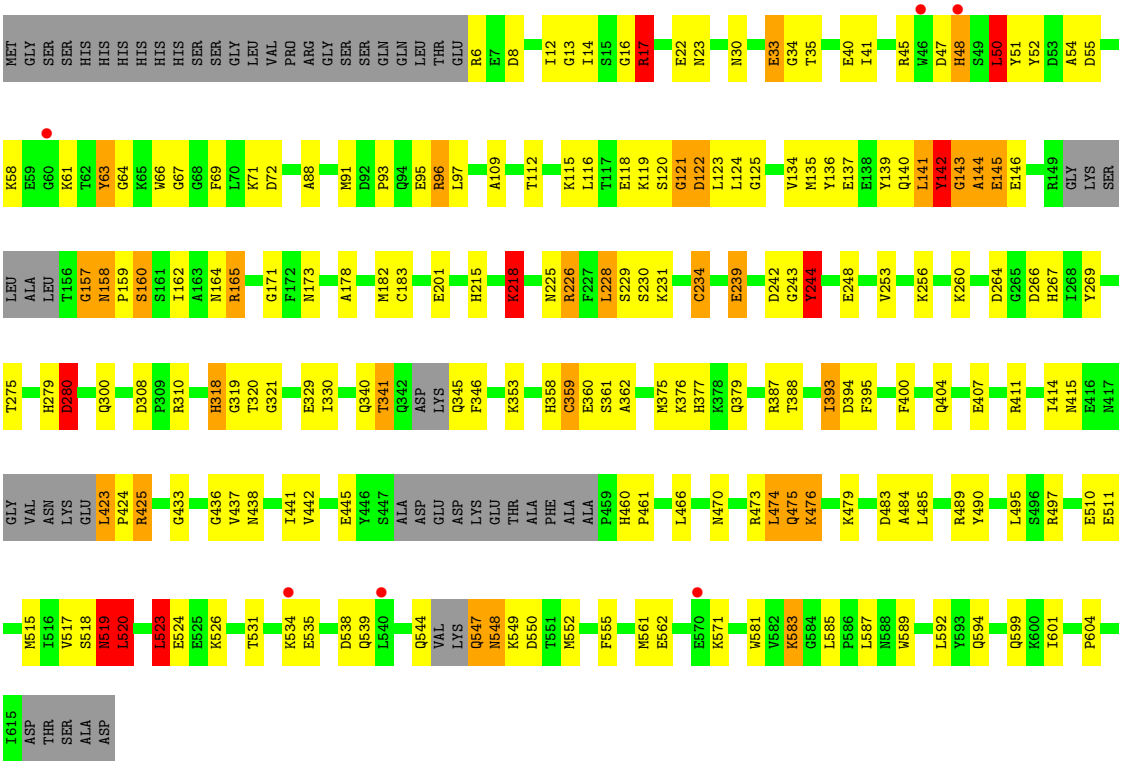
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q1RS72
D	-15	HIS	-	expression tag	UNP Q1RS72
D	-14	HIS	-	expression tag	UNP Q1RS72
D	-13	HIS	-	expression tag	UNP Q1RS72
D	-12	HIS	-	expression tag	UNP Q1RS72
D	-11	HIS	-	expression tag	UNP Q1RS72
D	-10	HIS	-	expression tag	UNP Q1RS72
D	-9	SER	-	expression tag	UNP Q1RS72
D	-8	SER	-	expression tag	UNP Q1RS72
D	-7	GLY	-	expression tag	UNP Q1RS72
D	-6	LEU	-	expression tag	UNP Q1RS72
D	-5	VAL	-	expression tag	UNP Q1RS72
D	-4	PRO	-	expression tag	UNP Q1RS72
D	-3	ARG	-	expression tag	UNP Q1RS72
D	-2	GLY	-	expression tag	UNP Q1RS72
D	-1	SER	-	expression tag	UNP Q1RS72
D	0	SER	-	expression tag	UNP Q1RS72

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

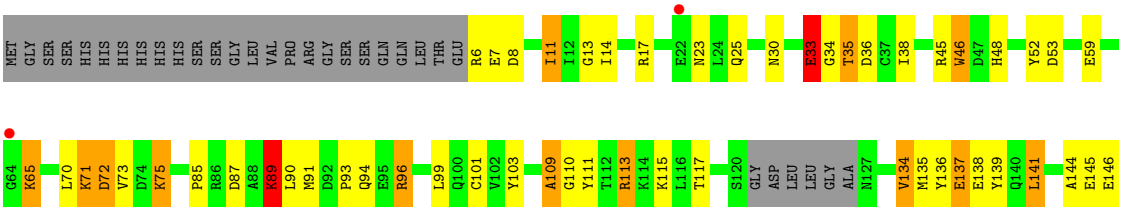
• Molecule 1: Polyketide synthase

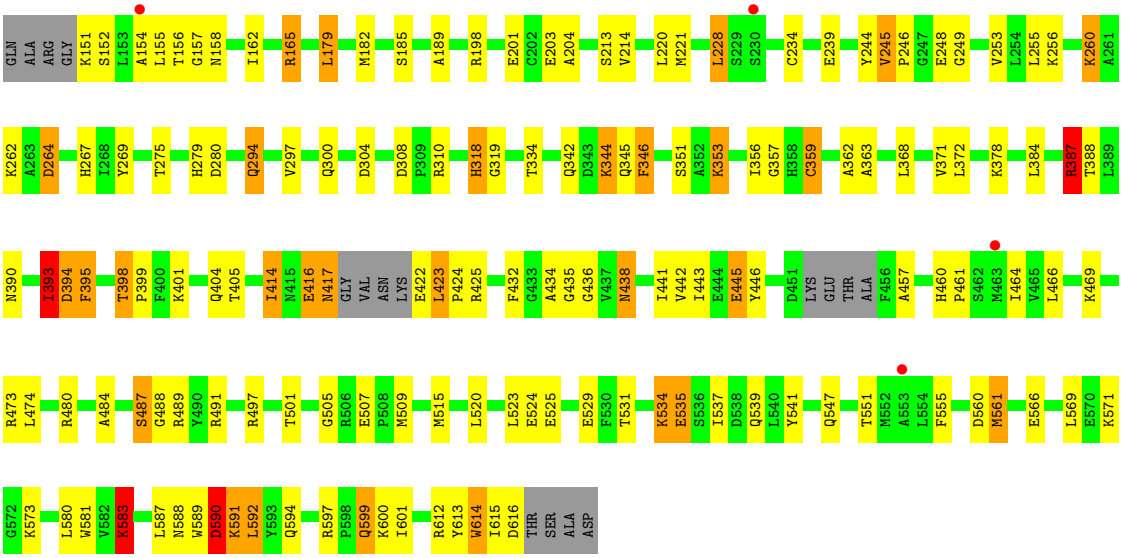
Chain A:



• Molecule 1: Polyketide synthase

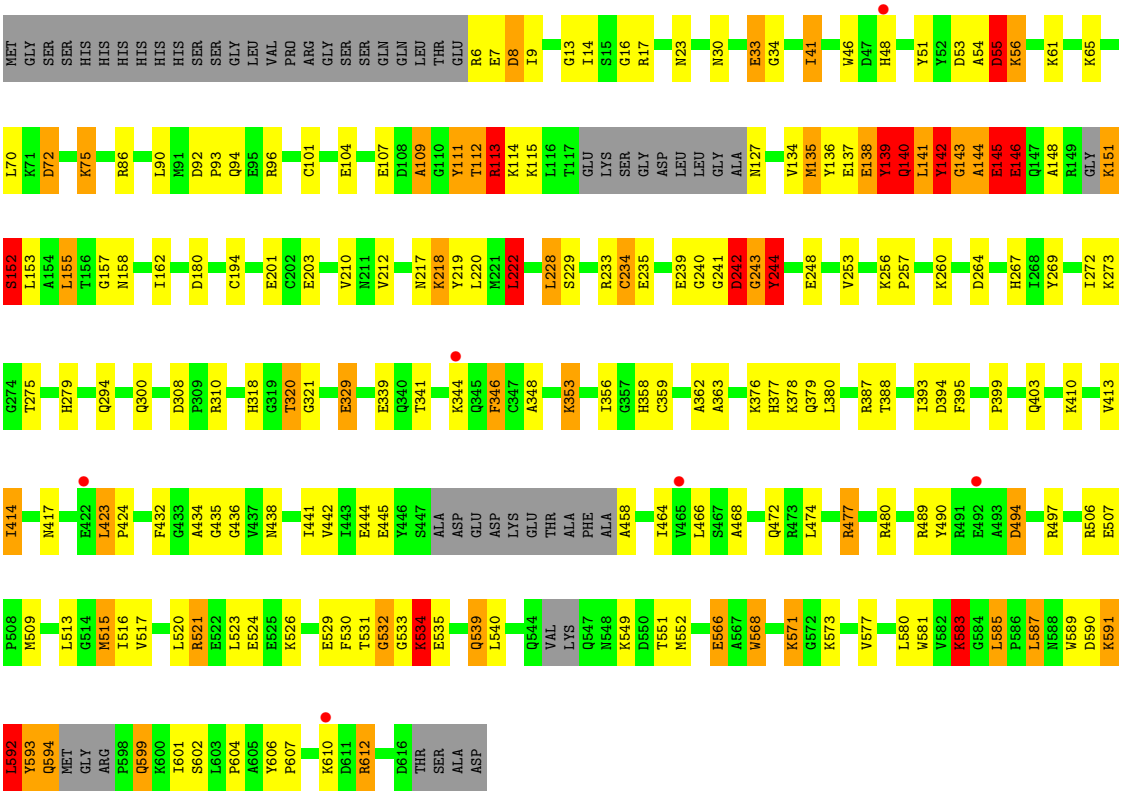
Chain B:





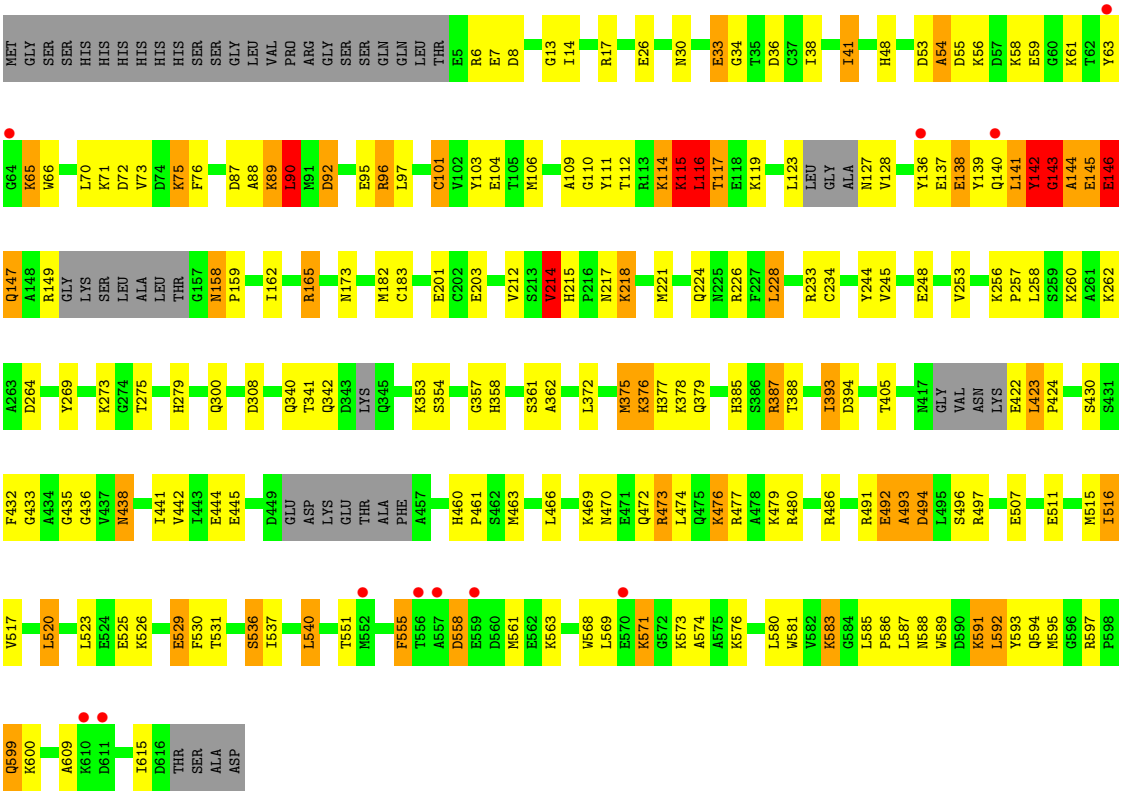
• Molecule 1: Polyketide synthase

Chain C:



• Molecule 1: Polyketide synthase

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER GLN GLN LEU THR E5 R6 E7 D8 G13 I14 R17 E26 N30 E33 G34 T35 D36 C37 I38 I41 H48 D53 A54 D55 K56 D57 K58 E59 G60 K61 T62 Y63
G64 K65 W66 L70 K71 D72 V73 D74 K75 F76 D87 A88 K89 L90 M91 D92 E95 R96 L97 C101 V102 Y103 E104 T105 M106 A109 G110 Y111 T112 R113 K114 K115 L116 T117 E118 K119 L123 LEU GLY ALA N127 V128 Y136 E137 E138 Y139 Q140 L141 Y142 G143 A144 E145 E146
Q147 A148 R149 GLY LYS SER LEU ALA LEU THR G157 N158 P159 I162 R165 N173 M182 C183 E201 C202 E203 V212 S213 V214 H215 P216 N217 K218 M221 Q224 N225 R226 F227 L228 R233 C234 Y244 V245 E248 V253 K256 P257 L258 S259 K260 A261 K262
A263 D264 Y269 K273 G274 T275 H279 Q300 D308 Q340 T341 Q342 D343 LYS Q345 K353 S354 G357 H358 S361 A362 L372 M375 K376 H377 K378 Q379 H385 S386 R387 T388 I393 D394 T405 N417 GLY VAL ASN LYS E422 L423 P424 S430 S431
F432 G433 A434 G435 G436 V437 N438 I441 V442 I443 E444 E445 D449 GLU ASP LYS GLU THR ALA PHE A457 H460 P461 S462 M463 L466 K469 N470 E471 Q472 R473 L474 Q475 K476 R477 A478 K479 R480 R486 R491 E492 A493 D494 L495 S496 R497 E507 E511 M515 I516
V517 L520 L523 E524 E525 K526 E529 F530 T531 S536 I537 L540 T551 M552 F555 T556 A557 D558 E559 D560 M561 E562 K563 W568 L569 E570 K571 G572 K573 A574 A575 K576 L580 W581 V582 K583 G584 L585 P586 L587 N588 W589 D590 K591 L592 Y593 Q594 M595 G596 R597 P598
Q599 K600 A609 K610 D611 I615 D616 THR SER ALA ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.76Å 319.13Å 103.47Å 90.00° 110.26° 90.00°	Depositor
Resolution (Å)	97.07 – 4.20 47.98 – 4.20	Depositor EDS
% Data completeness (in resolution range)	79.9 (97.07-4.20) 78.9 (47.98-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.288 , 0.341 0.281 , 0.330	Depositor DCC
R_{free} test set	1279 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	168.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 149.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.115 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18315	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0/4632	1.20	61/6245 (1.0%)
1	B	0.61	0/4709	1.28	56/6351 (0.9%)
1	C	0.62	0/4651	1.30	59/6272 (0.9%)
1	D	0.62	0/4681	1.22	50/6312 (0.8%)
All	All	0.62	0/18673	1.25	226/25180 (0.9%)

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	8
1	B	0	3
1	C	0	7
1	D	0	2
All	All	0	20

There are no bond length outliers.

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	54	ALA	CB-CA-C	24.75	147.22	110.10
1	C	152	SER	N-CA-C	17.36	157.87	111.00
1	C	152	SER	N-CA-CB	-17.30	84.55	110.50
1	B	144	ALA	N-CA-C	17.01	156.92	111.00
1	B	144	ALA	CB-CA-C	-15.76	86.46	110.10
1	A	51	TYR	N-CA-CB	-15.29	83.08	110.60
1	C	532	GLY	N-CA-C	-15.22	75.05	113.10
1	A	583	LYS	N-CA-C	-14.52	71.79	111.00
1	B	590	ASP	N-CA-C	-14.43	72.05	111.00
1	C	583	LYS	N-CA-C	-14.04	73.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	583	LYS	N-CA-C	-13.96	73.31	111.00
1	D	89	LYS	N-CA-C	-13.96	73.32	111.00
1	C	139	TYR	N-CA-C	-13.70	74.00	111.00
1	C	142	TYR	C-N-CA	13.55	150.75	122.30
1	D	142	TYR	N-CA-CB	-13.15	86.92	110.60
1	A	50	LEU	N-CA-C	-13.06	75.74	111.00
1	B	590	ASP	CB-CA-C	12.69	135.79	110.40
1	C	241	GLY	N-CA-C	-12.64	81.50	113.10
1	B	487	SER	N-CA-C	-12.42	77.47	111.00
1	B	591	LYS	N-CA-C	-12.34	77.69	111.00
1	B	146	GLU	N-CA-CB	-12.17	88.70	110.60
1	B	363	ALA	CB-CA-C	-12.05	92.02	110.10
1	C	144	ALA	C-N-CA	-11.93	91.88	121.70
1	C	142	TYR	N-CA-C	-11.91	78.85	111.00
1	D	143	GLY	N-CA-C	-11.89	83.38	113.10
1	D	493	ALA	N-CA-C	-11.65	79.55	111.00
1	C	264	ASP	N-CA-C	-11.43	80.13	111.00
1	B	591	LYS	CB-CA-C	11.41	133.23	110.40
1	D	264	ASP	N-CA-C	-11.40	80.22	111.00
1	B	583	LYS	N-CA-C	-11.15	80.90	111.00
1	B	614	TRP	N-CA-CB	-11.10	90.62	110.60
1	A	33	GLU	N-CA-C	-10.80	81.83	111.00
1	B	109	ALA	CB-CA-C	-10.50	94.35	110.10
1	C	143	GLY	N-CA-C	-10.39	87.12	113.10
1	A	143	GLY	N-CA-C	-10.36	87.21	113.10
1	C	244	TYR	CA-CB-CG	-10.23	93.97	113.40
1	B	613	TYR	N-CA-C	10.23	138.61	111.00
1	C	33	GLU	N-CA-C	-9.91	84.25	111.00
1	B	33	GLU	N-CA-C	-9.81	84.50	111.00
1	A	474	LEU	N-CA-C	9.73	137.28	111.00
1	C	222	LEU	CA-CB-CG	9.72	137.65	115.30
1	B	145	GLU	N-CA-C	-9.71	84.79	111.00
1	C	109	ALA	CB-CA-C	-9.66	95.61	110.10
1	D	214	VAL	N-CA-CB	-9.57	90.44	111.50
1	C	394	ASP	N-CA-C	-9.52	85.30	111.00
1	D	33	GLU	N-CA-C	-9.47	85.44	111.00
1	B	393	ILE	CB-CA-C	9.46	130.53	111.60
1	B	480	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	C	363	ALA	CB-CA-C	-9.12	96.42	110.10
1	B	489	ARG	N-CA-CB	-9.01	94.39	110.60
1	D	226	ARG	N-CA-CB	8.97	126.75	110.60
1	B	614	TRP	N-CA-C	8.91	135.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	142	TYR	O-C-N	-8.86	108.13	123.20
1	A	17	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	D	54	ALA	N-CA-C	-8.78	87.30	111.00
1	A	394	ASP	N-CA-C	-8.78	87.31	111.00
1	A	523	LEU	CB-CG-CD1	8.71	125.82	111.00
1	C	86	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	A	242	ASP	N-CA-C	-8.44	88.22	111.00
1	C	535	GLU	N-CA-CB	8.39	125.71	110.60
1	A	475	GLN	N-CA-CB	-8.39	95.50	110.60
1	B	34	GLY	N-CA-C	-8.36	92.21	113.10
1	D	90	LEU	N-CA-CB	8.33	127.06	110.40
1	C	146	GLU	N-CA-C	-8.31	88.55	111.00
1	A	361	SER	CB-CA-C	-8.31	94.31	110.10
1	B	33	GLU	CB-CA-C	-8.18	94.05	110.40
1	C	435	GLY	N-CA-C	-8.18	92.66	113.10
1	B	146	GLU	N-CA-C	8.15	133.01	111.00
1	A	495	LEU	CB-CG-CD1	8.15	124.85	111.00
1	D	142	TYR	CB-CA-C	-7.96	94.48	110.40
1	A	50	LEU	CA-CB-CG	7.95	133.59	115.30
1	C	55	ASP	CB-CA-C	7.94	126.28	110.40
1	A	50	LEU	CB-CA-C	-7.93	95.13	110.20
1	A	51	TYR	N-CA-C	7.90	132.34	111.00
1	B	35	THR	N-CA-CB	7.88	125.28	110.30
1	B	145	GLU	N-CA-CB	-7.88	96.42	110.60
1	C	240	GLY	N-CA-C	-7.85	93.47	113.10
1	D	144	ALA	N-CA-C	-7.83	89.86	111.00
1	C	138	GLU	N-CA-C	7.81	132.09	111.00
1	C	592	LEU	CB-CA-C	-7.73	95.51	110.20
1	D	361	SER	CB-CA-C	-7.73	95.41	110.10
1	A	359	CYS	N-CA-C	-7.71	90.19	111.00
1	C	593	TYR	N-CA-CB	-7.66	96.81	110.60
1	A	264	ASP	N-CA-C	-7.64	90.37	111.00
1	B	435	GLY	N-CA-C	-7.63	94.02	113.10
1	A	318	HIS	N-CA-C	-7.61	90.45	111.00
1	B	145	GLU	CB-CA-C	-7.56	95.29	110.40
1	A	318	HIS	CB-CA-C	-7.47	95.46	110.40
1	A	474	LEU	CB-CA-C	-7.45	96.04	110.20
1	C	112	THR	N-CA-C	7.34	130.82	111.00
1	B	35	THR	N-CA-C	-7.31	91.27	111.00
1	A	411	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	D	496	SER	CB-CA-C	-7.27	96.28	110.10
1	D	165	ARG	NE-CZ-NH1	7.21	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	394	ASP	N-CA-C	-7.13	91.74	111.00
1	A	165	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	121	GLY	N-CA-C	-7.08	95.41	113.10
1	C	113	ARG	CB-CA-C	7.06	124.52	110.40
1	A	280	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	140	GLN	N-CA-C	-6.98	92.15	111.00
1	B	71	LYS	CB-CA-C	-6.91	96.57	110.40
1	D	147	GLN	N-CA-CB	6.91	123.04	110.60
1	D	144	ALA	N-CA-CB	-6.86	100.50	110.10
1	C	242	ASP	N-CA-C	-6.83	92.55	111.00
1	B	111	TYR	N-CA-C	-6.80	92.63	111.00
1	D	114	LYS	N-CA-C	-6.77	92.71	111.00
1	C	243	GLY	N-CA-C	6.74	129.94	113.10
1	B	65	LYS	N-CA-CB	-6.70	98.54	110.60
1	B	480	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	17	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	D	595	MET	CB-CA-C	-6.63	97.14	110.40
1	C	242	ASP	O-C-N	-6.58	112.02	123.20
1	A	34	GLY	N-CA-C	-6.54	96.74	113.10
1	A	63	TYR	N-CA-C	-6.53	93.37	111.00
1	D	56	LYS	N-CA-C	-6.52	93.40	111.00
1	A	158	ASN	N-CA-CB	6.51	122.32	110.60
1	D	34	GLY	N-CA-C	-6.51	96.83	113.10
1	A	395	PHE	CB-CA-C	6.49	123.39	110.40
1	B	264	ASP	N-CA-C	-6.41	93.70	111.00
1	A	495	LEU	CB-CA-C	-6.41	98.03	110.20
1	B	65	LYS	N-CA-C	6.35	128.15	111.00
1	B	89	LYS	CB-CA-C	6.34	123.08	110.40
1	D	594	GLN	CB-CA-C	6.33	123.06	110.40
1	D	226	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	520	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	121	GLY	O-C-N	-6.30	112.62	122.70
1	B	488	GLY	N-CA-C	-6.26	97.44	113.10
1	D	387	ARG	CB-CA-C	-6.25	97.89	110.40
1	D	117	THR	CB-CA-C	-6.23	94.77	111.60
1	A	144	ALA	CB-CA-C	-6.23	100.76	110.10
1	A	225	ASN	N-CA-C	-6.22	94.21	111.00
1	D	115	LYS	CB-CA-C	-6.20	98.00	110.40
1	B	87	ASP	CB-CA-C	-6.19	98.02	110.40
1	D	537	ILE	CB-CA-C	6.18	123.95	111.60
1	D	33	GLU	CB-CA-C	-6.15	98.10	110.40
1	D	585	LEU	N-CA-C	-6.14	94.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	115	LYS	CB-CA-C	6.14	122.68	110.40
1	D	595	MET	N-CA-CB	-6.13	99.57	110.60
1	B	359	CYS	N-CA-C	-6.07	94.62	111.00
1	A	319	GLY	N-CA-C	-6.06	97.95	113.10
1	A	266	ASP	N-CA-CB	6.04	121.47	110.60
1	D	435	GLY	N-CA-C	-6.02	98.04	113.10
1	C	55	ASP	N-CA-C	-6.00	94.81	111.00
1	C	114	LYS	N-CA-C	5.99	127.17	111.00
1	D	362	ALA	N-CA-CB	5.93	118.41	110.10
1	B	387	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	115	LYS	N-CA-C	-5.88	95.11	111.00
1	C	494	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	414	ILE	CB-CA-C	5.87	123.34	111.60
1	B	203	GLU	CA-CB-CG	5.87	126.31	113.40
1	D	116	LEU	N-CA-C	5.86	126.83	111.00
1	A	54	ALA	CB-CA-C	5.85	118.87	110.10
1	A	437	VAL	N-CA-C	-5.83	95.25	111.00
1	B	464	ILE	N-CA-C	-5.82	95.30	111.00
1	C	152	SER	O-C-N	-5.81	113.40	122.70
1	A	473	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	D	56	LYS	N-CA-CB	5.79	121.02	110.60
1	A	35	THR	N-CA-CB	5.79	121.30	110.30
1	A	393	ILE	CB-CA-C	-5.77	100.07	111.60
1	B	393	ILE	CA-CB-CG1	5.76	121.94	111.00
1	A	425	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	C	434	ALA	CB-CA-C	-5.74	101.49	110.10
1	C	34	GLY	N-CA-C	-5.70	98.86	113.10
1	C	242	ASP	CA-C-N	5.68	127.56	116.20
1	D	592	LEU	CB-CA-C	5.66	120.96	110.20
1	D	146	GLU	CB-CA-C	5.65	121.71	110.40
1	B	434	ALA	CB-CA-C	-5.65	101.62	110.10
1	B	394	ASP	N-CA-CB	5.64	120.76	110.60
1	C	585	LEU	N-CA-C	-5.61	95.85	111.00
1	B	395	PHE	CB-CA-C	-5.61	99.19	110.40
1	D	393	ILE	CB-CA-C	-5.60	100.41	111.60
1	A	394	ASP	CB-CA-C	5.59	121.58	110.40
1	C	33	GLU	CB-CA-C	-5.58	99.24	110.40
1	D	116	LEU	N-CA-CB	-5.56	99.27	110.40
1	C	144	ALA	CA-C-N	5.55	129.42	117.20
1	C	242	ASP	N-CA-CB	5.54	120.57	110.60
1	A	144	ALA	N-CA-C	-5.54	96.05	111.00
1	D	394	ASP	N-CA-C	-5.54	96.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	86	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	C	395	PHE	N-CA-CB	5.51	120.52	110.60
1	B	53	ASP	CB-CA-C	5.51	121.41	110.40
1	C	601	ILE	CB-CA-C	5.49	122.58	111.60
1	B	346	PHE	CB-CG-CD2	-5.49	116.95	120.80
1	B	154	ALA	CB-CA-C	-5.49	101.87	110.10
1	A	594	GLN	N-CA-C	-5.48	96.20	111.00
1	A	119	LYS	CB-CA-C	-5.47	99.46	110.40
1	B	35	THR	CB-CA-C	5.46	126.33	111.60
1	D	143	GLY	O-C-N	-5.41	114.04	122.70
1	C	53	ASP	CB-CA-C	5.40	121.20	110.40
1	C	521	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	64	GLY	N-CA-C	-5.37	99.67	113.10
1	C	72	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	111	TYR	N-CA-C	5.37	125.50	111.00
1	A	280	ASP	N-CA-C	-5.37	96.51	111.00
1	B	36	ASP	N-CA-C	-5.37	96.52	111.00
1	D	585	LEU	CB-CA-C	5.35	120.36	110.20
1	A	58	LYS	CD-CE-NZ	5.35	124.00	111.70
1	D	61	LYS	N-CA-C	-5.33	96.60	111.00
1	A	160	SER	CB-CA-C	-5.33	99.98	110.10
1	C	140	GLN	CB-CA-C	5.32	121.05	110.40
1	B	113	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	145	GLU	N-CA-C	-5.30	96.69	111.00
1	A	124	LEU	N-CA-C	5.30	125.30	111.00
1	C	568	TRP	CB-CA-C	-5.29	99.81	110.40
1	C	144	ALA	N-CA-C	-5.28	96.75	111.00
1	A	362	ALA	N-CA-CB	5.26	117.46	110.10
1	A	473	ARG	CB-CG-CD	5.25	125.26	111.60
1	B	474	LEU	CA-CB-CG	5.25	127.39	115.30
1	B	318	HIS	N-CA-C	-5.25	96.83	111.00
1	A	55	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	226	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	239	GLU	N-CA-CB	5.24	120.03	110.60
1	D	123	LEU	N-CA-CB	5.24	120.88	110.40
1	D	55	ASP	N-CA-CB	-5.23	101.19	110.60
1	A	122	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	245	VAL	CB-CA-C	5.17	121.23	111.40
1	A	218	LYS	CA-CB-CG	5.17	124.78	113.40
1	A	225	ASN	CB-CA-C	5.14	120.68	110.40
1	A	411	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	D	594	GLN	N-CA-C	-5.11	97.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	539	GLN	CB-CA-C	-5.11	100.18	110.40
1	A	474	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	318	HIS	O-C-N	-5.08	114.57	123.20
1	C	111	TYR	N-CA-CB	-5.06	101.50	110.60
1	D	59	GLU	CB-CA-C	5.04	120.47	110.40
1	B	319	GLY	N-CA-C	-5.04	100.51	113.10

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	GLY	Mainchain
1	A	157	GLY	Mainchain
1	A	244	TYR	Mainchain
1	A	475	GLN	Peptide
1	A	518	SER	Peptide
1	A	519	ASN	Peptide
1	A	592	LEU	Peptide
1	A	72	ASP	Peptide
1	B	137	GLU	Peptide
1	B	457	ALA	Peptide
1	B	72	ASP	Peptide
1	C	139	TYR	Mainchain
1	C	142	TYR	Mainchain,Peptide
1	C	152	SER	Mainchain
1	C	242	ASP	Mainchain
1	C	244	TYR	Sidechain
1	C	534	LYS	Mainchain
1	D	137	GLU	Peptide
1	D	143	GLY	Mainchain

5.2 Too-close contacts (i)

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	4543	0	4470	151	0
1	B	4618	0	4540	145	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4562	0	4491	258	0
1	D	4592	0	4505	211	1
All	All	18315	0	18006	708	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (708) 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:141:LEU:HD21	1:A:215:HIS:CE1	1.26	1.63
1:D:142:TYR:CE2	1:D:615:ILE:HG12	1.29	1.56
1:D:142:TYR:CE2	1:D:615:ILE:CG1	1.77	1.56
1:C:135:MET:CG	1:D:159:PRO:HD2	1.18	1.52
1:C:458:ALA:N	1:C:594:GLN:HB3	1.30	1.46
1:C:458:ALA:HA	1:C:594:GLN:CG	1.51	1.40
1:A:141:LEU:HD23	1:A:215:HIS:CG	1.57	1.40
1:C:135:MET:CG	1:D:159:PRO:CD	1.97	1.38
1:C:458:ALA:CB	1:C:594:GLN:OE1	1.71	1.37
1:C:458:ALA:CA	1:C:594:GLN:HG2	1.55	1.35
1:C:135:MET:HG3	1:D:159:PRO:CD	1.52	1.34
1:D:117:THR:HG21	1:D:127:ASN:N	1.43	1.33
1:C:151:LYS:HZ2	1:D:224:GLN:NE2	1.28	1.32
1:A:141:LEU:CD2	1:A:215:HIS:CE1	2.16	1.29
1:C:458:ALA:N	1:C:594:GLN:CB	1.97	1.28
1:C:135:MET:SD	1:D:159:PRO:CD	2.16	1.27
1:C:135:MET:HB2	1:C:180:ASP:OD2	1.25	1.26
1:C:137:GLU:HG2	1:D:136:TYR:CE2	1.68	1.26
1:A:141:LEU:HD23	1:A:215:HIS:CD2	1.70	1.26
1:A:141:LEU:CD2	1:A:215:HIS:CG	2.19	1.23
1:A:136:TYR:OH	1:A:360:GLU:OE2	1.54	1.23
1:A:143:GLY:HA3	1:A:146:GLU:CG	1.67	1.22
1:C:93:PRO:HD2	1:C:138:GLU:OE1	1.05	1.21
1:D:141:LEU:HD21	1:D:215:HIS:NE2	1.56	1.21
1:D:142:TYR:CD2	1:D:615:ILE:HG13	1.75	1.21
1:C:55:ASP:O	1:C:56:LYS:HD2	1.39	1.20
1:B:484:ALA:O	1:B:487:SER:O	1.60	1.19
1:C:135:MET:HE1	1:D:158:ASN:ND2	1.56	1.19
1:C:135:MET:SD	1:D:159:PRO:HD2	1.79	1.19
1:C:497:ARG:CD	1:C:599:GLN:HE22	1.57	1.17
1:A:139:TYR:HD2	1:A:142:TYR:CE2	1.62	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:CD2	1:A:215:HIS:ND1	2.09	1.16
1:D:142:TYR:CE2	1:D:615:ILE:HG13	1.57	1.16
1:A:143:GLY:CA	1:A:146:GLU:HG2	1.74	1.15
1:D:340:GLN:O	1:D:341:THR:HG23	1.43	1.15
1:C:497:ARG:CG	1:C:599:GLN:HE22	1.60	1.14
1:C:589:TRP:O	1:C:592:LEU:CD2	1.94	1.14
1:A:141:LEU:HD21	1:A:215:HIS:NE2	1.62	1.13
1:A:141:LEU:CD2	1:A:215:HIS:CD2	2.30	1.13
1:A:16:GLY:O	1:A:17:ARG:NH1	1.82	1.12
1:C:529:GLU:O	1:C:532:GLY:O	1.64	1.11
1:B:310:ARG:HA	1:B:346:PHE:HZ	1.08	1.10
1:A:16:GLY:O	1:A:17:ARG:CZ	1.99	1.10
1:A:144:ALA:HB1	1:B:141:LEU:HD11	1.25	1.10
1:C:137:GLU:CG	1:D:136:TYR:CE2	2.35	1.10
1:C:497:ARG:CD	1:C:599:GLN:NE2	2.15	1.09
1:C:137:GLU:HG2	1:D:136:TYR:CD2	1.88	1.08
1:A:144:ALA:CB	1:B:141:LEU:HD11	1.83	1.07
1:C:93:PRO:CD	1:C:138:GLU:OE1	2.01	1.07
1:A:141:LEU:HD21	1:A:215:HIS:ND1	1.66	1.07
1:B:534:LYS:O	1:B:534:LYS:NZ	1.86	1.07
1:A:139:TYR:CD2	1:A:142:TYR:CE2	2.42	1.06
1:D:141:LEU:HD21	1:D:215:HIS:CD2	1.90	1.06
1:C:458:ALA:CA	1:C:594:GLN:CG	2.22	1.06
1:D:136:TYR:OH	1:D:140:GLN:OE1	1.72	1.05
1:C:151:LYS:NZ	1:D:224:GLN:NE2	2.04	1.05
1:C:458:ALA:HB2	1:C:594:GLN:OE1	0.88	1.05
1:C:497:ARG:HD2	1:C:599:GLN:OE1	1.57	1.04
1:A:139:TYR:CD2	1:A:142:TYR:HE2	1.73	1.03
1:C:151:LYS:NZ	1:D:224:GLN:HE21	1.56	1.02
1:C:135:MET:CB	1:C:180:ASP:OD2	2.08	1.01
1:A:393:ILE:O	1:A:393:ILE:HG13	1.61	1.00
1:C:93:PRO:HD2	1:C:138:GLU:CD	1.82	0.99
1:C:589:TRP:O	1:C:592:LEU:HD21	1.61	0.99
1:B:310:ARG:HA	1:B:346:PHE:CZ	1.97	0.99
1:C:136:TYR:CE1	1:C:218:LYS:HD2	1.98	0.99
1:C:135:MET:HE1	1:D:158:ASN:HD22	0.83	0.98
1:D:117:THR:CG2	1:D:127:ASN:N	2.25	0.98
1:B:353:LYS:O	1:B:356:ILE:O	1.80	0.98
1:B:529:GLU:OE1	1:B:535:GLU:CD	2.02	0.97
1:C:497:ARG:HG2	1:C:599:GLN:HE22	1.25	0.97
1:C:135:MET:CE	1:D:158:ASN:HD22	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:NZ	1:D:221:MET:HA	1.81	0.96
1:A:218:LYS:NZ	1:A:360:GLU:OE1	1.99	0.95
1:C:497:ARG:NE	1:C:599:GLN:NE2	2.15	0.95
1:C:9:ILE:HD11	1:C:194:CYS:SG	2.07	0.95
1:C:219:TYR:HA	1:C:222:LEU:HD13	1.45	0.94
1:C:497:ARG:HD2	1:C:599:GLN:CD	1.87	0.94
1:C:137:GLU:CD	1:D:136:TYR:CE2	2.41	0.94
1:D:142:TYR:CD2	1:D:615:ILE:CG1	2.43	0.94
1:D:117:THR:HG22	1:D:127:ASN:HB3	1.49	0.93
1:C:497:ARG:NE	1:C:599:GLN:HE22	1.65	0.93
1:C:137:GLU:OE1	1:D:140:GLN:OE1	1.87	0.93
1:A:393:ILE:O	1:A:393:ILE:CG1	2.15	0.92
1:C:144:ALA:O	1:C:146:GLU:N	2.01	0.92
1:B:30:ASN:O	1:B:33:GLU:O	1.88	0.92
1:A:310:ARG:HD3	1:A:341:THR:HG21	1.50	0.92
1:C:458:ALA:HB2	1:C:594:GLN:CD	1.90	0.91
1:D:115:LYS:NZ	1:D:117:THR:HG23	1.85	0.91
1:C:497:ARG:CG	1:C:599:GLN:NE2	2.30	0.91
1:B:110:GLY:HA3	1:B:600:LYS:HE2	1.53	0.90
1:D:114:LYS:HG3	1:D:114:LYS:O	1.71	0.90
1:D:115:LYS:HE2	1:D:128:VAL:CG2	2.02	0.89
1:D:393:ILE:HG13	1:D:393:ILE:O	1.70	0.89
1:D:141:LEU:CD2	1:D:215:HIS:NE2	2.35	0.89
1:D:581:TRP:O	1:D:583:LYS:O	1.90	0.89
1:A:581:TRP:O	1:A:583:LYS:O	1.90	0.89
1:D:393:ILE:O	1:D:393:ILE:CG1	2.20	0.89
1:C:151:LYS:HZ1	1:D:221:MET:HA	1.36	0.88
1:D:279:HIS:CD2	1:D:436:GLY:O	2.26	0.88
1:D:116:LEU:H	1:D:116:LEU:HD23	1.39	0.88
1:A:141:LEU:CD2	1:A:215:HIS:NE2	2.27	0.88
1:C:474:LEU:HD22	1:C:477:ARG:CZ	2.02	0.88
1:D:141:LEU:HD13	1:D:142:TYR:N	1.90	0.87
1:A:520:LEU:O	1:A:523:LEU:HD12	1.74	0.86
1:A:30:ASN:O	1:A:33:GLU:O	1.93	0.86
1:A:228:LEU:HD22	1:A:244:TYR:O	1.75	0.85
1:C:151:LYS:HG3	1:C:152:SER:H	1.41	0.85
1:C:279:HIS:CD2	1:C:436:GLY:O	2.28	0.85
1:D:142:TYR:HE2	1:D:615:ILE:CG1	1.39	0.85
1:C:137:GLU:OE1	1:D:140:GLN:CD	2.16	0.84
1:C:497:ARG:HG2	1:C:599:GLN:NE2	1.91	0.84
1:C:153:LEU:HD11	1:D:221:MET:HG3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:NH2	1:B:213:SER:O	2.09	0.84
1:C:30:ASN:O	1:C:33:GLU:O	1.96	0.84
1:C:136:TYR:CD1	1:C:218:LYS:HD2	2.13	0.83
1:D:256:LYS:HE2	1:D:260:LYS:HB2	1.60	0.83
1:C:135:MET:HB2	1:C:180:ASP:CG	1.99	0.83
1:C:135:MET:SD	1:D:159:PRO:HD3	2.16	0.83
1:D:115:LYS:HE2	1:D:128:VAL:HG23	1.59	0.83
1:A:40:GLU:OE2	1:A:48:HIS:HE1	1.61	0.83
1:A:310:ARG:HD3	1:A:341:THR:CG2	2.09	0.83
1:C:592:LEU:H	1:C:592:LEU:HD23	1.43	0.82
1:C:135:MET:CG	1:D:159:PRO:HD3	2.06	0.82
1:C:393:ILE:O	1:C:393:ILE:HG13	1.77	0.82
1:B:93:PRO:HG2	1:B:139:TYR:OH	1.80	0.82
1:D:233:ARG:NH2	1:D:354:SER:O	2.12	0.82
1:B:592:LEU:CD2	1:B:594:GLN:H	1.91	0.82
1:D:568:TRP:O	1:D:571:LYS:HE2	1.79	0.82
1:C:151:LYS:HZ1	1:D:221:MET:CA	1.92	0.82
1:A:140:GLN:C	1:A:142:TYR:H	1.81	0.82
1:B:359:CYS:HB2	1:B:362:ALA:O	1.79	0.82
1:A:144:ALA:CB	1:B:141:LEU:CD1	2.58	0.81
1:A:142:TYR:O	1:A:143:GLY:C	2.17	0.80
1:A:581:TRP:C	1:A:583:LYS:O	2.20	0.80
1:C:294:GLN:OE1	1:C:329:GLU:OE1	1.99	0.80
1:D:88:ALA:C	1:D:89:LYS:O	2.04	0.80
1:C:139:TYR:HB3	1:C:142:TYR:O	1.80	0.80
1:A:279:HIS:CD2	1:A:436:GLY:O	2.35	0.80
1:A:279:HIS:ND1	1:A:280:ASP:O	2.15	0.80
1:A:519:ASN:OD1	1:A:520:LEU:C	2.21	0.80
1:C:581:TRP:O	1:C:583:LYS:O	1.99	0.79
1:C:393:ILE:O	1:C:393:ILE:CG1	2.30	0.79
1:D:581:TRP:C	1:D:583:LYS:O	2.19	0.79
1:B:581:TRP:O	1:B:583:LYS:O	2.01	0.79
1:C:140:GLN:OE1	1:C:151:LYS:O	2.00	0.79
1:D:340:GLN:O	1:D:341:THR:CG2	2.30	0.79
1:B:588:ASN:O	1:B:590:ASP:O	2.01	0.78
1:D:30:ASN:O	1:D:33:GLU:O	2.00	0.78
1:C:9:ILE:CD1	1:C:194:CYS:SG	2.72	0.77
1:A:519:ASN:OD1	1:A:520:LEU:O	2.03	0.76
1:C:612:ARG:O	1:C:612:ARG:HG2	1.86	0.76
1:B:460:HIS:CG	1:B:461:PRO:HD3	2.20	0.76
1:C:135:MET:HG3	1:D:159:PRO:HD2	0.76	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLY:HA3	1:A:146:GLU:HG2	0.81	0.76
1:C:135:MET:HG3	1:D:159:PRO:CG	2.16	0.76
1:C:589:TRP:O	1:C:592:LEU:HD22	1.86	0.76
1:D:273:LYS:HE3	1:D:444:GLU:HB2	1.69	0.75
1:B:398:THR:HG22	1:B:399:PRO:HD2	1.68	0.75
1:C:137:GLU:HG2	1:D:136:TYR:HE2	1.47	0.75
1:B:156:THR:HG23	1:B:156:THR:O	1.87	0.75
1:C:152:SER:O	1:C:157:GLY:N	2.20	0.75
1:D:115:LYS:HZ3	1:D:117:THR:HG23	1.50	0.75
1:A:517:VAL:HB	1:A:519:ASN:HD22	1.51	0.74
1:A:218:LYS:CE	1:A:360:GLU:OE1	2.35	0.74
1:C:136:TYR:CE1	1:C:218:LYS:CD	2.69	0.74
1:C:592:LEU:HD23	1:C:592:LEU:N	2.03	0.74
1:D:73:VAL:O	1:D:96:ARG:NH2	2.20	0.74
1:B:345:GLN:HG2	1:B:401:LYS:HD2	1.68	0.74
1:B:560:ASP:OD1	1:B:561:MET:N	2.20	0.74
1:D:372:LEU:O	1:D:375:MET:HG3	1.86	0.74
1:C:497:ARG:CD	1:C:599:GLN:CD	2.51	0.74
1:C:497:ARG:CD	1:C:599:GLN:OE1	2.34	0.74
1:C:581:TRP:C	1:C:583:LYS:O	2.25	0.74
1:C:329:GLU:OE1	1:C:329:GLU:HA	1.87	0.73
1:B:346:PHE:HD2	1:B:399:PRO:HB3	1.54	0.73
1:C:273:LYS:HE3	1:C:444:GLU:HB2	1.69	0.73
1:B:70:LEU:HG	1:B:248:GLU:OE2	1.88	0.73
1:C:134:VAL:HG21	1:C:210:VAL:O	1.89	0.73
1:C:529:GLU:C	1:C:532:GLY:O	2.28	0.72
1:C:140:GLN:HA	1:C:140:GLN:NE2	2.03	0.72
1:A:523:LEU:HD13	1:A:524:GLU:H	1.53	0.72
1:D:492:GLU:C	1:D:493:ALA:O	2.18	0.72
1:C:228:LEU:HD22	1:C:244:TYR:O	1.88	0.72
1:A:485:LEU:HD13	1:A:523:LEU:HD23	1.72	0.72
1:C:138:GLU:HG2	1:C:139:TYR:CD2	2.25	0.71
1:D:76:PHE:CD1	1:D:96:ARG:HG3	2.24	0.71
1:C:151:LYS:NZ	1:D:221:MET:CA	2.50	0.71
1:D:591:LYS:HE3	1:D:591:LYS:N	2.06	0.70
1:A:91:MET:HG3	1:A:96:ARG:HH12	1.54	0.70
1:A:144:ALA:HB1	1:B:141:LEU:CD1	2.14	0.70
1:C:581:TRP:HD1	1:C:587:LEU:HD11	1.55	0.70
1:D:117:THR:HG22	1:D:127:ASN:CB	2.20	0.70
1:D:473:ARG:HD2	1:D:473:ARG:N	2.06	0.70
1:B:555:PHE:HA	1:B:561:MET:SD	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:HD3	1:C:610:LYS:HA	1.73	0.70
1:A:140:GLN:C	1:A:142:TYR:N	2.46	0.70
1:C:458:ALA:CA	1:C:594:GLN:CB	2.61	0.70
1:C:566:GLU:OE2	1:C:591:LYS:NZ	2.25	0.70
1:C:581:TRP:CD1	1:C:587:LEU:HD11	2.27	0.69
1:C:318:HIS:CE1	1:C:320:THR:HG22	2.27	0.69
1:D:141:LEU:CD2	1:D:215:HIS:CD2	2.74	0.69
1:C:144:ALA:HB3	1:C:146:GLU:OE1	1.92	0.69
1:A:173:ASN:OD1	1:B:279:HIS:O	2.11	0.69
1:B:110:GLY:CA	1:B:600:LYS:HE2	2.22	0.69
1:C:135:MET:CE	1:D:158:ASN:ND2	2.43	0.69
1:C:359:CYS:HB2	1:C:362:ALA:O	1.93	0.69
1:D:116:LEU:HD23	1:D:116:LEU:N	2.06	0.69
1:A:139:TYR:CE2	1:A:142:TYR:HE2	2.10	0.69
1:D:115:LYS:HZ1	1:D:117:THR:HG23	1.55	0.69
1:B:460:HIS:CD2	1:B:461:PRO:HD3	2.28	0.69
1:B:346:PHE:HD2	1:B:399:PRO:CB	2.05	0.68
1:A:142:TYR:O	1:A:144:ALA:N	2.26	0.68
1:C:235:GLU:H	1:C:244:TYR:HE1	1.42	0.68
1:A:340:GLN:HG3	1:A:340:GLN:O	1.93	0.68
1:A:318:HIS:O	1:A:329:GLU:OE1	2.11	0.67
1:B:581:TRP:C	1:B:583:LYS:O	2.32	0.67
1:B:589:TRP:HA	1:B:591:LYS:HG3	1.76	0.67
1:C:244:TYR:N	1:C:244:TYR:CD2	2.61	0.67
1:A:445:GLU:OE1	1:A:445:GLU:N	2.27	0.67
1:B:359:CYS:CB	1:B:362:ALA:O	2.43	0.67
1:A:122:ASP:O	1:A:123:LEU:HG	1.95	0.66
1:B:505:GLY:HA3	1:B:600:LYS:NZ	2.10	0.66
1:B:6:ARG:CZ	1:B:304:ASP:O	2.44	0.66
1:C:229:SER:HB2	1:C:243:GLY:O	1.95	0.66
1:C:458:ALA:CB	1:C:594:GLN:CD	2.56	0.66
1:C:497:ARG:HE	1:C:599:GLN:NE2	1.94	0.66
1:D:110:GLY:O	1:D:600:LYS:HE2	1.96	0.65
1:C:137:GLU:CD	1:D:136:TYR:CZ	2.69	0.65
1:D:256:LYS:CE	1:D:260:LYS:HB2	2.26	0.65
1:D:142:TYR:HE2	1:D:615:ILE:HG12	0.57	0.65
1:A:523:LEU:HD13	1:A:524:GLU:N	2.11	0.65
1:C:256:LYS:HD3	1:C:257:PRO:HD2	1.77	0.65
1:D:141:LEU:O	1:D:141:LEU:HD22	1.96	0.65
1:D:228:LEU:HD22	1:D:244:TYR:O	1.95	0.65
1:B:592:LEU:HD22	1:B:594:GLN:H	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD22	1:B:244:TYR:O	1.97	0.65
1:C:474:LEU:HD22	1:C:477:ARG:NH2	2.11	0.65
1:C:497:ARG:HE	1:C:599:GLN:HE22	1.45	0.65
1:C:137:GLU:CG	1:D:136:TYR:CD2	2.70	0.64
1:C:530:PHE:CE1	1:C:540:LEU:HD22	2.31	0.64
1:A:93:PRO:HA	1:A:96:ARG:HD2	1.79	0.64
1:B:501:THR:HG23	1:B:600:LYS:HE3	1.80	0.64
1:C:515:MET:SD	1:C:516:ILE:N	2.69	0.64
1:C:134:VAL:CG2	1:C:210:VAL:O	2.46	0.64
1:D:516:ILE:HD13	1:D:574:ALA:HB1	1.78	0.64
1:B:600:LYS:HG3	1:B:601:ILE:H	1.63	0.63
1:D:114:LYS:O	1:D:114:LYS:CG	2.46	0.63
1:B:529:GLU:OE1	1:B:535:GLU:OE2	2.15	0.63
1:C:16:GLY:O	1:C:17:ARG:HD3	1.98	0.63
1:C:533:GLY:O	1:C:534:LYS:HB2	1.97	0.63
1:A:218:LYS:HE2	1:A:360:GLU:OE1	1.97	0.63
1:B:353:LYS:HD3	1:B:353:LYS:N	2.13	0.63
1:C:148:ALA:O	1:C:151:LYS:HD3	1.98	0.63
1:D:141:LEU:CD2	1:D:215:HIS:CE1	2.82	0.63
1:D:141:LEU:HD13	1:D:141:LEU:C	2.19	0.62
1:A:116:LEU:HD13	1:A:171:GLY:O	1.99	0.62
1:A:375:MET:HG2	1:A:445:GLU:OE2	1.99	0.62
1:C:141:LEU:O	1:C:143:GLY:O	2.17	0.62
1:A:120:SER:OG	1:A:122:ASP:OD1	2.18	0.62
1:A:234:CYS:HA	1:A:244:TYR:CE1	2.35	0.61
1:D:101:CYS:HA	1:D:104:GLU:HG2	1.82	0.61
1:C:136:TYR:CE1	1:C:218:LYS:HG3	2.35	0.61
1:D:53:ASP:C	1:D:54:ALA:O	2.30	0.61
1:D:112:THR:HB	1:D:114:LYS:HG2	1.83	0.61
1:C:153:LEU:HG	1:D:221:MET:SD	2.41	0.61
1:D:115:LYS:HE2	1:D:128:VAL:HG21	1.81	0.61
1:C:310:ARG:NH1	1:C:341:THR:O	2.34	0.61
1:D:53:ASP:CG	1:D:54:ALA:O	2.38	0.61
1:B:70:LEU:N	1:B:248:GLU:OE1	2.34	0.60
1:C:17:ARG:NE	1:C:101:CYS:SG	2.74	0.60
1:C:592:LEU:CD2	1:C:592:LEU:H	2.12	0.60
1:D:141:LEU:HD21	1:D:215:HIS:HE2	1.63	0.60
1:D:76:PHE:CD1	1:D:96:ARG:CG	2.83	0.60
1:C:244:TYR:CE2	1:C:321:GLY:C	2.75	0.60
1:D:142:TYR:CZ	1:D:615:ILE:CG1	2.70	0.60
1:B:103:TYR:OH	1:B:507:GLU:OE2	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:LYS:HG3	1:C:152:SER:N	2.16	0.60
1:D:353:LYS:HD2	1:D:358:HIS:ND1	2.16	0.60
1:D:375:MET:O	1:D:378:LYS:HD2	2.02	0.60
1:D:119:LYS:HE2	1:D:173:ASN:CG	2.21	0.60
1:C:151:LYS:HZ3	1:D:224:GLN:HE21	1.49	0.60
1:A:63:TYR:HE2	1:A:230:SER:O	1.84	0.60
1:A:425:ARG:HB2	1:A:445:GLU:CD	2.21	0.60
1:B:529:GLU:HB3	1:B:535:GLU:HG3	1.83	0.60
1:B:11:ILE:HD11	1:B:372:LEU:CD1	2.31	0.59
1:C:458:ALA:CA	1:C:594:GLN:HB3	2.26	0.59
1:D:258:LEU:HG	1:D:262:LYS:HE3	1.85	0.59
1:C:54:ALA:O	1:C:55:ASP:C	2.40	0.59
1:C:93:PRO:CD	1:C:138:GLU:CD	2.59	0.59
1:C:606:TYR:HB3	1:C:607:PRO:HD2	1.85	0.59
1:A:139:TYR:O	1:A:142:TYR:CD2	2.54	0.59
1:B:35:THR:O	1:B:384:LEU:HD21	2.03	0.59
1:C:477:ARG:HH22	1:C:513:LEU:HB3	1.68	0.59
1:B:534:LYS:O	1:B:534:LYS:CG	2.50	0.59
1:C:468:ALA:CB	1:C:474:LEU:HD21	2.33	0.59
1:B:592:LEU:CD2	1:B:594:GLN:N	2.66	0.59
1:C:222:LEU:HG	1:C:228:LEU:HG	1.85	0.59
1:C:591:LYS:O	1:C:593:TYR:CD2	2.56	0.59
1:D:430:SER:HB3	1:D:432:PHE:HE1	1.68	0.59
1:B:155:LEU:O	1:B:156:THR:HG22	2.03	0.58
1:C:135:MET:CG	1:C:180:ASP:OD2	2.51	0.58
1:A:120:SER:OG	1:A:122:ASP:CG	2.42	0.58
1:C:9:ILE:HG13	1:C:272:ILE:HB	1.85	0.58
1:C:90:LEU:HB3	1:C:155:LEU:HG	1.86	0.58
1:C:592:LEU:HG	1:C:592:LEU:O	2.03	0.58
1:A:134:VAL:HG11	1:A:162:ILE:HD13	1.86	0.58
1:B:580:LEU:O	1:B:583:LYS:O	2.22	0.58
1:C:477:ARG:NH2	1:C:513:LEU:HB3	2.19	0.58
1:C:539:GLN:C	1:C:540:LEU:HD12	2.23	0.58
1:A:244:TYR:CD2	1:A:320:THR:O	2.56	0.58
1:B:534:LYS:HD3	1:B:534:LYS:N	2.17	0.58
1:C:474:LEU:HD22	1:C:477:ARG:NE	2.17	0.58
1:D:95:GLU:CB	1:D:162:ILE:HD13	2.34	0.58
1:A:91:MET:SD	1:A:96:ARG:NH1	2.77	0.58
1:C:138:GLU:OE2	1:C:139:TYR:CE2	2.57	0.58
1:C:137:GLU:CG	1:D:136:TYR:HE2	2.09	0.57
1:C:55:ASP:O	1:C:56:LYS:CD	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:TYR:CE1	1:C:218:LYS:CG	2.88	0.57
1:C:141:LEU:O	1:C:141:LEU:HD12	2.05	0.57
1:C:148:ALA:HB3	1:C:151:LYS:HD2	1.86	0.57
1:C:136:TYR:HE1	1:C:218:LYS:HG3	1.68	0.57
1:D:17:ARG:HB3	1:D:70:LEU:HD11	1.87	0.57
1:D:115:LYS:CE	1:D:128:VAL:CG2	2.82	0.57
1:A:91:MET:CG	1:A:96:ARG:HH12	2.17	0.57
1:A:555:PHE:CD2	1:A:585:LEU:HD13	2.39	0.57
1:B:589:TRP:CA	1:B:591:LYS:HG3	2.35	0.56
1:C:494:ASP:OD1	1:C:494:ASP:O	2.23	0.56
1:C:242:ASP:O	1:C:244:TYR:CE2	2.58	0.56
1:C:592:LEU:HD12	1:C:594:GLN:HE22	1.70	0.56
1:A:50:LEU:HD23	1:A:50:LEU:O	2.05	0.56
1:A:139:TYR:CD2	1:A:142:TYR:CD2	2.91	0.56
1:C:70:LEU:HG	1:C:248:GLU:OE1	2.04	0.56
1:C:497:ARG:HG3	1:C:599:GLN:OE1	2.05	0.56
1:C:135:MET:HG2	1:D:159:PRO:CD	2.24	0.56
1:D:143:GLY:O	1:D:144:ALA:C	2.40	0.56
1:A:93:PRO:HA	1:A:96:ARG:CD	2.35	0.56
1:B:529:GLU:OE1	1:B:535:GLU:OE1	2.24	0.56
1:A:318:HIS:CD2	1:A:320:THR:HG22	2.41	0.56
1:A:318:HIS:HD2	1:A:320:THR:HG22	1.71	0.56
1:B:534:LYS:O	1:B:534:LYS:HG2	2.05	0.56
1:D:116:LEU:H	1:D:116:LEU:CD2	2.01	0.56
1:A:17:ARG:NE	1:A:17:ARG:HA	2.21	0.55
1:B:310:ARG:HG3	1:B:346:PHE:CZ	2.40	0.55
1:D:142:TYR:CZ	1:D:615:ILE:HG12	2.20	0.55
1:B:93:PRO:CG	1:B:139:TYR:OH	2.54	0.55
1:D:217:ASN:OD1	1:D:218:LYS:N	2.40	0.55
1:A:244:TYR:CG	1:A:320:THR:O	2.60	0.55
1:B:580:LEU:HD12	1:B:583:LYS:HE2	1.87	0.55
1:C:566:GLU:CD	1:C:591:LYS:NZ	2.61	0.55
1:A:135:MET:HB3	1:A:136:TYR:CE2	2.41	0.54
1:A:484:ALA:HB1	1:A:489:ARG:CZ	2.37	0.54
1:C:497:ARG:CG	1:C:599:GLN:OE1	2.55	0.54
1:B:351:SER:OG	1:B:353:LYS:HB2	2.07	0.54
1:D:14:ILE:HG22	1:D:253:VAL:HG12	1.90	0.54
1:A:330:ILE:CG2	1:A:400:PHE:CZ	2.91	0.54
1:D:432:PHE:CD2	1:D:438:ASN:HB3	2.42	0.54
1:B:371:VAL:HG11	1:B:443:ILE:HD12	1.89	0.54
1:C:94:GLN:OE1	1:C:162:ILE:HD11	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:TYR:HD1	1:C:142:TYR:HB2	1.73	0.54
1:C:592:LEU:HD12	1:C:594:GLN:NE2	2.21	0.54
1:B:592:LEU:HD23	1:B:594:GLN:H	1.71	0.54
1:C:144:ALA:O	1:C:145:GLU:C	2.22	0.54
1:B:279:HIS:CD2	1:B:436:GLY:O	2.61	0.54
1:A:14:ILE:HG22	1:A:253:VAL:HG12	1.90	0.54
1:B:134:VAL:HG11	1:B:162:ILE:HD13	1.90	0.53
1:C:489:ARG:NH1	1:C:490:TYR:OH	2.41	0.53
1:B:414:ILE:HG12	1:B:422:GLU:N	2.24	0.53
1:C:144:ALA:C	1:C:146:GLU:N	2.60	0.53
1:D:115:LYS:NZ	1:D:117:THR:CG2	2.67	0.53
1:A:63:TYR:CE2	1:A:230:SER:O	2.61	0.53
1:A:137:GLU:OE2	1:A:158:ASN:N	2.42	0.53
1:B:14:ILE:HG22	1:B:253:VAL:HG12	1.90	0.53
1:B:136:TYR:OH	1:B:139:TYR:N	2.41	0.53
1:A:66:TRP:HE3	1:A:67:GLY:N	2.06	0.53
1:C:51:TYR:HA	1:C:61:LYS:HE3	1.91	0.53
1:C:140:GLN:NE2	1:C:140:GLN:CA	2.72	0.53
1:B:505:GLY:HA3	1:B:600:LYS:HZ3	1.72	0.53
1:C:152:SER:O	1:C:157:GLY:CA	2.57	0.53
1:D:591:LYS:HE3	1:D:591:LYS:H	1.71	0.53
1:C:234:CYS:HA	1:C:244:TYR:CD1	2.43	0.53
1:D:87:ASP:C	1:D:89:LYS:O	2.47	0.53
1:A:88:ALA:O	1:A:91:MET:HG2	2.09	0.53
1:A:160:SER:O	1:A:164:ASN:CG	2.48	0.52
1:C:530:PHE:CZ	1:C:540:LEU:HD22	2.43	0.52
1:A:330:ILE:HG23	1:A:400:PHE:CZ	2.44	0.52
1:B:179:LEU:HD21	1:B:189:ALA:HB2	1.90	0.52
1:C:458:ALA:N	1:C:594:GLN:HB2	2.11	0.52
1:A:47:ASP:O	1:A:50:LEU:HD22	2.09	0.52
1:C:497:ARG:CG	1:C:599:GLN:CD	2.75	0.52
1:C:111:TYR:O	1:C:111:TYR:CG	2.62	0.52
1:A:244:TYR:CE1	1:A:321:GLY:HA3	2.44	0.52
1:C:75:LYS:HD3	1:C:610:LYS:CA	2.40	0.52
1:D:95:GLU:CA	1:D:162:ILE:HD13	2.40	0.52
1:D:116:LEU:HD12	1:D:203:GLU:OE1	2.09	0.52
1:D:593:TYR:N	1:D:593:TYR:CD2	2.77	0.52
1:B:368:LEU:HD13	1:B:443:ILE:HD11	1.91	0.52
1:C:566:GLU:OE1	1:C:591:LYS:NZ	2.42	0.52
1:C:6:ARG:HG3	1:C:7:GLU:OE2	2.10	0.51
1:A:182:MET:SD	1:B:158:ASN:ND2	2.81	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:ALA:HA	1:C:594:GLN:HG2	0.64	0.51
1:D:234:CYS:SG	1:D:245:VAL:HG12	2.51	0.51
1:D:430:SER:HB3	1:D:432:PHE:CE1	2.46	0.51
1:D:492:GLU:HG3	1:D:520:LEU:CD2	2.40	0.51
1:B:592:LEU:HD21	1:B:594:GLN:HA	1.92	0.51
1:C:359:CYS:CB	1:C:362:ALA:O	2.57	0.51
1:C:14:ILE:HG22	1:C:253:VAL:HG12	1.91	0.51
1:C:136:TYR:CE2	1:C:218:LYS:NZ	2.62	0.51
1:B:6:ARG:NH2	1:B:304:ASP:O	2.43	0.51
1:B:344:LYS:O	1:B:345:GLN:C	2.48	0.51
1:C:138:GLU:OE2	1:C:139:TYR:HE2	1.92	0.51
1:B:255:LEU:O	1:B:256:LYS:HG3	2.09	0.51
1:C:90:LEU:O	1:C:155:LEU:HD12	2.10	0.51
1:D:87:ASP:HA	1:D:90:LEU:HD23	1.92	0.51
1:D:141:LEU:HD22	1:D:141:LEU:C	2.30	0.51
1:D:491:ARG:O	1:D:493:ALA:O	2.29	0.51
1:B:234:CYS:SG	1:B:245:VAL:HG12	2.51	0.51
1:C:244:TYR:CZ	1:C:321:GLY:HA3	2.45	0.51
1:B:46:TRP:NE1	1:B:214:VAL:O	2.32	0.51
1:C:414:ILE:HB	1:C:423:LEU:HD12	1.92	0.51
1:C:580:LEU:HD12	1:C:583:LYS:HE2	1.92	0.51
1:C:55:ASP:N	1:C:55:ASP:OD1	2.43	0.51
1:C:203:GLU:O	1:C:256:LYS:HD3	2.11	0.51
1:D:551:THR:HG21	1:D:583:LYS:NZ	2.25	0.51
1:C:458:ALA:CB	1:C:594:GLN:CG	2.89	0.50
1:D:96:ARG:HE	1:D:97:LEU:HG	1.76	0.50
1:D:173:ASN:CG	1:D:173:ASN:O	2.49	0.50
1:B:425:ARG:NH2	1:B:445:GLU:HG3	2.27	0.50
1:B:501:THR:HG23	1:B:600:LYS:CE	2.41	0.50
1:C:135:MET:HG3	1:C:180:ASP:OD2	2.11	0.50
1:C:458:ALA:CA	1:C:594:GLN:CD	2.76	0.50
1:A:17:ARG:CZ	1:A:23:ASN:HA	2.41	0.50
1:A:158:ASN:OD1	1:A:159:PRO:HD2	2.10	0.50
1:B:438:ASN:OD1	1:B:438:ASN:N	2.44	0.50
1:A:393:ILE:O	1:A:393:ILE:CD1	2.58	0.50
1:C:139:TYR:CD1	1:C:142:TYR:HB2	2.46	0.50
1:D:145:GLU:OE1	1:D:146:GLU:CD	2.50	0.50
1:A:544:GLN:HB3	1:A:547:GLN:HB2	1.94	0.50
1:A:136:TYR:OH	1:A:360:GLU:CD	2.41	0.50
1:C:93:PRO:CD	1:C:138:GLU:OE2	2.60	0.50
1:C:242:ASP:O	1:C:244:TYR:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLN:O	1:A:142:TYR:N	2.45	0.50
1:A:555:PHE:HD2	1:A:585:LEU:HD13	1.76	0.50
1:D:103:TYR:OH	1:D:507:GLU:HG3	2.11	0.50
1:D:536:SER:HA	1:D:540:LEU:HD21	1.94	0.50
1:A:66:TRP:HE3	1:A:67:GLY:CA	2.25	0.50
1:D:141:LEU:HD23	1:D:215:HIS:CE1	2.47	0.50
1:A:555:PHE:O	1:A:561:MET:SD	2.70	0.49
1:B:497:ARG:HG2	1:B:599:GLN:O	2.12	0.49
1:D:599:GLN:OE1	1:D:600:LYS:O	2.29	0.49
1:A:135:MET:HB3	1:A:136:TYR:CD2	2.47	0.49
1:A:515:MET:HG3	1:A:526:LYS:CD	2.42	0.49
1:B:416:GLU:O	1:B:417:ASN:HB2	2.12	0.49
1:D:573:LYS:HG3	1:D:576:LYS:HD3	1.94	0.49
1:A:310:ARG:O	1:A:345:GLN:HG2	2.12	0.49
1:A:158:ASN:ND2	1:B:182:MET:SD	2.82	0.49
1:A:497:ARG:HG2	1:A:599:GLN:O	2.11	0.49
1:B:93:PRO:HG2	1:B:139:TYR:CZ	2.48	0.49
1:B:137:GLU:HB2	1:B:138:GLU:HG3	1.95	0.49
1:C:222:LEU:HG	1:C:228:LEU:CG	2.43	0.49
1:D:95:GLU:HA	1:D:162:ILE:HD13	1.95	0.49
1:D:256:LYS:HD2	1:D:257:PRO:HD2	1.95	0.49
1:A:489:ARG:HH22	1:A:604:PRO:HD3	1.77	0.49
1:C:16:GLY:C	1:C:17:ARG:HD3	2.32	0.49
1:D:116:LEU:N	1:D:116:LEU:CD2	2.72	0.49
1:D:393:ILE:O	1:D:393:ILE:CD1	2.60	0.49
1:A:414:ILE:O	1:A:414:ILE:HG22	2.13	0.49
1:B:535:GLU:HB3	1:B:537:ILE:CD1	2.43	0.49
1:C:267:HIS:HE1	1:C:602:SER:HB2	1.78	0.49
1:B:534:LYS:O	1:B:534:LYS:CD	2.60	0.48
1:B:334:THR:HG23	1:B:398:THR:HG23	1.95	0.48
1:C:445:GLU:OE1	1:C:445:GLU:HA	2.13	0.48
1:A:17:ARG:CZ	1:A:17:ARG:HA	2.43	0.48
1:D:95:GLU:HA	1:D:162:ILE:CD1	2.43	0.48
1:D:87:ASP:O	1:D:89:LYS:O	2.31	0.48
1:D:474:LEU:HD11	1:D:511:GLU:HB3	1.94	0.48
1:A:145:GLU:O	1:A:145:GLU:CD	2.52	0.48
1:C:212:VAL:HA	1:C:248:GLU:HG2	1.95	0.48
1:A:310:ARG:CD	1:A:341:THR:HG21	2.32	0.48
1:A:476:LYS:HA	1:A:479:LYS:HB2	1.96	0.48
1:B:91:MET:CE	1:B:96:ARG:HE	2.27	0.48
1:B:368:LEU:CD1	1:B:443:ILE:HD11	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:GLN:HB3	1:B:541:TYR:CE1	2.49	0.48
1:C:112:THR:HG23	1:C:113:ARG:N	2.29	0.48
1:C:243:GLY:C	1:C:244:TYR:CD2	2.86	0.48
1:D:445:GLU:OE1	1:D:445:GLU:HA	2.14	0.48
1:D:497:ARG:HG3	1:D:599:GLN:O	2.14	0.48
1:A:48:HIS:C	1:A:48:HIS:CD2	2.87	0.48
1:A:358:HIS:O	1:A:359:CYS:C	2.50	0.48
1:C:590:ASP:C	1:C:592:LEU:HD23	2.34	0.48
1:D:75:LYS:NZ	1:D:609:ALA:O	2.38	0.48
1:A:66:TRP:CE3	1:A:67:GLY:N	2.82	0.47
1:B:11:ILE:HD11	1:B:372:LEU:HD11	1.94	0.47
1:B:38:ILE:HD11	1:B:357:GLY:N	2.29	0.47
1:D:529:GLU:OE1	1:D:530:PHE:N	2.46	0.47
1:A:137:GLU:OE2	1:A:157:GLY:HA2	2.13	0.47
1:B:505:GLY:HA3	1:B:600:LYS:HZ1	1.79	0.47
1:A:116:LEU:HB3	1:A:125:GLY:HA2	1.96	0.47
1:A:474:LEU:HD11	1:A:511:GLU:HB3	1.96	0.47
1:A:489:ARG:NH2	1:A:604:PRO:HD3	2.30	0.47
1:B:134:VAL:HG21	1:B:162:ILE:HD13	1.97	0.47
1:C:568:TRP:CD2	1:C:577:VAL:HG21	2.49	0.47
1:C:107:GLU:OE1	1:C:506:ARG:NH1	2.48	0.47
1:A:143:GLY:O	1:A:146:GLU:O	2.31	0.47
1:B:248:GLU:HG3	1:B:249:GLY:N	2.28	0.47
1:C:229:SER:CB	1:C:243:GLY:O	2.61	0.47
1:B:99:LEU:HD11	1:B:165:ARG:HG3	1.95	0.47
1:D:183:CYS:HB2	1:D:433:GLY:HA2	1.97	0.47
1:C:219:TYR:O	1:C:222:LEU:HD22	2.15	0.47
1:C:256:LYS:NZ	1:C:260:LYS:HD2	2.30	0.47
1:A:144:ALA:HB2	1:B:141:LEU:CD1	2.41	0.47
1:C:72:ASP:HB2	1:C:75:LYS:HE3	1.96	0.47
1:C:107:GLU:OE2	1:C:606:TYR:CE2	2.68	0.47
1:D:139:TYR:CD1	1:D:139:TYR:C	2.88	0.47
1:B:262:LYS:HE3	1:B:446:TYR:CZ	2.50	0.47
1:B:294:GLN:NE2	1:B:432:PHE:CZ	2.83	0.47
1:A:229:SER:HB2	1:A:243:GLY:O	2.15	0.47
1:D:551:THR:HG21	1:D:583:LYS:HZ2	1.79	0.47
1:C:151:LYS:HZ1	1:D:221:MET:N	2.13	0.46
1:B:179:LEU:HD11	1:B:185:SER:O	2.16	0.46
1:C:606:TYR:HB3	1:C:607:PRO:CD	2.45	0.46
1:D:212:VAL:HA	1:D:248:GLU:HG2	1.97	0.46
1:C:244:TYR:CG	1:C:320:THR:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:MET:HG3	1:D:526:LYS:HZ3	1.80	0.46
1:D:127:ASN:N	1:D:173:ASN:H	2.13	0.46
1:B:445:GLU:OE1	1:B:446:TYR:O	2.34	0.46
1:D:515:MET:HG3	1:D:526:LYS:NZ	2.30	0.46
1:A:122:ASP:O	1:A:123:LEU:CG	2.63	0.46
1:B:414:ILE:HD12	1:B:414:ILE:H	1.79	0.46
1:B:587:LEU:HD11	1:B:589:TRP:CD2	2.51	0.46
1:C:234:CYS:HA	1:C:244:TYR:CE1	2.51	0.46
1:D:569:LEU:HD13	1:D:592:LEU:HA	1.96	0.46
1:C:137:GLU:CD	1:D:136:TYR:HH	2.19	0.46
1:C:423:LEU:HD23	1:C:424:PRO:HD2	1.98	0.46
1:D:515:MET:SD	1:D:517:VAL:HG13	2.56	0.46
1:A:587:LEU:HD11	1:A:589:TRP:CD2	2.50	0.46
1:B:395:PHE:CD1	1:B:395:PHE:C	2.89	0.46
1:B:539:GLN:HB3	1:B:541:TYR:CZ	2.51	0.46
1:A:520:LEU:O	1:A:523:LEU:CD1	2.57	0.46
1:B:589:TRP:C	1:B:591:LYS:HG3	2.35	0.46
1:C:135:MET:HE3	1:C:135:MET:HB3	1.70	0.45
1:C:137:GLU:OE1	1:D:140:GLN:CG	2.63	0.45
1:D:555:PHE:CZ	1:D:586:PRO:O	2.69	0.45
1:D:587:LEU:HD11	1:D:589:TRP:CD2	2.52	0.45
1:B:378:LYS:HG2	1:B:425:ARG:NH1	2.31	0.45
1:B:390:ASN:O	1:B:393:ILE:HG23	2.15	0.45
1:C:151:LYS:HZ3	1:D:221:MET:CB	2.29	0.45
1:C:509:MET:CE	1:C:606:TYR:CE2	2.99	0.45
1:D:377:HIS:O	1:D:379:GLN:HG3	2.16	0.45
1:C:348:ALA:HB1	1:C:403:GLN:CG	2.46	0.45
1:D:38:ILE:HG12	1:D:233:ARG:NH1	2.32	0.45
1:B:432:PHE:HD1	1:B:438:ASN:HB3	1.82	0.45
1:C:153:LEU:CD1	1:D:221:MET:HG3	2.37	0.45
1:A:423:LEU:HD23	1:A:424:PRO:HD2	1.99	0.45
1:B:423:LEU:HD23	1:B:424:PRO:HD2	1.98	0.45
1:C:464:ILE:HD11	1:C:517:VAL:HG21	1.98	0.45
1:D:92:ASP:OD1	1:D:92:ASP:N	2.49	0.45
1:C:151:LYS:HZ3	1:D:221:MET:HA	1.77	0.45
1:A:183:CYS:HB2	1:A:433:GLY:HA2	1.97	0.45
1:B:152:SER:O	1:B:157:GLY:HA3	2.16	0.45
1:C:137:GLU:OE1	1:D:136:TYR:CE2	2.69	0.45
1:D:493:ALA:O	1:D:494:ASP:OD1	2.35	0.45
1:C:17:ARG:NH2	1:C:104:GLU:OE1	2.50	0.45
1:C:135:MET:HG2	1:C:135:MET:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:CD1	1:A:171:GLY:O	2.65	0.44
1:C:580:LEU:O	1:C:583:LYS:O	2.35	0.44
1:D:101:CYS:HA	1:D:104:GLU:CG	2.47	0.44
1:A:40:GLU:CD	1:A:48:HIS:HE1	2.19	0.44
1:B:35:THR:O	1:B:384:LEU:CD2	2.65	0.44
1:B:297:VAL:HG21	1:B:438:ASN:HB2	1.97	0.44
1:C:571:LYS:H	1:C:571:LYS:HG2	1.69	0.44
1:D:516:ILE:CD1	1:D:574:ALA:HB1	2.44	0.44
1:C:348:ALA:HB1	1:C:403:GLN:CD	2.38	0.44
1:C:135:MET:HG2	1:D:159:PRO:HD3	1.95	0.44
1:D:423:LEU:HD23	1:D:424:PRO:HD2	1.98	0.44
1:A:13:GLY:HA3	1:A:109:ALA:HB2	1.99	0.44
1:A:515:MET:SD	1:A:517:VAL:HG13	2.57	0.44
1:C:135:MET:HE2	1:D:158:ASN:HB3	1.62	0.44
1:A:12:ILE:HD13	1:A:256:LYS:HG2	1.99	0.44
1:A:69:PHE:HA	1:A:248:GLU:OE2	2.18	0.44
1:A:112:THR:O	1:A:115:LYS:HB2	2.18	0.44
1:A:135:MET:HE2	1:A:360:GLU:HG2	1.99	0.44
1:A:460:HIS:ND1	1:A:461:PRO:O	2.51	0.44
1:C:380:LEU:HD13	1:C:403:GLN:HE22	1.83	0.44
1:D:13:GLY:HA3	1:D:109:ALA:HB2	2.00	0.44
1:D:588:ASN:CG	1:D:591:LYS:NZ	2.72	0.44
1:A:244:TYR:CE2	1:A:320:THR:O	2.71	0.44
1:B:93:PRO:HD2	1:B:139:TYR:CE1	2.52	0.43
1:D:106:MET:HG2	1:D:111:TYR:O	2.17	0.43
1:C:468:ALA:CB	1:C:474:LEU:CD2	2.96	0.43
1:D:53:ASP:CB	1:D:54:ALA:O	2.67	0.43
1:D:460:HIS:HB3	1:D:461:PRO:HD3	1.99	0.43
1:B:535:GLU:HB3	1:B:537:ILE:HD11	2.00	0.43
1:C:13:GLY:HA3	1:C:109:ALA:HB2	1.99	0.43
1:D:117:THR:HG21	1:D:127:ASN:CA	2.38	0.43
1:D:138:GLU:HB3	1:D:214:VAL:HG21	2.00	0.43
1:B:73:VAL:O	1:B:96:ARG:NH1	2.51	0.43
1:B:260:LYS:CE	1:B:264:ASP:HB2	2.48	0.43
1:C:152:SER:C	1:C:157:GLY:H	2.19	0.43
1:C:8:ASP:N	1:C:8:ASP:OD1	2.51	0.43
1:D:183:CYS:HG	1:D:358:HIS:HE2	1.63	0.43
1:A:12:ILE:HD13	1:A:256:LYS:CG	2.49	0.43
1:B:13:GLY:HA3	1:B:109:ALA:HB2	1.99	0.43
1:B:589:TRP:O	1:B:591:LYS:HG3	2.19	0.43
1:C:468:ALA:HB2	1:C:474:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:GLN:HB2	1:C:540:LEU:HD12	2.01	0.43
1:D:95:GLU:CA	1:D:162:ILE:CD1	2.97	0.43
1:B:94:GLN:NE2	1:B:134:VAL:HG12	2.34	0.43
1:C:468:ALA:HB3	1:C:474:LEU:HD21	2.00	0.43
1:C:515:MET:HG2	1:C:526:LYS:HD3	2.01	0.43
1:A:561:MET:SD	1:A:561:MET:C	2.97	0.43
1:C:587:LEU:N	1:C:587:LEU:HD12	2.34	0.43
1:D:115:LYS:HD2	1:D:128:VAL:HG21	2.01	0.43
1:A:415:ASN:ND2	1:C:387:ARG:O	2.51	0.43
1:B:260:LYS:HE3	1:B:264:ASP:HB2	2.00	0.43
1:B:318:HIS:CE1	1:B:432:PHE:O	2.72	0.43
1:B:487:SER:O	1:B:487:SER:OG	2.34	0.43
1:C:127:ASN:OD1	1:C:203:GLU:HG3	2.18	0.43
1:C:585:LEU:HG	1:C:587:LEU:HG	2.00	0.43
1:D:90:LEU:O	1:D:90:LEU:HG	2.19	0.42
1:D:476:LYS:HG2	1:D:479:LYS:HE3	2.01	0.42
1:D:615:ILE:N	1:D:615:ILE:HD13	2.33	0.42
1:C:458:ALA:HA	1:C:594:GLN:CD	2.31	0.42
1:D:38:ILE:HD11	1:D:357:GLY:N	2.34	0.42
1:D:145:GLU:OE1	1:D:145:GLU:C	2.58	0.42
1:B:204:ALA:HB2	1:B:256:LYS:CG	2.49	0.42
1:C:41:ILE:HG12	1:C:65:LYS:O	2.19	0.42
1:C:158:ASN:ND2	1:D:182:MET:SD	2.83	0.42
1:D:14:ILE:HG12	1:D:269:TYR:CE2	2.54	0.42
1:D:233:ARG:HE	1:D:385:HIS:CD2	2.37	0.42
1:D:571:LYS:H	1:D:571:LYS:HG3	1.71	0.42
1:B:139:TYR:OH	1:B:614:TRP:CH2	2.64	0.42
1:B:535:GLU:CB	1:B:537:ILE:HD12	2.49	0.42
1:C:14:ILE:HG12	1:C:269:TYR:CE2	2.55	0.42
1:D:393:ILE:O	1:D:393:ILE:HD12	2.20	0.42
1:A:14:ILE:HG12	1:A:269:TYR:CE2	2.55	0.42
1:D:88:ALA:CA	1:D:89:LYS:O	2.68	0.42
1:D:115:LYS:CE	1:D:128:VAL:HG21	2.47	0.42
1:A:66:TRP:CE3	1:A:67:GLY:CA	3.01	0.42
1:A:490:TYR:CE2	1:A:601:ILE:HD11	2.54	0.42
1:C:318:HIS:CE1	1:C:432:PHE:O	2.72	0.42
1:C:526:LYS:CG	1:C:540:LEU:HD21	2.49	0.42
1:D:117:THR:CG2	1:D:127:ASN:CA	2.96	0.42
1:A:226:ARG:O	1:A:226:ARG:HG2	2.20	0.42
1:B:52:TYR:HA	1:B:65:LYS:HE3	2.02	0.42
1:C:346:PHE:CD2	1:C:399:PRO:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LEU:O	1:D:90:LEU:CG	2.67	0.42
1:D:117:THR:CG2	1:D:127:ASN:HB3	2.35	0.42
1:D:526:LYS:O	1:D:529:GLU:OE1	2.38	0.42
1:B:346:PHE:HD2	1:B:399:PRO:HB2	1.82	0.42
1:B:535:GLU:HB2	1:B:537:ILE:HD12	2.02	0.42
1:C:566:GLU:CD	1:C:591:LYS:HZ3	2.22	0.42
1:D:41:ILE:HG12	1:D:65:LYS:O	2.19	0.42
1:D:65:LYS:HB3	1:D:66:TRP:CE3	2.55	0.42
1:D:599:GLN:HG2	1:D:600:LYS:N	2.34	0.42
1:B:432:PHE:CD1	1:B:438:ASN:HB3	2.55	0.41
1:C:9:ILE:HD13	1:C:194:CYS:SG	2.58	0.41
1:D:143:GLY:O	1:D:144:ALA:O	2.38	0.41
1:B:11:ILE:CD1	1:B:372:LEU:HD11	2.50	0.41
1:B:535:GLU:CB	1:B:537:ILE:CD1	2.97	0.41
1:B:592:LEU:HD23	1:B:594:GLN:N	2.34	0.41
1:B:398:THR:CG2	1:B:399:PRO:HD2	2.46	0.41
1:B:566:GLU:HA	1:B:569:LEU:HD23	2.02	0.41
1:C:275:THR:HG22	1:C:441:ILE:HD12	2.03	0.41
1:D:76:PHE:CD1	1:D:96:ARG:HG2	2.55	0.41
1:A:275:THR:HG22	1:A:441:ILE:HD12	2.02	0.41
1:C:353:LYS:HD3	1:C:358:HIS:CD2	2.55	0.41
1:C:506:ARG:NH2	1:C:604:PRO:O	2.51	0.41
1:B:275:THR:HG22	1:B:441:ILE:HD12	2.03	0.41
1:C:509:MET:HE2	1:C:606:TYR:CE2	2.55	0.41
1:D:600:LYS:HD2	1:D:600:LYS:HA	1.90	0.41
1:A:96:ARG:HG2	1:A:97:LEU:N	2.36	0.41
1:A:561:MET:SD	1:A:562:GLU:HG2	2.61	0.41
1:B:14:ILE:HG12	1:B:269:TYR:CE2	2.55	0.41
1:B:589:TRP:O	1:B:591:LYS:N	2.54	0.41
1:C:137:GLU:OE1	1:D:140:GLN:HG2	2.21	0.41
1:C:377:HIS:O	1:C:379:GLN:HG3	2.20	0.41
1:D:36:ASP:CG	1:D:233:ARG:NH1	2.73	0.41
1:A:144:ALA:HB2	1:B:141:LEU:HD13	2.03	0.41
1:A:377:HIS:O	1:A:379:GLN:HG3	2.21	0.41
1:D:115:LYS:HZ3	1:D:117:THR:CG2	2.25	0.41
1:A:159:PRO:O	1:A:178:ALA:HB2	2.21	0.41
1:B:592:LEU:CD2	1:B:592:LEU:C	2.89	0.41
1:C:151:LYS:NZ	1:D:221:MET:CB	2.84	0.41
1:C:217:ASN:HD22	1:D:140:GLN:HE22	1.68	0.41
1:C:515:MET:SD	1:C:539:GLN:O	2.79	0.41
1:D:36:ASP:OD1	1:D:233:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:MET:SD	1:D:376:LYS:N	2.94	0.41
1:C:140:GLN:OE1	1:C:152:SER:HB3	2.21	0.41
1:A:490:TYR:CZ	1:A:601:ILE:HD11	2.56	0.40
1:B:6:ARG:NH1	1:B:304:ASP:O	2.53	0.40
1:B:85:PRO:O	1:B:89:LYS:HG2	2.22	0.40
1:C:93:PRO:CG	1:C:138:GLU:OE2	2.69	0.40
1:C:474:LEU:HD23	1:C:474:LEU:HA	1.79	0.40
1:D:96:ARG:HD2	1:D:97:LEU:N	2.36	0.40
1:B:72:ASP:HB2	1:B:75:LYS:HD3	2.03	0.40
1:B:507:GLU:CG	1:B:509:MET:HE2	2.52	0.40
1:A:489:ARG:HD2	1:A:490:TYR:CE2	2.57	0.40
1:A:548:ASN:ND2	1:A:548:ASN:H	2.20	0.40
1:B:342:GLN:HE21	1:B:342:GLN:HB2	1.58	0.40
1:C:353:LYS:HB2	1:C:353:LYS:HE2	1.83	0.40
1:D:72:ASP:HB2	1:D:75:LYS:HD3	2.03	0.40
1:D:183:CYS:SG	1:D:358:HIS:NE2	2.83	0.40
1:D:555:PHE:O	1:D:558:ASP:OD2	2.38	0.40
1:A:183:CYS:SG	1:A:358:HIS:NE2	2.93	0.40
1:C:356:ILE:HD12	1:C:359:CYS:SG	2.62	0.40
1:D:275:THR:HG22	1:D:441:ILE:HD12	2.02	0.40
1:B:294:GLN:HE21	1:B:294:GLN:HB3	1.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ARG:O	1:D:405:THR:OG1[2_646]	2.01	0.19

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	572/640 (89%)	529 (92%)	40 (7%)	3 (0%)	29 68
1	B	583/640 (91%)	543 (93%)	38 (6%)	2 (0%)	41 76
1	C	574/640 (90%)	533 (93%)	41 (7%)	0	100 100
1	D	578/640 (90%)	543 (94%)	35 (6%)	0	100 100
All	All	2307/2560 (90%)	2148 (93%)	154 (7%)	5 (0%)	47 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	ASP
1	A	141	LEU
1	A	142	TYR
1	B	113	ARG
1	B	246	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	479/524 (91%)	420 (88%)	59 (12%)	4 22
1	B	488/524 (93%)	411 (84%)	77 (16%)	2 16
1	C	482/524 (92%)	414 (86%)	68 (14%)	3 19
1	D	484/524 (92%)	414 (86%)	70 (14%)	3 18
All	All	1933/2096 (92%)	1659 (86%)	274 (14%)	3 19

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	8	ASP
1	A	17	ARG
1	A	22	GLU
1	A	41	ILE
1	A	45	ARG

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Mol	Chain	Res	Type
1	A	48	HIS
1	A	50	LEU
1	A	52	TYR
1	A	61	LYS
1	A	71	LYS
1	A	95	GLU
1	A	96	ARG
1	A	118	GLU
1	A	142	TYR
1	A	145	GLU
1	A	165	ARG
1	A	201	GLU
1	A	218	LYS
1	A	226	ARG
1	A	228	LEU
1	A	231	LYS
1	A	234	CYS
1	A	239	GLU
1	A	244	TYR
1	A	260	LYS
1	A	267	HIS
1	A	280	ASP
1	A	300	GLN
1	A	308	ASP
1	A	341	THR
1	A	346	PHE
1	A	353	LYS
1	A	376	LYS
1	A	387	ARG
1	A	388	THR
1	A	404	GLN
1	A	407	GLU
1	A	423	LEU
1	A	438	ASN
1	A	442	VAL
1	A	466	LEU
1	A	470	ASN
1	A	476	LYS
1	A	483	ASP
1	A	510	GLU
1	A	519	ASN
1	A	520	LEU

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Mol	Chain	Res	Type
1	A	523	LEU
1	A	531	THR
1	A	534	LYS
1	A	535	GLU
1	A	539	GLN
1	A	547	GLN
1	A	548	ASN
1	A	549	LYS
1	A	550	ASP
1	A	552	MET
1	A	571	LYS
1	B	7	GLU
1	B	8	ASP
1	B	11	ILE
1	B	17	ARG
1	B	23	ASN
1	B	25	GLN
1	B	33	GLU
1	B	46	TRP
1	B	48	HIS
1	B	59	GLU
1	B	71	LYS
1	B	75	LYS
1	B	89	LYS
1	B	90	LEU
1	B	96	ARG
1	B	101	CYS
1	B	115	LYS
1	B	117	THR
1	B	134	VAL
1	B	135	MET
1	B	141	LEU
1	B	151	LYS
1	B	165	ARG
1	B	179	LEU
1	B	198	ARG
1	B	201	GLU
1	B	220	LEU
1	B	221	MET
1	B	228	LEU
1	B	239	GLU
1	B	260	LYS

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Mol	Chain	Res	Type
1	B	267	HIS
1	B	280	ASP
1	B	294	GLN
1	B	300	GLN
1	B	308	ASP
1	B	344	LYS
1	B	353	LYS
1	B	387	ARG
1	B	388	THR
1	B	393	ILE
1	B	394	ASP
1	B	398	THR
1	B	404	GLN
1	B	405	THR
1	B	414	ILE
1	B	416	GLU
1	B	417	ASN
1	B	423	LEU
1	B	438	ASN
1	B	442	VAL
1	B	445	GLU
1	B	466	LEU
1	B	469	LYS
1	B	473	ARG
1	B	491	ARG
1	B	515	MET
1	B	520	LEU
1	B	523	LEU
1	B	524	GLU
1	B	525	GLU
1	B	531	THR
1	B	534	LYS
1	B	535	GLU
1	B	547	GLN
1	B	551	THR
1	B	561	MET
1	B	571	LYS
1	B	573	LYS
1	B	583	LYS
1	B	590	ASP
1	B	592	LEU
1	B	597	ARG

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Mol	Chain	Res	Type
1	B	599	GLN
1	B	612	ARG
1	B	615	ILE
1	B	616	ASP
1	C	8	ASP
1	C	23	ASN
1	C	41	ILE
1	C	46	TRP
1	C	48	HIS
1	C	55	ASP
1	C	56	LYS
1	C	75	LYS
1	C	92	ASP
1	C	96	ARG
1	C	113	ARG
1	C	135	MET
1	C	140	GLN
1	C	141	LEU
1	C	145	GLU
1	C	146	GLU
1	C	151	LYS
1	C	155	LEU
1	C	201	GLU
1	C	218	LYS
1	C	220	LEU
1	C	222	LEU
1	C	228	LEU
1	C	233	ARG
1	C	234	CYS
1	C	239	GLU
1	C	300	GLN
1	C	308	ASP
1	C	320	THR
1	C	329	GLU
1	C	339	GLU
1	C	344	LYS
1	C	346	PHE
1	C	353	LYS
1	C	376	LYS
1	C	378	LYS
1	C	388	THR
1	C	410	LYS

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Mol	Chain	Res	Type
1	C	413	VAL
1	C	417	ASN
1	C	423	LEU
1	C	438	ASN
1	C	442	VAL
1	C	466	LEU
1	C	472	GLN
1	C	477	ARG
1	C	480	ARG
1	C	507	GLU
1	C	515	MET
1	C	520	LEU
1	C	521	ARG
1	C	523	LEU
1	C	524	GLU
1	C	531	THR
1	C	534	LYS
1	C	549	LYS
1	C	551	THR
1	C	552	MET
1	C	566	GLU
1	C	571	LYS
1	C	573	LYS
1	C	583	LYS
1	C	587	LEU
1	C	591	LYS
1	C	592	LEU
1	C	594	GLN
1	C	599	GLN
1	C	612	ARG
1	D	6	ARG
1	D	7	GLU
1	D	8	ASP
1	D	26	GLU
1	D	41	ILE
1	D	48	HIS
1	D	58	LYS
1	D	63	TYR
1	D	65	LYS
1	D	71	LYS
1	D	75	LYS
1	D	90	LEU

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Mol	Chain	Res	Type
1	D	92	ASP
1	D	96	ARG
1	D	101	CYS
1	D	115	LYS
1	D	116	LEU
1	D	138	GLU
1	D	141	LEU
1	D	142	TYR
1	D	145	GLU
1	D	146	GLU
1	D	147	GLN
1	D	149	ARG
1	D	158	ASN
1	D	165	ARG
1	D	201	GLU
1	D	214	VAL
1	D	218	LYS
1	D	228	LEU
1	D	300	GLN
1	D	308	ASP
1	D	342	GLN
1	D	375	MET
1	D	376	LYS
1	D	387	ARG
1	D	388	THR
1	D	422	GLU
1	D	423	LEU
1	D	438	ASN
1	D	442	VAL
1	D	463	MET
1	D	466	LEU
1	D	469	LYS
1	D	470	ASN
1	D	472	GLN
1	D	473	ARG
1	D	476	LYS
1	D	477	ARG
1	D	480	ARG
1	D	486	ARG
1	D	492	GLU
1	D	494	ASP
1	D	516	ILE

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Mol	Chain	Res	Type
1	D	520	LEU
1	D	523	LEU
1	D	525	GLU
1	D	529	GLU
1	D	531	THR
1	D	536	SER
1	D	540	LEU
1	D	555	PHE
1	D	558	ASP
1	D	561	MET
1	D	563	LYS
1	D	571	LYS
1	D	580	LEU
1	D	591	LYS
1	D	597	ARG
1	D	599	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	173	ASN
1	A	211	ASN
1	A	377	HIS
1	A	385	HIS
1	A	548	ASN
1	B	48	HIS
1	B	279	HIS
1	B	318	HIS
1	B	342	GLN
1	B	404	GLN
1	B	547	GLN
1	C	217	ASN
1	C	225	ASN
1	C	267	HIS
1	C	318	HIS
1	C	377	HIS
1	C	403	GLN
1	C	417	ASN
1	C	599	GLN
1	D	158	ASN
1	D	164	ASN

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Mol	Chain	Res	Type
1	D	224	GLN
1	D	225	ASN
1	D	279	HIS
1	D	292	ASN
1	D	377	HIS
1	D	385	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	584/640 (91%)	-0.23	6 (1%)	82	74	23, 191, 295, 377	0
1	B	593/640 (92%)	-0.20	6 (1%)	82	74	30, 189, 285, 364	0
1	C	586/640 (91%)	-0.18	6 (1%)	82	74	23, 193, 285, 402	0
1	D	590/640 (92%)	-0.19	11 (1%)	66	58	23, 191, 285, 399	0
All	All	2353/2560 (91%)	-0.20	29 (1%)	79	70	23, 191, 290, 402	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	557	ALA	4.8
1	A	60	GLY	3.5
1	C	344	LYS	3.4
1	C	422	GLU	3.4
1	B	154	ALA	3.3
1	D	559	GLU	2.8
1	D	136	TYR	2.8
1	A	570	GLU	2.7
1	A	48	HIS	2.7
1	B	230	SER	2.6
1	D	140	GLN	2.6
1	D	556	THR	2.6
1	D	63	TYR	2.6
1	D	611	ASP	2.5
1	D	64	GLY	2.4
1	C	48	HIS	2.4
1	B	553	ALA	2.3
1	B	22	GLU	2.3
1	D	570	GLU	2.2
1	B	463	MET	2.2
1	C	610	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	540	LEU	2.1
1	D	552	MET	2.1
1	C	492	GLU	2.1
1	A	534	LYS	2.1
1	B	64	GLY	2.0
1	A	46	TRP	2.0
1	D	610	LYS	2.0
1	C	465	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.