Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 06:59 PM EDT

PDB ID	:	3T8L
Title	:	Crystal Structure of adenine deaminase with Mn/Fe
Authors	:	Bagaria, A.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2011-08-01
Resolution	:	2.80 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:

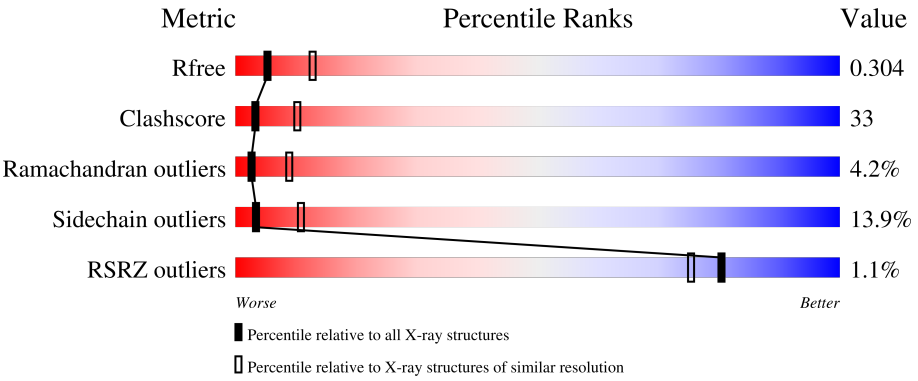
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	608	41% 37% 14%
1	B	608	2% 34% 40% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	606	-	-	-	X
2	UNX	A	607	-	-	-	X
2	UNX	A	608	-	-	-	X
2	UNX	B	606	-	-	-	X
2	UNX	B	607	-	-	-	X
2	UNX	B	608	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8761 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 Adenine deaminase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	Se	0	0	0
			4337	2723	775	817	6	16			
1	B	587	Total	C	N	O	S	Se	0	0	0
			4335	2721	775	817	6	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	expression tag	UNP Q7CUX4
A	-1	SER	-	expression tag	UNP Q7CUX4
A	0	LEU	-	expression tag	UNP Q7CUX4
A	598	GLU	-	expression tag	UNP Q7CUX4
A	599	GLY	-	expression tag	UNP Q7CUX4
A	600	HIS	-	expression tag	UNP Q7CUX4
A	601	HIS	-	expression tag	UNP Q7CUX4
A	602	HIS	-	expression tag	UNP Q7CUX4
A	603	HIS	-	expression tag	UNP Q7CUX4
A	604	HIS	-	expression tag	UNP Q7CUX4
A	605	HIS	-	expression tag	UNP Q7CUX4
B	-2	MSE	-	expression tag	UNP Q7CUX4
B	-1	SER	-	expression tag	UNP Q7CUX4
B	0	LEU	-	expression tag	UNP Q7CUX4
B	598	GLU	-	expression tag	UNP Q7CUX4
B	599	GLY	-	expression tag	UNP Q7CUX4
B	600	HIS	-	expression tag	UNP Q7CUX4
B	601	HIS	-	expression tag	UNP Q7CUX4
B	602	HIS	-	expression tag	UNP Q7CUX4
B	603	HIS	-	expression tag	UNP Q7CUX4
B	604	HIS	-	expression tag	UNP Q7CUX4
B	605	HIS	-	expression tag	UNP Q7CUX4

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 3 is water.

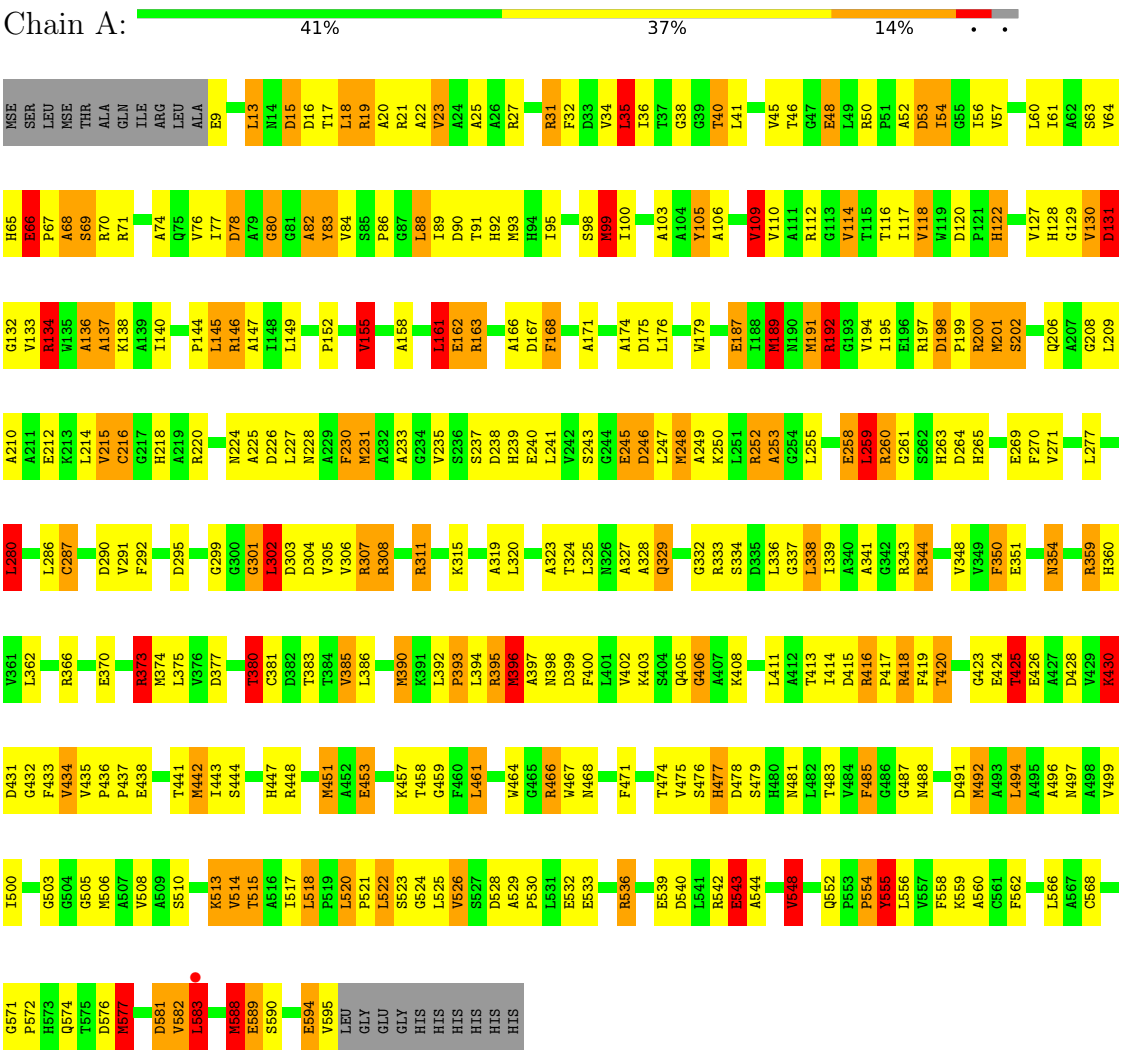
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	33	Total O 33 33	0	0
3	B	50	Total O 50 50	0	0

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.

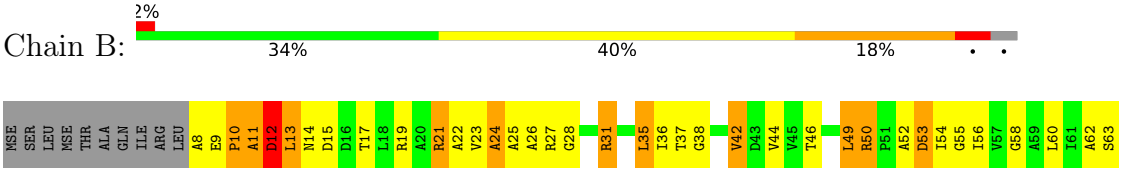
• Molecule 1: Adenine deaminase 2

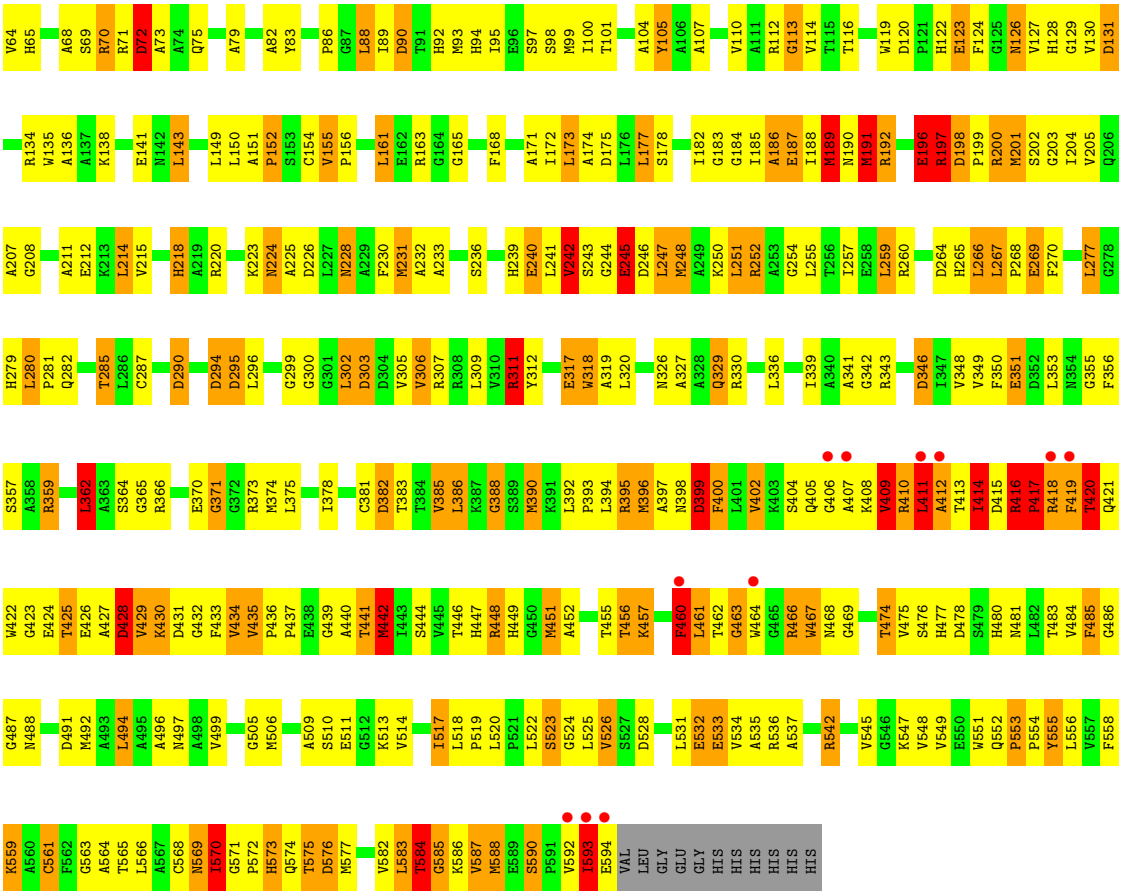
Chain A:



• Molecule 1: Adenine deaminase 2

Chain B:




V64 H65 A68 S69 R70 R71 D72 A73 A74 Q75 A79 A82 Y83 P86 G87 L88 I89 D90 T91 H92 M93 H94 I95 E96 S97 S98 M99 I100 T101 A104 Y105 A106 A107 V110 A111 R112 G113 V114 T115 T116 W119 D120 P121 H122 E123 F124 G125 N126 V127 H128 G129 V130 D131
R134 W135 A136 A137 K138 E141 N142 L143 L149 L150 A151 P152 S153 C154 V155 P156 L161 E162 R163 G164 G165 F168 A171 I172 L173 A174 D175 L176 L177 S178 I182 G183 G184 I185 A186 E187 I188 M189 N190 M191 R192 E196 R197 D198 P199 R200 M201 S202 G203 I204 V205 Q206
A207 G208 A211 E212 K213 L214 V215 H218 A219 R220 K223 N224 A225 D226 L227 N228 A229 F230 M231 A232 A233 S236 H239 E240 L241 V242 S243 G244 E245 D246 L247 M248 A249 K250 L251 R252 A253 G254 L255 T256 I257 E258 L259 R260 D264 H265 L266 L267 P268 E269 F270 L277 G278
H279 L280 P281 Q282 T285 L286 C287 D290 D294 D295 L296 G299 G300 G301 L302 D303 D304 V305 V306 R307 R308 L309 V310 R311 Y312 E317 W318 A319 L320 N326 A327 A328 Q329 R330 L336 I339 A340 A341 G342 R343 D346 I347 V348 V349 F350 E351 D352 L353 N354 G355 F356
S357 A358 R359 L362 A363 S364 G365 R366 E370 G371 G372 R373 M374 L375 I378 C381 D382 T383 T384 V385 L386 K387 G388 S389 M390 K391 L392 P393 L394 R395 M396 A397 N398 D399 F400 L401 V402 K403 S404 Q405 G406 A407 K408 V409 R410 L411 A412 T413 I414 D415 R416 P417 R418 F419 T420 Q421
W422 G423 E424 T425 E426 A427 D428 V429 K430 D431 G432 F433 V434 V435 P436 P437 E438 G439 A440 T441 M442 I443 S444 V445 T446 H447 R448 H449 G450 M451 A452 T455 T456 K457 F460 L461 T462 G463 W464 G465 R466 W467 N468 G469 T474 V475 S476 H477 D478 S479 H480 N481 L482 T483 V484 P485 G486
G487 N488 D491 M492 A493 L494 A495 A496 N497 A498 V499 G505 M506 A509 S510 E511 G512 K513 V514 I517 L518 P519 L520 P521 L522 S523 G524 L525 V526 S527 D528 L531 E532 E533 V534 A535 R536 A537 R542 V545 G546 K547 V548 V549 E550 W551 Q552 P553 P554 Y555 L556 V557 F558
K559 A560 C561 F562 G563 A564 T565 L566 A567 C568 N569 I570 G571 P572 H573 Q574 T575 D576 M577 V582 L583 T584 G585 K586 V587 M588 E589 S590 P591 V592 I593 E594 VAL LEU GLY GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.54Å 131.17Å 69.28Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	48.73 – 2.80 47.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.73-2.80) 99.7 (47.46-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.301 0.182 , 0.304	Depositor DCC
R_{free} test set	1362 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8761	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 (i)

5.1 Standard geometry (i)

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

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	2.10	137/4402 (3.1%)	1.79	93/5964 (1.6%)
1	B	1.96	105/4400 (2.4%)	1.75	77/5961 (1.3%)
All	All	2.03	242/8802 (2.7%)	1.77	170/11925 (1.4%)

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	2
1	B	0	6
All	All	0	8

All (242) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	GLU	CD-OE2	12.79	1.39	1.25
1	A	451	MSE	SE-CE	12.26	2.67	1.95
1	A	396	MSE	SE-CE	11.74	2.64	1.95
1	A	163	ARG	CZ-NH1	11.57	1.48	1.33
1	B	189	MSE	SE-CE	11.45	2.63	1.95
1	A	385	VAL	CB-CG1	11.45	1.76	1.52
1	A	189	MSE	SE-CE	11.36	2.62	1.95
1	A	212	GLU	CG-CD	11.26	1.68	1.51
1	A	532	GLU	CD-OE1	10.88	1.37	1.25
1	B	245	GLU	CG-CD	10.00	1.67	1.51
1	B	191	MSE	SE-CE	9.97	2.54	1.95
1	B	396	MSE	SE-CE	9.81	2.53	1.95
1	B	435	VAL	CB-CG2	9.00	1.71	1.52
1	A	130	VAL	CB-CG1	9.00	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	VAL	CB-CG1	-8.99	1.33	1.52
1	A	216	CYS	CB-SG	-8.82	1.67	1.82
1	A	577	MSE	SE-CE	8.80	2.47	1.95
1	A	99	MSE	SE-CE	8.68	2.46	1.95
1	A	233	ALA	CA-CB	-8.61	1.34	1.52
1	A	192	ARG	CG-CD	8.51	1.73	1.51
1	B	355	GLY	C-O	8.50	1.37	1.23
1	A	533	GLU	CD-OE2	8.45	1.34	1.25
1	B	141	GLU	CD-OE1	8.43	1.34	1.25
1	A	105	TYR	CD2-CE2	8.40	1.51	1.39
1	A	532	GLU	CD-OE2	8.35	1.34	1.25
1	B	254	GLY	C-O	-8.25	1.10	1.23
1	A	479	SER	CB-OG	8.24	1.52	1.42
1	A	287	CYS	CB-SG	-8.24	1.68	1.82
1	B	451	MSE	SE-CE	8.17	2.43	1.95
1	B	215	VAL	CB-CG1	-8.16	1.35	1.52
1	A	48	GLU	CD-OE1	8.15	1.34	1.25
1	A	52	ALA	CA-CB	-8.15	1.35	1.52
1	A	543	GLU	CG-CD	8.03	1.64	1.51
1	B	31	ARG	CZ-NH2	7.95	1.43	1.33
1	A	350	PHE	CD1-CE1	7.94	1.55	1.39
1	A	162	GLU	CG-CD	7.94	1.63	1.51
1	B	105	TYR	CE1-CZ	7.89	1.48	1.38
1	A	499	VAL	CB-CG2	-7.85	1.36	1.52
1	A	319	ALA	CA-CB	-7.74	1.36	1.52
1	B	38	GLY	C-O	7.74	1.36	1.23
1	A	595	VAL	CA-CB	7.68	1.70	1.54
1	B	105	TYR	CE2-CZ	7.65	1.48	1.38
1	A	129	GLY	C-O	7.60	1.35	1.23
1	A	166	ALA	CA-CB	7.58	1.68	1.52
1	A	305	VAL	CB-CG2	7.57	1.68	1.52
1	B	44	VAL	CB-CG2	-7.53	1.37	1.52
1	A	208	GLY	N-CA	-7.52	1.34	1.46
1	B	533	GLU	CG-CD	7.50	1.63	1.51
1	A	212	GLU	CD-OE1	7.39	1.33	1.25
1	A	245	GLU	CG-CD	7.38	1.63	1.51
1	B	236	SER	CA-CB	-7.24	1.42	1.52
1	B	171	ALA	CA-CB	7.08	1.67	1.52
1	A	103	ALA	CA-CB	7.03	1.67	1.52
1	A	240	GLU	CG-CD	7.00	1.62	1.51
1	A	168	PHE	CE2-CZ	7.00	1.50	1.37
1	A	543	GLU	CD-OE2	6.99	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	TYR	CD2-CE2	6.95	1.49	1.39
1	B	212	GLU	CG-CD	6.84	1.62	1.51
1	B	201	MSE	SE-CE	6.83	2.35	1.95
1	B	42	VAL	CB-CG1	-6.77	1.38	1.52
1	B	318	TRP	CB-CG	-6.71	1.38	1.50
1	A	560	ALA	CA-CB	-6.67	1.38	1.52
1	A	588	MSE	SE-CE	6.66	2.34	1.95
1	A	499	VAL	CB-CG1	-6.65	1.38	1.52
1	A	582	VAL	CA-CB	-6.65	1.40	1.54
1	A	269	GLU	CD-OE1	6.62	1.32	1.25
1	B	113	GLY	C-O	6.62	1.34	1.23
1	A	329	GLN	CD-NE2	6.62	1.49	1.32
1	B	134	ARG	CZ-NH1	6.60	1.41	1.33
1	B	110	VAL	CB-CG2	-6.59	1.39	1.52
1	B	542	ARG	CZ-NH2	6.56	1.41	1.33
1	B	533	GLU	CB-CG	6.53	1.64	1.52
1	B	21	ARG	CZ-NH2	6.51	1.41	1.33
1	B	124	PHE	CE2-CZ	6.51	1.49	1.37
1	A	390	MSE	CG-SE	6.48	2.17	1.95
1	A	137	ALA	CA-CB	-6.47	1.38	1.52
1	B	197	ARG	CZ-NH2	6.46	1.41	1.33
1	A	301	GLY	N-CA	-6.45	1.36	1.46
1	B	123	GLU	CD-OE2	-6.44	1.18	1.25
1	A	174	ALA	N-CA	6.44	1.59	1.46
1	A	248	MSE	SE-CE	6.43	2.33	1.95
1	B	201	MSE	CG-SE	6.36	2.17	1.95
1	B	511	GLU	CG-CD	6.36	1.61	1.51
1	A	48	GLU	CB-CG	6.34	1.64	1.52
1	B	127	VAL	CB-CG1	-6.32	1.39	1.52
1	A	595	VAL	CB-CG1	6.30	1.66	1.52
1	B	588	MSE	SE-CE	6.29	2.32	1.95
1	B	399	ASP	CB-CG	6.26	1.65	1.51
1	B	196	GLU	CD-OE1	6.25	1.32	1.25
1	B	211	ALA	CA-CB	-6.23	1.39	1.52
1	B	240	GLU	CD-OE1	6.22	1.32	1.25
1	A	536	ARG	CG-CD	6.20	1.67	1.51
1	A	23	VAL	CB-CG1	6.19	1.65	1.52
1	B	188	ILE	N-CA	-6.19	1.33	1.46
1	B	570	ILE	CB-CG2	6.17	1.72	1.52
1	B	280	LEU	C-O	-6.15	1.11	1.23
1	B	165	GLY	N-CA	6.15	1.55	1.46
1	A	373	ARG	CG-CD	6.13	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	GLU	CD-OE2	6.12	1.32	1.25
1	A	291	VAL	CB-CG2	-6.11	1.40	1.52
1	A	80	GLY	N-CA	6.11	1.55	1.46
1	A	430	LYS	CD-CE	6.09	1.66	1.51
1	A	559	LYS	CD-CE	6.06	1.66	1.51
1	B	467	TRP	CB-CG	6.06	1.61	1.50
1	A	133	VAL	CB-CG1	-6.06	1.40	1.52
1	A	548	VAL	CA-CB	6.05	1.67	1.54
1	A	48	GLU	CG-CD	6.01	1.60	1.51
1	B	584	THR	CA-CB	5.99	1.69	1.53
1	B	373	ARG	CG-CD	5.97	1.66	1.51
1	A	393	PRO	CB-CG	5.94	1.79	1.50
1	B	245	GLU	CD-OE2	5.94	1.32	1.25
1	B	559	LYS	CD-CE	5.94	1.66	1.51
1	B	260	ARG	CG-CD	5.93	1.66	1.51
1	A	138	LYS	CG-CD	5.93	1.72	1.52
1	A	315	LYS	CE-NZ	5.92	1.63	1.49
1	A	292	PHE	CB-CG	-5.91	1.41	1.51
1	B	124	PHE	CG-CD1	5.91	1.47	1.38
1	B	351	GLU	CG-CD	5.90	1.60	1.51
1	A	377	ASP	CB-CG	5.89	1.64	1.51
1	A	433	PHE	CE1-CZ	5.88	1.48	1.37
1	B	232	ALA	CA-CB	5.88	1.64	1.52
1	A	9	GLU	N-CA	5.87	1.58	1.46
1	A	270	PHE	CB-CG	-5.87	1.41	1.51
1	B	231	MSE	SE-CE	5.86	2.29	1.95
1	A	208	GLY	C-O	5.85	1.33	1.23
1	A	350	PHE	CG-CD2	5.81	1.47	1.38
1	B	127	VAL	C-O	-5.78	1.12	1.23
1	B	400	PHE	CE1-CZ	5.78	1.48	1.37
1	A	31	ARG	CZ-NH2	5.76	1.40	1.33
1	A	21	ARG	CZ-NH1	5.76	1.40	1.33
1	A	66	GLU	CD-OE1	5.75	1.31	1.25
1	B	532	GLU	CD-OE1	5.74	1.31	1.25
1	B	231	MSE	CG-SE	5.73	2.15	1.95
1	B	114	VAL	CB-CG2	5.73	1.64	1.52
1	B	24	ALA	CA-CB	-5.73	1.40	1.52
1	B	207	ALA	CA-CB	-5.70	1.40	1.52
1	B	306	VAL	CB-CG2	-5.70	1.40	1.52
1	A	155	VAL	CB-CG2	-5.69	1.41	1.52
1	A	306	VAL	CB-CG2	5.69	1.64	1.52
1	A	264	ASP	CB-CG	5.68	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	174	ALA	CA-CB	-5.68	1.40	1.52
1	A	328	ALA	CA-CB	-5.67	1.40	1.52
1	A	555	TYR	CG-CD2	5.60	1.46	1.39
1	A	543	GLU	CB-CG	5.59	1.62	1.52
1	B	105	TYR	CZ-OH	5.58	1.47	1.37
1	B	460	PHE	CD2-CE2	5.58	1.50	1.39
1	B	230	PHE	CD1-CE1	5.57	1.50	1.39
1	B	28	GLY	CA-C	5.57	1.60	1.51
1	B	242	VAL	CB-CG1	5.56	1.64	1.52
1	B	534	VAL	CB-CG2	5.56	1.64	1.52
1	B	499	VAL	CB-CG2	-5.54	1.41	1.52
1	B	526	VAL	CB-CG1	-5.53	1.41	1.52
1	A	559	LYS	CE-NZ	5.53	1.62	1.49
1	B	196	GLU	CD-OE2	5.52	1.31	1.25
1	A	66	GLU	CG-CD	5.51	1.60	1.51
1	B	225	ALA	CA-CB	5.51	1.64	1.52
1	B	135	TRP	CZ3-CH2	5.50	1.48	1.40
1	B	135	TRP	C-O	5.50	1.33	1.23
1	A	320	LEU	C-O	5.48	1.33	1.23
1	B	248	MSE	CG-SE	5.48	2.14	1.95
1	A	40	THR	C-O	5.47	1.33	1.23
1	A	82	ALA	CA-CB	5.47	1.64	1.52
1	A	146	ARG	CB-CG	5.47	1.67	1.52
1	A	533	GLU	CG-CD	5.47	1.60	1.51
1	A	543	GLU	CD-OE1	5.47	1.31	1.25
1	A	215	VAL	CB-CG1	-5.46	1.41	1.52
1	B	248	MSE	SE-CE	5.43	2.27	1.95
1	B	52	ALA	CA-CB	-5.42	1.41	1.52
1	A	354	ASN	CG-OD1	5.42	1.35	1.24
1	A	230	PHE	CE1-CZ	5.42	1.47	1.37
1	B	569	ASN	CB-CG	5.42	1.63	1.51
1	A	258	GLU	CB-CG	-5.41	1.41	1.52
1	A	246	ASP	CB-CG	5.41	1.63	1.51
1	B	329	GLN	CG-CD	5.40	1.63	1.51
1	A	201	MSE	SE-CE	5.39	2.27	1.95
1	B	439	GLY	C-O	5.38	1.32	1.23
1	A	539	GLU	CD-OE2	5.38	1.31	1.25
1	A	138	LYS	CD-CE	5.38	1.64	1.51
1	B	442	MSE	SE-CE	5.36	2.27	1.95
1	A	311	ARG	CD-NE	5.36	1.55	1.46
1	A	105	TYR	CZ-OH	-5.35	1.28	1.37
1	A	562	PHE	C-O	5.35	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	TYR	CG-CD2	5.33	1.46	1.39
1	A	466	ARG	CB-CG	5.33	1.67	1.52
1	B	187	GLU	CD-OE1	-5.32	1.19	1.25
1	B	420	THR	N-CA	5.31	1.56	1.46
1	A	80	GLY	C-O	5.31	1.32	1.23
1	B	336	LEU	CG-CD2	5.30	1.71	1.51
1	A	344	ARG	CZ-NH2	-5.29	1.26	1.33
1	A	259	LEU	CG-CD1	-5.27	1.32	1.51
1	A	253	ALA	CA-CB	-5.26	1.41	1.52
1	A	400	PHE	CB-CG	-5.26	1.42	1.51
1	A	269	GLU	CG-CD	5.25	1.59	1.51
1	A	83	TYR	CE2-CZ	5.25	1.45	1.38
1	B	434	VAL	CA-CB	5.23	1.65	1.54
1	A	594	GLU	N-CA	5.23	1.56	1.46
1	A	41	LEU	N-CA	-5.21	1.35	1.46
1	B	189	MSE	CG-SE	5.21	2.13	1.95
1	B	409	VAL	N-CA	5.19	1.56	1.46
1	A	134	ARG	CZ-NH1	5.18	1.39	1.33
1	B	349	VAL	CB-CG1	-5.18	1.42	1.52
1	A	68	ALA	CA-CB	5.17	1.63	1.52
1	A	225	ALA	CA-CB	-5.16	1.41	1.52
1	A	589	GLU	CB-CG	5.14	1.61	1.52
1	A	109	VAL	CB-CG2	-5.13	1.42	1.52
1	A	548	VAL	CB-CG2	-5.13	1.42	1.52
1	A	581	ASP	CB-CG	5.13	1.62	1.51
1	B	200	ARG	CG-CD	5.13	1.64	1.51
1	A	131	ASP	C-O	5.12	1.33	1.23
1	B	559	LYS	CG-CD	5.12	1.69	1.52
1	A	54	ILE	CB-CG2	5.11	1.68	1.52
1	A	249	ALA	CA-CB	-5.11	1.41	1.52
1	A	539	GLU	CG-CD	5.11	1.59	1.51
1	B	88	LEU	C-O	5.11	1.33	1.23
1	A	71	ARG	CG-CD	5.11	1.64	1.51
1	A	187	GLU	CB-CG	-5.11	1.42	1.52
1	A	514	VAL	CA-CB	5.09	1.65	1.54
1	A	64	VAL	C-O	5.09	1.33	1.23
1	B	317	GLU	CD-OE1	5.09	1.31	1.25
1	A	100	ILE	CB-CG2	5.08	1.68	1.52
1	A	114	VAL	CB-CG2	-5.08	1.42	1.52
1	A	485	PHE	CA-CB	-5.08	1.42	1.53
1	A	559	LYS	CG-CD	5.08	1.69	1.52
1	A	332	GLY	N-CA	-5.08	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	ALA	C-O	5.07	1.32	1.23
1	B	203	GLY	N-CA	5.07	1.53	1.46
1	A	83	TYR	CG-CD2	5.07	1.45	1.39
1	B	330	ARG	CZ-NH1	5.07	1.39	1.33
1	B	307	ARG	C-O	5.07	1.32	1.23
1	B	496	ALA	CA-CB	-5.06	1.41	1.52
1	A	202	SER	CB-OG	5.06	1.48	1.42
1	A	292	PHE	CE2-CZ	5.05	1.47	1.37
1	A	479	SER	CA-CB	5.05	1.60	1.52
1	B	353	LEU	C-O	-5.05	1.13	1.23
1	A	477	HIS	CA-CB	-5.04	1.42	1.53
1	B	11	ALA	CA-CB	-5.03	1.41	1.52
1	B	269	GLU	CD-OE2	5.03	1.31	1.25
1	B	342	GLY	C-O	-5.03	1.15	1.23
1	B	561	CYS	CB-SG	-5.02	1.73	1.81
1	A	171	ALA	C-O	5.02	1.32	1.23
1	A	56	ILE	CA-CB	5.01	1.66	1.54
1	A	245	GLU	CD-OE1	5.01	1.31	1.25

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ARG	NE-CZ-NH2	-20.65	109.97	120.30
1	B	197	ARG	NE-CZ-NH1	-18.11	111.25	120.30
1	A	343	ARG	NE-CZ-NH1	17.08	128.84	120.30
1	A	163	ARG	NE-CZ-NH1	15.14	127.87	120.30
1	A	343	ARG	NE-CZ-NH2	-13.68	113.46	120.30
1	B	192	ARG	NE-CZ-NH2	-11.79	114.40	120.30
1	A	21	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	B	173	LEU	CA-CB-CG	-11.04	89.90	115.30
1	B	53	ASP	CB-CG-OD1	10.05	127.35	118.30
1	B	252	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	A	15	ASP	CB-CG-OD1	-10.04	109.27	118.30
1	B	197	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	B	343	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	B	252	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	B	27	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	19	ARG	NE-CZ-NH2	-9.63	115.49	120.30
1	A	214	LEU	CB-CG-CD1	-9.35	95.11	111.00
1	A	238	ASP	CB-CG-OD1	9.33	126.69	118.30
1	B	395	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	B	359	ARG	NE-CZ-NH1	9.05	124.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	492	MSE	CG-SE-CE	8.91	118.50	98.90
1	A	27	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	359	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	189	MSE	CG-SE-CE	8.73	118.11	98.90
1	B	528	ASP	CB-CG-OD1	8.70	126.13	118.30
1	B	214	LEU	CB-CG-CD2	-8.69	96.23	111.00
1	B	72	ASP	N-CA-CB	-8.68	94.97	110.60
1	A	344	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	A	264	ASP	CB-CG-OD1	8.54	125.99	118.30
1	B	311	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	238	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	333	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	A	359	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	131	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	A	231	MSE	CG-SE-CE	8.11	116.73	98.90
1	B	218	HIS	N-CA-C	-8.03	89.33	111.00
1	B	396	MSE	CG-SE-CE	8.00	116.50	98.90
1	B	138	LYS	CD-CE-NZ	-7.97	93.38	111.70
1	A	385	VAL	CG1-CB-CG2	7.79	123.36	110.90
1	A	252	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	259	LEU	CB-CG-CD1	-7.69	97.93	111.00
1	B	355	GLY	N-CA-C	-7.59	94.11	113.10
1	B	50	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	520	LEU	CA-CB-CG	7.51	132.57	115.30
1	A	241	LEU	CB-CG-CD1	-7.46	98.32	111.00
1	A	373	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	16	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	27	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	B	420	THR	N-CA-C	7.31	130.73	111.00
1	B	70	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	290	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	B	386	LEU	CA-CB-CG	7.10	131.63	115.30
1	B	277	LEU	CA-CB-CG	7.09	131.61	115.30
1	A	338	LEU	CA-CB-CG	7.05	131.53	115.30
1	B	143	LEU	CA-CB-CG	-7.03	99.14	115.30
1	A	41	LEU	CB-CG-CD1	7.00	122.90	111.00
1	B	448	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	416	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	362	LEU	CA-CB-CG	-6.87	99.49	115.30
1	B	330	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	78	ASP	CB-CG-OD2	-6.86	112.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	LEU	CA-CB-CG	-6.85	99.54	115.30
1	A	308	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	395	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	396	MSE	CB-CA-C	-6.80	96.79	110.40
1	B	120	ASP	N-CA-CB	-6.72	98.50	110.60
1	B	451	MSE	CG-SE-CE	6.72	113.67	98.90
1	A	325	LEU	CB-CG-CD1	6.70	122.39	111.00
1	B	346	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	64	VAL	N-CA-C	-6.69	92.94	111.00
1	A	260	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	161	LEU	CB-CG-CD2	-6.66	99.68	111.00
1	A	198	ASP	CB-CG-OD1	-6.65	112.32	118.30
1	B	359	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	373	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	18	LEU	CB-CG-CD2	-6.57	99.83	111.00
1	A	64	VAL	CB-CA-C	-6.53	99.00	111.40
1	B	264	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	390	MSE	CG-SE-CE	6.51	113.22	98.90
1	B	192	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	198	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	A	192	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	362	LEU	CA-CB-CG	6.43	130.10	115.30
1	B	336	LEU	CB-CG-CD2	6.35	121.79	111.00
1	A	35	LEU	CB-CG-CD2	6.32	121.75	111.00
1	A	134	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	382	ASP	N-CA-CB	-6.26	99.32	110.60
1	B	463	GLY	N-CA-C	-6.26	97.45	113.10
1	B	309	LEU	CA-CB-CG	6.18	129.51	115.30
1	B	366	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	50	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	A	399	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	A	118	VAL	N-CA-C	-6.10	94.52	111.00
1	B	307	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	141	GLU	OE1-CD-OE2	6.03	130.54	123.30
1	A	146	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	336	LEU	CB-CG-CD2	-5.95	100.89	111.00
1	A	187	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	A	16	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	105	TYR	CZ-CE2-CD2	-5.85	114.53	119.80
1	B	266	LEU	CA-CB-CG	-5.79	101.97	115.30
1	A	176	LEU	CB-CG-CD2	5.76	120.80	111.00
1	B	491	ASP	CB-CG-OD1	5.76	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	VAL	O-C-N	-5.75	113.50	122.70
1	A	338	LEU	CB-CA-C	-5.73	99.31	110.20
1	A	241	LEU	CB-CG-CD2	5.72	120.73	111.00
1	B	294	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	554	PRO	N-CA-C	-5.70	97.27	112.10
1	A	226	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	131	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	200	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	176	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	B	177	LEU	CB-CG-CD2	5.63	120.58	111.00
1	A	280	LEU	CB-CG-CD1	5.63	120.57	111.00
1	B	442	MSE	CB-CG-SE	-5.62	95.82	112.70
1	B	187	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	A	247	LEU	CB-CG-CD2	5.60	120.52	111.00
1	A	431	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	513	LYS	CD-CE-NZ	-5.59	98.83	111.70
1	B	542	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	B	466	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	311	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	53	ASP	N-CA-C	-5.52	96.10	111.00
1	A	307	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	15	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	145	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	B	381	CYS	N-CA-C	-5.49	96.19	111.00
1	A	526	VAL	CG1-CB-CG2	5.48	119.67	110.90
1	A	194	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	A	77	ILE	C-N-CA	-5.47	108.03	121.70
1	A	492	MSE	CA-CB-CG	-5.46	104.02	113.30
1	A	76	VAL	CB-CA-C	-5.44	101.06	111.40
1	A	411	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	A	88	LEU	CA-CB-CG	-5.38	102.93	115.30
1	B	90	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	218	HIS	CB-CA-C	-5.36	99.67	110.40
1	B	12	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	13	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	581	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	231	MSE	CA-CB-CG	-5.33	104.24	113.30
1	A	566	LEU	CB-CG-CD1	5.32	120.05	111.00
1	A	91	THR	OG1-CB-CG2	-5.31	97.78	110.00
1	A	325	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	A	311	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	B	260	ARG	CG-CD-NE	-5.28	100.71	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	ASN	N-CA-C	5.27	125.24	111.00
1	B	536	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	411	LEU	CA-CB-CG	5.24	127.36	115.30
1	B	416	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	320	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	A	522	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	B	134	ARG	CG-CD-NE	5.19	122.70	111.80
1	B	382	ASP	CB-CA-C	5.19	120.78	110.40
1	B	285	THR	CB-CA-C	-5.19	97.60	111.60
1	B	343	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	214	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	210	ALA	N-CA-C	-5.16	97.08	111.00
1	B	410	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	109	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	B	205	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	271	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	A	201	MSE	CG-SE-CE	5.11	110.13	98.90
1	A	302	LEU	CA-CB-CG	-5.10	103.58	115.30
1	A	9	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	A	395	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	503	GLY	N-CA-C	5.07	125.77	113.10
1	B	320	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	259	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	A	540	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	MSE	Peptide
1	A	430	LYS	Peptide
1	B	152	PRO	Peptide
1	B	412	ALA	Peptide
1	B	417	PRO	Peptide
1	B	419	PHE	Peptide
1	B	460	PHE	Peptide
1	B	553	PRO	Peptide

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	4337	0	4344	222	0
1	B	4335	0	4339	363	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	33	0	0	5	0
3	B	50	0	0	16	0
All	All	8761	0	8683	572	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 33.

All (572) 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:385:VAL:CB	1:A:385:VAL:CG1	1.76	1.58
1:B:231:MSE:SE	1:B:231:MSE:CG	2.14	1.44
1:A:492:MSE:SE	1:A:492:MSE:CE	2.14	1.44
1:A:393:PRO:CB	1:A:393:PRO:CG	1.79	1.43
1:A:231:MSE:SE	1:A:231:MSE:CE	2.17	1.42
1:A:390:MSE:CG	1:A:390:MSE:SE	2.17	1.42
1:B:577:MSE:CE	1:B:577:MSE:SE	2.15	1.42
1:B:201:MSE:CG	1:B:201:MSE:SE	2.17	1.42
1:A:374:MSE:SE	1:A:374:MSE:CE	2.22	1.36
1:B:189:MSE:HG3	1:B:568:CYS:SG	1.64	1.36
1:B:390:MSE:CE	1:B:390:MSE:SE	2.23	1.35
1:B:427:ALA:O	1:B:429:VAL:N	1.60	1.33
1:A:201:MSE:SE	1:A:201:MSE:CE	2.27	1.33
1:B:442:MSE:SE	1:B:442:MSE:CE	2.27	1.32
1:B:248:MSE:SE	1:B:248:MSE:CE	2.27	1.32
1:B:231:MSE:SE	1:B:231:MSE:CE	2.30	1.30
1:B:412:ALA:HA	1:B:423:GLY:O	1.25	1.29
1:B:588:MSE:SE	1:B:588:MSE:CE	2.32	1.27
1:A:248:MSE:SE	1:A:248:MSE:CE	2.33	1.26
1:A:588:MSE:SE	1:A:588:MSE:CE	2.34	1.26
1:B:201:MSE:SE	1:B:201:MSE:CE	2.35	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:MSE:CE	1:B:451:MSE:SE	2.43	1.17
1:B:420:THR:HB	1:B:572:PRO:HD2	1.29	1.15
1:B:552:GLN:H	1:B:556:LEU:HD23	1.09	1.14
1:A:99:MSE:SE	1:A:99:MSE:CE	2.46	1.12
1:A:577:MSE:SE	1:A:577:MSE:CE	2.47	1.11
1:A:120:ASP:OD1	1:A:122:HIS:HB3	1.50	1.11
1:B:412:ALA:CA	1:B:423:GLY:O	2.00	1.09
1:B:191:MSE:SE	1:B:191:MSE:CE	2.54	1.05
1:B:396:MSE:SE	1:B:396:MSE:CE	2.53	1.05
1:B:552:GLN:H	1:B:556:LEU:CD2	1.70	1.02
1:B:552:GLN:N	1:B:556:LEU:HD23	1.73	1.02
1:A:588:MSE:HE2	1:A:590:SER:O	1.60	1.00
1:B:583:LEU:O	1:B:585:GLY:N	1.94	1.00
1:B:410:ARG:HB2	1:B:593:ILE:HG22	1.42	1.00
1:A:189:MSE:SE	1:A:189:MSE:CE	2.62	0.97
1:A:308:ARG:HG2	1:A:311:ARG:NH2	1.80	0.97
1:B:189:MSE:SE	1:B:189:MSE:CE	2.63	0.96
1:A:396:MSE:SE	1:A:396:MSE:CE	2.64	0.95
1:A:396:MSE:HB3	1:A:398:ASN:H	1.31	0.94
1:B:488:ASN:O	1:B:492:MSE:HG3	1.67	0.93
1:A:451:MSE:SE	1:A:451:MSE:CE	2.67	0.93
1:B:476:SER:H	1:B:480:HIS:HD2	1.05	0.93
1:B:411:LEU:O	1:B:424:GLU:HA	1.68	0.92
1:B:415:ASP:O	1:B:416:ARG:HB2	1.69	0.91
1:B:31:ARG:HA	1:B:72:ASP:OD2	1.71	0.91
1:B:416:ARG:CZ	1:B:421:GLN:OE1	2.18	0.91
1:B:416:ARG:HD2	1:B:421:GLN:HG2	1.53	0.91
1:B:402:VAL:HB	1:B:434:VAL:HG23	1.54	0.90
1:A:448:ARG:H	1:A:481:ASN:HD22	1.19	0.90
1:A:420:THR:HG21	1:A:572:PRO:O	1.71	0.90
1:B:427:ALA:C	1:B:429:VAL:N	2.21	0.89
1:A:518:LEU:C	1:A:518:LEU:HD12	1.92	0.89
1:A:286:LEU:HD12	1:A:323:ALA:HB2	1.55	0.89
1:B:412:ALA:C	1:B:413:THR:CG2	2.41	0.89
1:B:412:ALA:C	1:B:413:THR:HG23	1.91	0.88
1:A:200:ARG:HB3	3:A:635:HOH:O	1.74	0.88
1:B:189:MSE:CG	1:B:568:CYS:SG	2.57	0.88
1:B:476:SER:H	1:B:480:HIS:CD2	1.93	0.86
1:B:505:GLY:HA2	1:B:520:LEU:HB2	1.58	0.86
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.39	0.85
1:B:412:ALA:CB	1:B:423:GLY:O	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ARG:HB3	1:A:419:PHE:O	1.77	0.84
1:A:99:MSE:HG2	1:A:520:LEU:HD21	1.60	0.84
1:B:477:HIS:HB3	1:B:478:ASP:OD1	1.78	0.84
1:B:64:VAL:HG21	3:B:643:HOH:O	1.78	0.83
1:B:351:GLU:OE1	1:B:359:ARG:HB2	1.78	0.82
1:B:196:GLU:HG3	3:B:646:HOH:O	1.78	0.82
1:B:190:ASN:HB3	1:B:201:MSE:SE	2.30	0.81
1:B:462:THR:HG22	1:B:463:GLY:N	1.94	0.81
1:B:486:GLY:HA3	1:B:492:MSE:SE	2.31	0.81
1:B:424:GLU:O	1:B:425:THR:HG22	1.81	0.81
1:A:448:ARG:H	1:A:481:ASN:ND2	1.78	0.81
1:B:420:THR:HB	1:B:572:PRO:CD	2.09	0.81
1:B:295:ASP:O	1:B:300:GLY:HA2	1.80	0.81
1:B:374:MSE:HE2	1:B:378:ILE:HD11	1.62	0.80
1:A:259:LEU:HD12	1:A:259:LEU:C	1.98	0.80
1:A:554:PRO:O	1:A:555:TYR:HB2	1.82	0.79
1:A:308:ARG:CG	1:A:311:ARG:NH2	2.45	0.79
1:B:79:ALA:O	1:B:82:ALA:HB3	1.83	0.78
1:B:551:TRP:C	1:B:553:PRO:HD3	2.04	0.77
1:B:239:HIS:CD2	1:B:240:GLU:HG2	2.19	0.77
1:B:239:HIS:HD2	1:B:240:GLU:HG2	1.50	0.77
1:B:407:ALA:O	1:B:429:VAL:HB	1.85	0.77
1:B:476:SER:N	1:B:480:HIS:HD2	1.83	0.77
1:A:373:ARG:HH11	1:A:373:ARG:CG	1.97	0.77
1:B:440:ALA:HB1	1:B:461:LEU:O	1.83	0.76
1:A:496:ALA:O	1:A:500:ILE:HG13	1.83	0.76
1:B:267:LEU:HD23	1:B:267:LEU:N	1.99	0.76
1:B:161:LEU:N	1:B:161:LEU:HD12	2.00	0.76
1:B:90:ASP:OD1	1:B:287:CYS:HA	1.86	0.75
1:B:462:THR:CG2	1:B:463:GLY:N	2.49	0.75
1:B:410:ARG:HD3	1:B:594:GLU:HB2	1.67	0.75
1:A:110:VAL:HG23	1:A:145:LEU:HD13	1.68	0.75
1:A:92:HIS:HE1	1:A:187:GLU:HG2	1.52	0.74
1:A:259:LEU:HD12	1:A:260:ARG:N	2.02	0.74
1:B:505:GLY:CA	1:B:520:LEU:HB2	2.17	0.74
1:B:415:ASP:O	1:B:416:ARG:CB	2.35	0.74
1:B:231:MSE:SE	1:B:231:MSE:CB	2.85	0.74
1:B:267:LEU:HD23	1:B:267:LEU:H	1.52	0.74
1:A:380:THR:OG1	1:A:381:CYS:N	2.21	0.73
1:A:93:MSE:HE1	1:A:95:ILE:HG12	1.70	0.73
1:A:99:MSE:HE2	1:A:506:MSE:HE1	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASP:HB3	3:B:658:HOH:O	1.87	0.73
1:A:385:VAL:CG1	1:A:385:VAL:HB	2.12	0.73
1:A:488:ASN:ND2	1:A:491:ASP:H	1.85	0.73
1:A:88:LEU:HB3	1:A:302:LEU:HD23	1.68	0.72
1:A:468:ASN:O	1:A:548:VAL:HG22	1.88	0.72
1:A:420:THR:HG22	1:A:571:GLY:HA3	1.70	0.72
1:B:248:MSE:O	1:B:252:ARG:HG3	1.89	0.72
1:A:63:SER:OG	1:A:65:HIS:HD2	1.73	0.72
1:B:294:ASP:HA	1:B:535:ALA:HB1	1.72	0.71
1:B:464:TRP:O	1:B:556:LEU:CD1	2.38	0.71
1:B:63:SER:OG	1:B:65:HIS:HD2	1.73	0.71
1:A:99:MSE:HG2	1:A:520:LEU:CD2	2.20	0.71
1:B:425:THR:HG22	3:B:615:HOH:O	1.91	0.70
1:A:383:THR:O	1:A:386:LEU:HB2	1.90	0.70
1:B:427:ALA:HB1	1:B:434:VAL:HG13	1.72	0.70
1:B:122:HIS:HB3	1:B:152:PRO:HB3	1.73	0.70
1:B:551:TRP:O	1:B:553:PRO:HD3	1.91	0.69
1:B:410:ARG:HB2	1:B:593:ILE:CG2	2.20	0.69
1:B:485:PHE:HZ	1:B:561:CYS:O	1.75	0.69
1:B:419:PHE:HA	3:B:647:HOH:O	1.92	0.69
1:B:427:ALA:O	1:B:429:VAL:HG23	1.92	0.69
1:A:110:VAL:CG2	1:A:145:LEU:HD13	2.22	0.69
1:B:416:ARG:HD2	1:B:421:GLN:CG	2.21	0.69
1:B:428:ASP:O	1:B:429:VAL:C	2.30	0.68
1:B:427:ALA:CB	1:B:434:VAL:HG13	2.24	0.68
1:B:583:LEU:C	1:B:585:GLY:H	1.95	0.68
1:A:385:VAL:CG1	1:A:385:VAL:CA	2.70	0.68
1:B:476:SER:O	1:B:480:HIS:CD2	2.46	0.68
1:B:402:VAL:HB	1:B:434:VAL:CG2	2.24	0.68
1:A:414:ILE:HG23	1:A:572:PRO:HB2	1.75	0.68
1:B:128:HIS:HE1	3:B:656:HOH:O	1.75	0.67
1:B:189:MSE:HG3	1:B:568:CYS:HG	1.53	0.67
1:B:122:HIS:CB	1:B:152:PRO:HB3	2.23	0.67
1:A:228:ASN:ND2	1:B:64:VAL:H	1.93	0.67
1:B:414:ILE:CG2	1:B:420:THR:HG21	2.25	0.67
1:B:474:THR:HG21	1:B:505:GLY:H	1.59	0.67
1:A:99:MSE:HE2	1:A:506:MSE:CE	2.25	0.67
1:B:416:ARG:NE	1:B:421:GLN:OE1	2.27	0.67
1:A:402:VAL:HB	1:A:434:VAL:HG13	1.77	0.66
1:B:425:THR:CG2	3:B:615:HOH:O	2.43	0.66
1:B:417:PRO:O	1:B:418:ARG:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:VAL:HG23	1:B:593:ILE:N	2.10	0.66
1:A:82:ALA:HB1	1:A:350:PHE:O	1.97	0.65
1:B:182:ILE:HG22	1:B:184:GLY:H	1.62	0.65
1:A:458:THR:CG2	1:A:459:GLY:N	2.59	0.65
1:B:412:ALA:CA	1:B:413:THR:HG23	2.27	0.65
1:B:430:LYS:HD2	1:B:431:ASP:N	2.12	0.64
1:B:161:LEU:N	1:B:161:LEU:CD1	2.60	0.64
1:B:464:TRP:O	1:B:556:LEU:HD13	1.98	0.64
1:A:341:ALA:HB2	1:B:228:ASN:HD22	1.63	0.64
1:A:396:MSE:HB3	1:A:398:ASN:N	2.08	0.64
1:B:428:ASP:O	1:B:435:VAL:HG12	1.98	0.64
1:A:405:GLN:O	1:A:406:GLY:O	2.16	0.64
1:B:163:ARG:O	1:B:447:HIS:HD2	1.79	0.64
1:B:410:ARG:CB	1:B:593:ILE:HG22	2.25	0.63
1:B:556:LEU:O	1:B:556:LEU:HG	1.99	0.63
1:A:38:GLY:O	1:A:80:GLY:HA2	1.98	0.63
1:A:428:ASP:O	1:A:435:VAL:HG23	1.99	0.63
1:B:393:PRO:O	1:B:395:ARG:NH1	2.30	0.63
1:A:467:TRP:O	1:A:487:GLY:HA3	1.99	0.63
1:A:146:ARG:NH2	1:A:344:ARG:HD3	2.14	0.63
1:A:202:SER:O	1:A:206:GLN:HG2	1.99	0.63
1:A:22:ALA:HA	1:A:57:VAL:HG21	1.81	0.62
1:B:296:LEU:O	1:B:300:GLY:HA3	1.99	0.62
1:B:406:GLY:O	1:B:429:VAL:HG11	1.98	0.62
1:B:446:THR:OG1	1:B:456:THR:HB	1.98	0.62
1:A:250:LYS:HB3	1:A:255:LEU:HD12	1.82	0.62
1:B:485:PHE:CZ	1:B:561:CYS:O	2.52	0.62
1:A:453:GLU:OE2	1:A:453:GLU:HA	2.00	0.62
1:B:318:TRP:O	1:B:319:ALA:C	2.36	0.62
1:B:570:ILE:HG13	1:B:583:LEU:HD11	1.81	0.62
1:A:448:ARG:HG3	1:A:481:ASN:HD22	1.65	0.62
1:A:403:LYS:HE3	1:A:432:GLY:CA	2.31	0.61
1:B:143:LEU:HD23	1:B:143:LEU:N	2.15	0.61
1:B:395:ARG:HD2	1:B:395:ARG:N	2.14	0.61
1:B:416:ARG:CD	1:B:421:GLN:HG2	2.30	0.61
1:B:542:ARG:O	1:B:545:VAL:HG12	2.00	0.61
1:A:239:HIS:HB3	1:A:258:GLU:HB2	1.82	0.61
1:B:572:PRO:O	1:B:573:HIS:CG	2.54	0.61
1:B:247:LEU:O	1:B:251:LEU:HB2	2.01	0.61
1:B:405:GLN:HG3	3:B:619:HOH:O	2.00	0.61
1:B:410:ARG:O	1:B:411:LEU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:OE1	1:A:359:ARG:HB2	2.00	0.60
1:B:464:TRP:O	1:B:556:LEU:HD11	2.00	0.60
1:A:505:GLY:HA2	1:A:520:LEU:HB2	1.81	0.60
1:B:177:LEU:HD21	1:B:185:ILE:HG13	1.83	0.60
1:B:305:VAL:O	1:B:306:VAL:C	2.38	0.60
1:B:425:THR:OG1	1:B:426:GLU:N	2.35	0.59
1:A:554:PRO:O	1:A:555:TYR:CB	2.48	0.59
1:B:414:ILE:HG22	1:B:420:THR:CG2	2.32	0.59
1:A:90:ASP:HB3	1:A:117:ILE:HG22	1.84	0.59
1:B:386:LEU:HD12	1:B:522:LEU:HB3	1.85	0.59
1:A:304:ASP:OD1	1:A:307:ARG:HD2	2.01	0.59
1:B:267:LEU:N	1:B:267:LEU:CD2	2.65	0.59
1:B:415:ASP:HA	1:B:462:THR:HB	1.84	0.59
1:A:215:VAL:HG12	1:A:235:VAL:HA	1.83	0.59
1:B:417:PRO:C	1:B:418:ARG:O	2.39	0.59
1:A:373:ARG:CG	1:A:373:ARG:NH1	2.65	0.59
1:B:590:SER:HB3	1:B:592:VAL:HG13	1.85	0.59
1:B:409:VAL:O	1:B:426:GLU:HA	2.03	0.58
1:B:474:THR:CG2	1:B:505:GLY:H	2.16	0.58
1:B:128:HIS:O	1:B:131:ASP:HB2	2.02	0.58
1:B:112:ARG:HD3	1:B:303:ASP:OD2	2.03	0.58
1:A:518:LEU:C	1:A:518:LEU:CD1	2.70	0.58
1:B:150:LEU:O	1:B:152:PRO:HD3	2.04	0.58
1:B:466:ARG:O	1:B:549:VAL:HG23	2.04	0.58
1:B:414:ILE:CG2	1:B:420:THR:CG2	2.82	0.57
1:B:416:ARG:NH1	1:B:421:GLN:OE1	2.36	0.57
1:B:86:PRO:HD3	1:B:339:ILE:HD12	1.87	0.57
1:B:154:CYS:O	1:B:189:MSE:HE2	2.03	0.57
1:B:412:ALA:HB1	1:B:423:GLY:O	2.05	0.57
1:B:477:HIS:CB	1:B:478:ASP:OD1	2.51	0.57
1:A:86:PRO:HG3	1:A:339:ILE:HG12	1.85	0.57
1:B:172:ILE:HA	1:B:175:ASP:OD2	2.05	0.57
1:B:417:PRO:O	1:B:418:ARG:C	2.42	0.57
1:B:570:ILE:HG12	1:B:571:GLY:N	2.18	0.57
1:B:583:LEU:C	1:B:585:GLY:N	2.55	0.57
1:A:53:ASP:OD2	1:A:67:PRO:HA	2.04	0.57
1:A:243:SER:OG	1:A:246:ASP:HB2	2.05	0.57
1:A:581:ASP:OD1	1:A:583:LEU:HD22	2.05	0.56
1:B:461:LEU:HD22	1:B:464:TRP:NE1	2.19	0.56
1:B:21:ARG:O	1:B:24:ALA:HB3	2.06	0.56
1:B:136:ALA:HB1	1:B:149:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:HG22	1:B:168:PHE:CG	2.40	0.56
1:B:412:ALA:O	1:B:413:THR:HG22	2.06	0.56
1:B:441:THR:O	1:B:461:LEU:HB2	2.05	0.56
1:A:67:PRO:O	1:A:69:SER:N	2.38	0.56
1:A:556:LEU:HG	1:A:556:LEU:O	2.05	0.56
1:B:163:ARG:O	1:B:447:HIS:CD2	2.58	0.56
1:A:588:MSE:CE	1:A:590:SER:O	2.47	0.56
1:A:485:PHE:N	1:A:485:PHE:CD2	2.73	0.56
1:A:105:TYR:CE2	1:A:109:VAL:HG11	2.41	0.56
1:A:308:ARG:CG	1:A:311:ARG:HH21	2.19	0.55
1:B:244:GLY:O	1:B:247:LEU:HB3	2.06	0.55
1:A:197:ARG:HH22	1:A:206:GLN:NE2	2.04	0.55
1:A:488:ASN:HD21	1:A:491:ASP:H	1.52	0.55
1:A:18:LEU:HD12	1:A:57:VAL:HG12	1.89	0.55
1:B:63:SER:OG	1:B:65:HIS:CD2	2.58	0.55
1:A:420:THR:CG2	1:A:572:PRO:O	2.52	0.55
1:A:329:GLN:HB3	1:B:329:GLN:HE21	1.71	0.55
1:B:93:MSE:HE3	1:B:105:TYR:CZ	2.42	0.55
1:B:586:LYS:C	1:B:587:VAL:HG23	2.26	0.55
1:A:413:THR:OG1	1:A:423:GLY:HA3	2.07	0.55
1:B:430:LYS:HB2	1:B:435:VAL:CG1	2.37	0.55
1:A:529:ALA:HB1	1:A:530:PRO:CD	2.38	0.54
1:B:31:ARG:CA	1:B:72:ASP:OD2	2.49	0.54
1:B:462:THR:CG2	1:B:463:GLY:H	2.21	0.54
1:A:416:ARG:CB	1:A:419:PHE:O	2.53	0.54
1:B:441:THR:OG1	1:B:467:TRP:CD1	2.58	0.54
1:B:58:GLY:O	1:B:365:GLY:HA3	2.08	0.54
1:B:494:LEU:O	1:B:494:LEU:HD12	2.08	0.54
1:A:370:GLU:HB3	1:A:375:LEU:HD21	1.90	0.54
1:A:442:MSE:N	1:A:442:MSE:HE3	2.23	0.54
1:B:187:GLU:OE2	1:B:218:HIS:HB2	2.07	0.54
1:B:410:ARG:HD3	1:B:593:ILE:HG22	1.89	0.54
1:A:474:THR:HG23	1:A:524:GLY:O	2.07	0.54
1:B:440:ALA:HB1	1:B:462:THR:HA	1.90	0.53
1:A:197:ARG:HH22	1:A:206:GLN:HE21	1.57	0.53
1:A:522:LEU:HB2	1:A:526:VAL:CG2	2.38	0.53
1:A:386:LEU:HD22	1:A:523:SER:OG	2.08	0.53
1:B:551:TRP:CH2	1:B:558:PHE:HA	2.43	0.53
1:A:441:THR:C	1:A:442:MSE:HE3	2.28	0.53
1:B:413:THR:HB	1:B:460:PHE:O	2.09	0.53
1:B:467:TRP:O	1:B:487:GLY:HA3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PRO:C	1:A:69:SER:H	2.12	0.53
1:B:447:HIS:CE1	1:B:451:MSE:H	2.26	0.53
1:B:424:GLU:C	1:B:425:THR:HG22	2.29	0.53
1:B:280:LEU:HB2	1:B:318:TRP:CE3	2.43	0.53
1:B:554:PRO:O	1:B:555:TYR:HB2	2.08	0.53
1:B:49:LEU:HD11	1:B:317:GLU:OE2	2.08	0.53
1:A:106:ALA:O	1:A:110:VAL:HB	2.09	0.52
1:A:394:LEU:C	1:A:395:ARG:HD2	2.30	0.52
1:B:239:HIS:HD2	1:B:240:GLU:CG	2.20	0.52
1:B:196:GLU:O	1:B:197:ARG:CB	2.55	0.52
1:A:68:ALA:O	1:A:70:ARG:N	2.43	0.52
1:B:532:GLU:CD	1:B:532:GLU:H	2.12	0.52
1:A:53:ASP:C	1:A:54:ILE:HD13	2.30	0.52
1:A:415:ASP:O	1:A:416:ARG:HB2	2.08	0.52
1:A:66:GLU:CG	1:A:69:SER:HB3	2.39	0.52
1:A:263:HIS:HB3	1:A:265:HIS:CE1	2.44	0.52
1:B:94:HIS:O	1:B:95:ILE:C	2.45	0.52
1:B:449:HIS:CD2	1:B:481:ASN:ND2	2.78	0.52
1:B:410:ARG:CD	1:B:594:GLU:HB2	2.38	0.52
1:B:245:GLU:O	1:B:246:ASP:C	2.48	0.51
1:B:414:ILE:HG22	1:B:420:THR:HG22	1.91	0.51
1:B:409:VAL:HB	1:B:429:VAL:CG2	2.40	0.51
1:A:20:ALA:HB2	1:B:197:ARG:HE	1.75	0.51
1:A:162:GLU:HA	1:A:577:MSE:HG3	1.93	0.51
1:A:359:ARG:HG2	1:A:360:HIS:CD2	2.45	0.51
1:A:458:THR:HG22	1:A:459:GLY:N	2.23	0.51
1:A:395:ARG:HD2	1:A:395:ARG:N	2.26	0.51
1:A:23:VAL:CG2	1:B:233:ALA:HB2	2.41	0.51
1:B:126:ASN:N	1:B:126:ASN:HD22	2.08	0.51
1:B:505:GLY:HA2	1:B:520:LEU:HD12	1.92	0.51
1:B:574:GLN:HG3	1:B:575:THR:N	2.26	0.51
1:B:414:ILE:O	1:B:415:ASP:C	2.49	0.51
1:B:35:LEU:HD12	1:B:73:ALA:HB2	1.93	0.51
1:A:46:THR:HB	1:B:277:LEU:HD11	1.93	0.50
1:A:137:ALA:O	1:A:140:ILE:HG13	2.11	0.50
1:A:403:LYS:HA	1:A:432:GLY:O	2.11	0.50
1:B:414:ILE:O	1:B:416:ARG:O	2.28	0.50
1:B:558:PHE:O	1:B:561:CYS:HB2	2.11	0.50
1:B:83:TYR:N	1:B:83:TYR:CD2	2.79	0.50
1:A:341:ALA:HB2	1:B:228:ASN:ND2	2.26	0.50
1:B:311:ARG:HB3	1:B:312:TYR:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD23	1:B:54:ILE:O	2.12	0.50
1:B:427:ALA:HB1	1:B:434:VAL:CG1	2.40	0.50
1:A:324:THR:HB	1:A:337:GLY:HA2	1.94	0.50
1:A:520:LEU:N	1:A:521:PRO:HD3	2.25	0.50
1:B:427:ALA:HB2	1:B:437:PRO:HG3	1.92	0.50
1:B:513:LYS:HG2	1:B:514:VAL:N	2.27	0.50
1:B:168:PHE:O	1:B:200:ARG:NH2	2.45	0.49
1:B:416:ARG:HD2	1:B:421:GLN:CD	2.31	0.49
1:A:475:VAL:HB	1:A:506:MSE:HE2	1.94	0.49
1:B:268:PRO:HD3	1:B:312:TYR:CD1	2.47	0.49
1:B:37:THR:HA	1:B:53:ASP:CG	2.32	0.49
1:A:187:GLU:HA	1:A:216:CYS:O	2.12	0.49
1:B:432:GLY:HA2	3:B:640:HOH:O	2.12	0.49
1:B:440:ALA:CB	1:B:462:THR:HA	2.43	0.49
1:B:551:TRP:CH2	1:B:558:PHE:HD1	2.31	0.49
1:A:131:ASP:HB2	3:A:612:HOH:O	2.12	0.49
1:B:572:PRO:O	1:B:573:HIS:CD2	2.65	0.49
1:A:179:TRP:N	1:A:179:TRP:CD1	2.80	0.49
1:A:191:MSE:HE1	1:A:220:ARG:O	2.13	0.49
1:B:414:ILE:HB	1:B:461:LEU:HD23	1.94	0.49
1:A:15:ASP:OD2	1:A:17:THR:HB	2.13	0.49
1:A:542:ARG:HG3	1:A:558:PHE:HD2	1.78	0.49
1:B:191:MSE:HE1	1:B:220:ARG:O	2.12	0.49
1:B:92:HIS:O	1:B:287:CYS:HB2	2.13	0.49
1:B:505:GLY:N	1:B:520:LEU:HB2	2.28	0.49
1:A:447:HIS:HE1	1:A:451:MSE:H	1.60	0.48
1:A:467:TRP:CD1	1:A:467:TRP:N	2.79	0.48
1:A:542:ARG:HG3	1:A:558:PHE:CD2	2.48	0.48
1:B:88:LEU:HG	1:B:113:GLY:O	2.13	0.48
1:B:469:GLY:HA3	1:B:509:ALA:O	2.13	0.48
1:A:63:SER:OG	1:A:65:HIS:CD2	2.59	0.48
1:B:586:LYS:C	1:B:587:VAL:CG2	2.81	0.48
1:B:223:LYS:O	1:B:224:ASN:C	2.51	0.48
1:A:442:MSE:HG2	1:A:458:THR:HG21	1.95	0.48
1:A:413:THR:HG23	1:A:425:THR:HG22	1.95	0.48
1:B:8:ALA:O	1:B:12:ASP:HB3	2.14	0.48
1:B:416:ARG:HB3	3:B:626:HOH:O	2.13	0.48
1:B:430:LYS:HD2	1:B:431:ASP:H	1.77	0.48
1:B:488:ASN:O	1:B:492:MSE:CG	2.52	0.48
1:B:56:ILE:HG23	1:B:60:LEU:O	2.13	0.48
1:B:410:ARG:CD	1:B:593:ILE:HG22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:HD1	1:A:508:VAL:HG23	1.78	0.48
1:B:55:GLY:O	1:B:62:ALA:N	2.44	0.48
1:B:409:VAL:O	1:B:426:GLU:HG3	2.13	0.48
1:B:448:ARG:O	1:B:448:ARG:CD	2.62	0.48
1:A:40:THR:O	1:A:83:TYR:HA	2.14	0.47
1:A:144:PRO:HG2	1:A:374:MSE:HE1	1.95	0.47
1:B:395:ARG:C	1:B:396:MSE:HG3	2.34	0.47
1:B:485:PHE:CZ	1:B:561:CYS:HA	2.48	0.47
1:A:392:LEU:HG	1:A:392:LEU:O	2.12	0.47
1:A:34:VAL:HG12	1:A:35:LEU:N	2.29	0.47
1:B:242:VAL:HG22	1:B:246:ASP:OD2	2.15	0.47
1:A:161:LEU:N	1:A:161:LEU:HD13	2.30	0.47
1:A:228:ASN:HD21	1:B:64:VAL:H	1.60	0.47
1:B:346:ASP:HA	1:B:362:LEU:O	2.13	0.47
1:B:469:GLY:N	1:B:548:VAL:HG13	2.29	0.47
1:B:592:VAL:O	1:B:593:ILE:HG13	2.15	0.47
1:A:92:HIS:O	1:A:287:CYS:HB2	2.14	0.47
1:A:395:ARG:N	1:A:497:ASN:OD1	2.41	0.47
1:B:185:ILE:HG22	1:B:186:ALA:O	2.15	0.47
1:B:251:LEU:HD12	1:B:251:LEU:HA	1.64	0.47
1:A:99:MSE:HA	1:A:526:VAL:HA	1.97	0.47
1:A:216:CYS:HB3	1:A:237:SER:OG	2.14	0.47
1:B:485:PHE:CD2	1:B:485:PHE:N	2.80	0.47
1:B:409:VAL:HB	1:B:429:VAL:HG23	1.96	0.47
1:B:204:ILE:HD13	1:B:204:ILE:HG21	1.61	0.47
1:A:248:MSE:O	1:A:252:ARG:HG3	2.15	0.46
1:B:412:ALA:O	1:B:413:THR:CG2	2.60	0.46
1:B:416:ARG:HA	1:B:417:PRO:HD2	1.72	0.46
1:B:517:ILE:O	1:B:519:PRO:HD3	2.15	0.46
1:B:593:ILE:HG22	1:B:594:GLU:H	1.80	0.46
1:A:136:ALA:HB1	1:A:149:LEU:HD21	1.97	0.46
1:A:522:LEU:HB2	1:A:526:VAL:HG23	1.98	0.46
1:B:311:ARG:HG2	1:B:311:ARG:HH11	1.79	0.46
1:A:231:MSE:HE1	1:A:253:ALA:O	2.15	0.46
1:B:182:ILE:CG2	1:B:184:GLY:H	2.28	0.46
1:B:266:LEU:CD2	1:B:269:GLU:OE1	2.63	0.46
1:B:533:GLU:CB	3:B:645:HOH:O	2.63	0.46
1:A:195:ILE:O	1:A:195:ILE:HG22	2.15	0.46
1:A:403:LYS:HE3	1:A:432:GLY:HA2	1.96	0.46
1:B:318:TRP:N	1:B:318:TRP:CD1	2.81	0.46
1:A:25:ALA:HB1	1:A:32:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:HIS:CD2	1:B:266:LEU:HG	2.50	0.46
1:B:468:ASN:N	1:B:548:VAL:HG13	2.31	0.46
1:A:89:ILE:HA	1:A:116:THR:O	2.16	0.46
1:B:122:HIS:CA	1:B:152:PRO:HB3	2.45	0.46
1:B:89:ILE:HG12	1:B:116:THR:HB	1.98	0.45
1:B:449:HIS:HD2	1:B:481:ASN:HD21	1.64	0.45
1:A:112:ARG:NH1	1:A:303:ASP:OD2	2.49	0.45
1:B:566:LEU:HG	1:B:566:LEU:O	2.16	0.45
1:B:95:ILE:HG13	1:B:119:TRP:CD2	2.51	0.45
1:B:113:GLY:HA3	1:B:348:VAL:HG21	1.97	0.45
1:B:250:LYS:HE2	3:B:649:HOH:O	2.16	0.45
1:A:66:GLU:HG3	1:A:69:SER:HB3	1.98	0.45
1:A:109:VAL:HG23	1:A:114:VAL:HB	1.98	0.45
1:A:144:PRO:HG2	1:A:374:MSE:CE	2.46	0.45
1:A:508:VAL:HG12	1:A:515:THR:OG1	2.16	0.45
1:B:449:HIS:CD2	1:B:481:ASN:HD21	2.34	0.45
1:B:556:LEU:O	1:B:556:LEU:CG	2.63	0.45
1:B:348:VAL:O	1:B:348:VAL:HG13	2.15	0.45
1:A:568:CYS:HB3	3:A:628:HOH:O	2.16	0.45
1:B:185:ILE:CD1	1:B:208:GLY:HA3	2.47	0.45
1:B:398:ASN:O	1:B:400:PHE:N	2.50	0.45
1:A:140:ILE:HD13	1:A:147:ALA:HB3	1.99	0.45
1:B:9:GLU:HA	1:B:10:PRO:HA	1.50	0.45
1:B:317:GLU:HB3	3:B:638:HOH:O	2.17	0.45
1:B:410:ARG:CZ	1:B:593:ILE:HG21	2.45	0.45
1:B:414:ILE:HG23	1:B:420:THR:HG21	1.99	0.45
1:B:457:LYS:HA	1:B:457:LYS:NZ	2.32	0.45
1:A:494:LEU:HD22	1:A:514:VAL:HG23	1.99	0.45
1:B:282:GLN:HA	1:B:326:ASN:ND2	2.32	0.45
1:B:383:THR:HB	1:B:522:LEU:HD22	1.98	0.45
1:B:592:VAL:CG2	1:B:593:ILE:N	2.78	0.45
1:A:146:ARG:HH22	1:A:344:ARG:HD3	1.82	0.45
1:B:279:HIS:O	1:B:281:PRO:HD3	2.17	0.45
1:B:422:TRP:NE1	1:B:572:PRO:HG3	2.32	0.45
1:A:146:ARG:HB2	1:A:146:ARG:CZ	2.48	0.44
1:A:529:ALA:HB1	1:A:530:PRO:HD2	2.00	0.44
1:B:259:LEU:HD11	1:B:270:PHE:CD2	2.52	0.44
1:B:474:THR:HG23	1:B:524:GLY:O	2.16	0.44
1:A:295:ASP:O	1:A:299:GLY:N	2.51	0.44
1:A:420:THR:CG2	1:A:571:GLY:HA3	2.45	0.44
1:B:93:MSE:HE1	1:B:95:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:VAL:O	1:B:385:VAL:HG13	2.17	0.44
1:A:327:ALA:HB2	3:A:634:HOH:O	2.18	0.44
1:A:477:HIS:HA	1:A:478:ASP:HA	1.60	0.44
1:A:23:VAL:HG21	1:B:233:ALA:HB2	1.99	0.44
1:A:161:LEU:N	1:A:161:LEU:CD1	2.80	0.44
1:B:151:ALA:N	1:B:184:GLY:O	2.49	0.44
1:B:447:HIS:HE1	1:B:451:MSE:H	1.66	0.44
1:A:280:LEU:HD23	3:A:632:HOH:O	2.18	0.44
1:B:19:ARG:HA	1:B:19:ARG:HD3	1.81	0.44
1:B:477:HIS:HA	1:B:478:ASP:HA	1.40	0.44
1:A:436:PRO:HA	1:A:437:PRO:HD3	1.84	0.44
1:B:36:ILE:O	1:B:53:ASP:HA	2.18	0.44
1:A:45:VAL:HG23	1:A:338:LEU:HD13	1.99	0.44
1:B:350:PHE:CE1	1:B:356:PHE:HB3	2.53	0.44
1:B:370:GLU:O	1:B:371:GLY:C	2.56	0.44
1:B:584:THR:O	1:B:586:LYS:N	2.51	0.44
1:B:90:ASP:HA	1:B:302:LEU:HD13	1.99	0.43
1:B:270:PHE:CD1	1:B:270:PHE:N	2.84	0.43
1:B:435:VAL:HG23	1:B:436:PRO:HD2	1.99	0.43
1:B:446:THR:O	1:B:481:ASN:HB3	2.17	0.43
1:B:494:LEU:HD13	1:B:494:LEU:HA	1.66	0.43
1:B:533:GLU:HB2	3:B:645:HOH:O	2.18	0.43
1:A:158:ALA:HB1	1:A:161:LEU:HD22	2.00	0.43
1:B:582:VAL:HG13	1:B:583:LEU:H	1.82	0.43
1:B:98:SER:O	1:B:100:ILE:HG23	2.18	0.43
1:B:435:VAL:CG2	1:B:436:PRO:HD2	2.49	0.43
1:A:192:ARG:HA	1:A:192:ARG:HD3	1.59	0.43
1:B:257:ILE:O	1:B:285:THR:OG1	2.31	0.43
1:A:522:LEU:HB2	1:A:526:VAL:HG22	2.01	0.43
1:B:390:MSE:HE3	1:B:392:LEU:HD21	2.01	0.43
1:B:569:ASN:HA	3:B:635:HOH:O	2.18	0.43
1:A:461:LEU:HD13	1:A:464:TRP:CE2	2.53	0.43
1:B:182:ILE:HG22	1:B:184:GLY:N	2.30	0.43
1:B:520:LEU:HD22	1:B:526:VAL:C	2.38	0.43
1:A:301:GLY:O	1:A:302:LEU:C	2.56	0.43
1:A:548:VAL:HG13	1:A:548:VAL:O	2.18	0.43
1:A:554:PRO:O	1:A:554:PRO:CD	2.62	0.43
1:B:122:HIS:HA	1:B:152:PRO:HB3	2.01	0.43
1:B:311:ARG:HG2	1:B:311:ARG:NH1	2.34	0.43
1:B:545:VAL:C	1:B:547:LYS:H	2.22	0.43
1:A:145:LEU:HA	1:A:145:LEU:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLY:O	1:A:308:ARG:NH2	2.52	0.43
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.17	0.43
1:A:510:SER:N	1:A:513:LYS:O	2.39	0.43
1:B:89:ILE:HG21	1:B:327:ALA:HB1	2.00	0.43
1:B:123:GLU:OE1	1:B:480:HIS:CE1	2.72	0.43
1:A:20:ALA:HB2	1:B:197:ARG:NE	2.34	0.42
1:A:128:HIS:HB2	1:A:132:GLY:CA	2.49	0.42
1:B:86:PRO:N	1:B:339:ILE:HD11	2.35	0.42
1:B:168:PHE:CD1	1:B:172:ILE:HG21	2.54	0.42
1:B:183:GLY:O	1:B:214:LEU:HD12	2.18	0.42
1:B:457:LYS:HB3	1:B:574:GLN:HE21	1.84	0.42
1:B:484:VAL:HG12	1:B:492:MSE:HE3	2.00	0.42
1:B:520:LEU:HD23	1:B:520:LEU:HA	1.93	0.42
1:B:394:LEU:C	1:B:395:ARG:HD2	2.40	0.42
1:B:513:LYS:HE2	1:B:513:LYS:HB3	1.41	0.42
1:A:228:ASN:HD22	1:B:341:ALA:HB2	1.85	0.42
1:B:23:VAL:O	1:B:26:ALA:HB3	2.19	0.42
1:A:35:LEU:HA	1:A:54:ILE:O	2.20	0.42
1:B:22:ALA:HB1	1:B:62:ALA:HB2	2.00	0.42
1:B:104:ALA:O	1:B:107:ALA:HB3	2.20	0.42
1:B:231:MSE:SE	1:B:231:MSE:HB3	2.70	0.42
1:A:18:LEU:HG	1:A:60:LEU:HD12	2.01	0.42
1:A:130:VAL:O	1:A:134:ARG:N	2.48	0.42
1:A:417:PRO:O	1:A:418:ARG:HB3	2.20	0.42
1:A:475:VAL:HG22	1:A:525:LEU:HD23	2.00	0.42
1:B:11:ALA:HA	1:B:14:ASN:ND2	2.34	0.42
1:B:518:LEU:HD13	1:B:537:ALA:HB3	2.01	0.42
1:A:34:VAL:CG1	1:A:35:LEU:N	2.82	0.42
1:A:67:PRO:C	1:A:69:SER:N	2.72	0.42
1:A:416:ARG:HA	1:A:417:PRO:HD3	1.91	0.42
1:B:99:MSE:HA	1:B:526:VAL:HA	2.01	0.42
1:B:268:PRO:HD3	1:B:312:TYR:CE1	2.55	0.42
1:B:474:THR:CG2	1:B:524:GLY:O	2.68	0.42
1:A:514:VAL:HG11	1:A:517:ILE:HD11	2.00	0.42
1:B:475:VAL:HG22	1:B:525:LEU:HA	2.01	0.42
1:B:571:GLY:O	1:B:573:HIS:CD2	2.73	0.42
1:A:448:ARG:N	1:A:481:ASN:ND2	2.58	0.42
1:B:395:ARG:O	1:B:396:MSE:HG3	2.20	0.42
1:B:416:ARG:CD	1:B:421:GLN:OE1	2.66	0.42
1:B:424:GLU:C	1:B:425:THR:CG2	2.88	0.42
1:A:457:LYS:HB3	1:A:574:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:VAL:O	1:B:548:VAL:CG1	2.68	0.42
1:A:582:VAL:H	1:A:582:VAL:HG12	1.42	0.42
1:B:198:ASP:O	1:B:202:SER:HB2	2.19	0.42
1:B:505:GLY:HA2	1:B:520:LEU:CB	2.37	0.42
1:B:506:MSE:HE3	1:B:520:LEU:HD11	2.02	0.42
1:A:167:ASP:O	1:A:168:PHE:HD1	2.03	0.41
1:A:198:ASP:HA	1:A:199:PRO:HD3	1.83	0.41
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.64	0.41
1:A:418:ARG:HD3	1:A:419:PHE:CE2	2.55	0.41
1:B:282:GLN:HA	1:B:326:ASN:HD21	1.85	0.41
1:A:66:GLU:HG2	1:A:69:SER:HB3	2.02	0.41
1:A:252:ARG:HG2	1:B:46:THR:HG21	2.00	0.41
1:B:520:LEU:HD22	1:B:526:VAL:CA	2.50	0.41
1:A:46:THR:OG1	1:A:48:GLU:HG3	2.20	0.41
1:B:294:ASP:CA	1:B:535:ALA:HB1	2.47	0.41
1:B:593:ILE:HG22	1:B:594:GLU:N	2.35	0.41
1:A:90:ASP:O	1:A:118:VAL:HB	2.20	0.41
1:A:155:VAL:HG22	1:A:168:PHE:CG	2.56	0.41
1:A:443:ILE:HB	1:A:461:LEU:HD21	2.02	0.41
1:B:129:GLY:O	1:B:130:VAL:C	2.59	0.41
1:B:155:VAL:O	1:B:155:VAL:HG23	2.20	0.41
1:A:92:HIS:CE1	1:A:187:GLU:HG2	2.42	0.41
1:A:386:LEU:HD22	1:A:523:SER:HG	1.85	0.41
1:A:520:LEU:HD13	1:A:525:LEU:O	2.21	0.41
1:B:175:ASP:O	1:B:178:SER:OG	2.38	0.41
1:B:24:ALA:O	1:B:25:ALA:C	2.56	0.41
1:B:410:ARG:O	1:B:411:LEU:CB	2.66	0.41
1:B:429:VAL:HA	1:B:435:VAL:H	1.86	0.41
1:A:54:ILE:CG2	1:A:61:ILE:HG23	2.51	0.41
1:A:136:ALA:O	1:A:140:ILE:HG12	2.21	0.41
1:A:424:GLU:C	1:A:425:THR:HG22	2.40	0.41
1:B:31:ARG:CB	1:B:72:ASP:OD2	2.69	0.41
1:B:155:VAL:HA	1:B:156:PRO:HA	1.65	0.41
1:B:447:HIS:HB2	1:B:576:ASP:OD1	2.21	0.41
1:B:399:ASP:OD1	1:B:456:THR:HG23	2.21	0.41
1:A:36:ILE:N	1:A:54:ILE:O	2.45	0.40
1:A:447:HIS:HD2	1:A:576:ASP:OD1	2.04	0.40
1:B:13:LEU:HD23	1:B:13:LEU:HA	1.93	0.40
1:B:196:GLU:O	1:B:197:ARG:HB3	2.21	0.40
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.92	0.40
1:B:433:PHE:CD2	1:B:433:PHE:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ARG:C	1:B:448:ARG:HD2	2.41	0.40
1:B:451:MSE:O	1:B:452:ALA:HB2	2.20	0.40
1:B:554:PRO:O	1:B:555:TYR:CB	2.70	0.40
1:A:252:ARG:HB3	1:B:50:ARG:NH2	2.36	0.40
1:A:485:PHE:N	1:A:485:PHE:HD2	2.18	0.40
1:A:13:LEU:O	1:A:19:ARG:NE	2.53	0.40
1:A:471:PHE:CD1	1:A:508:VAL:HG23	2.55	0.40
1:B:155:VAL:O	1:B:155:VAL:CG2	2.69	0.40
1:B:161:LEU:CD1	1:B:161:LEU:H	2.31	0.40
1:B:185:ILE:HD11	1:B:208:GLY:CA	2.51	0.40
1:B:415:ASP:HB3	1:B:421:GLN:HG3	2.04	0.40
1:B:448:ARG:CD	1:B:448:ARG:C	2.90	0.40
1:A:413:THR:OG1	1:A:423:GLY:CA	2.70	0.40
1:B:69:SER:O	1:B:70:ARG:HG2	2.22	0.40
1:B:388:GLY:HA2	3:B:634:HOH:O	2.21	0.40
1:B:395:ARG:N	1:B:497:ASN:OD1	2.49	0.40
1:B:506:MSE:HE3	1:B:520:LEU:CD1	2.52	0.40
1:B:563:GLY:O	1:B:565:THR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	585/608 (96%)	520 (89%)	49 (8%)	16 (3%)	5 17
1	B	585/608 (96%)	483 (83%)	69 (12%)	33 (6%)	2 5
All	All	1170/1216 (96%)	1003 (86%)	118 (10%)	49 (4%)	3 9

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	406	GLY
1	B	72	ASP
1	B	224	ASN
1	B	418	ARG
1	B	428	ASP
1	B	429	VAL
1	B	461	LEU
1	B	583	LEU
1	B	584	THR
1	B	585	GLY
1	B	593	ILE
1	A	69	SER
1	A	418	ARG
1	A	555	TYR
1	A	589	GLU
1	B	299	GLY
1	B	303	ASP
1	B	364	SER
1	B	371	GLY
1	B	399	ASP
1	B	555	TYR
1	A	74	ALA
1	A	380	THR
1	A	397	ALA
1	A	416	ARG
1	A	543	GLU
1	A	544	ALA
1	B	247	LEU
1	B	311	ARG
1	B	388	GLY
1	B	397	ALA
1	A	583	LEU
1	B	186	ALA
1	B	197	ARG
1	B	404	SER
1	B	411	LEU
1	B	416	ARG
1	B	523	SER
1	B	564	ALA
1	B	573	HIS
1	B	576	ASP
1	A	136	ALA

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Mol	Chain	Res	Type
1	A	302	LEU
1	A	425	THR
1	B	68	ALA
1	B	414	ILE
1	B	587	VAL
1	B	417	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	445/444 (100%)	386 (87%)	59 (13%)	4 12
1	B	444/444 (100%)	379 (85%)	65 (15%)	3 9
All	All	889/888 (100%)	765 (86%)	124 (14%)	3 11

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	31	ARG
1	A	35	LEU
1	A	66	GLU
1	A	78	ASP
1	A	84	VAL
1	A	98	SER
1	A	99	MSE
1	A	109	VAL
1	A	122	HIS
1	A	131	ASP
1	A	134	ARG
1	A	152	PRO
1	A	155	VAL
1	A	161	LEU
1	A	163	ARG
1	A	175	ASP

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Mol	Chain	Res	Type
1	A	189	MSE
1	A	191	MSE
1	A	192	ARG
1	A	209	LEU
1	A	227	LEU
1	A	230	PHE
1	A	245	GLU
1	A	259	LEU
1	A	280	LEU
1	A	290	ASP
1	A	334	SER
1	A	354	ASN
1	A	366	ARG
1	A	373	ARG
1	A	380	THR
1	A	396	MSE
1	A	408	LYS
1	A	420	THR
1	A	425	THR
1	A	426	GLU
1	A	430	LYS
1	A	434	VAL
1	A	438	GLU
1	A	442	MSE
1	A	444	SER
1	A	453	GLU
1	A	461	LEU
1	A	466	ARG
1	A	476	SER
1	A	483	THR
1	A	494	LEU
1	A	515	THR
1	A	518	LEU
1	A	528	ASP
1	A	536	ARG
1	A	543	GLU
1	A	548	VAL
1	A	552	GLN
1	A	577	MSE
1	A	583	LEU
1	A	588	MSE
1	A	594	GLU

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Mol	Chain	Res	Type
1	B	10	PRO
1	B	12	ASP
1	B	15	ASP
1	B	17	THR
1	B	35	LEU
1	B	42	VAL
1	B	71	ARG
1	B	75	GLN
1	B	97	SER
1	B	101	THR
1	B	126	ASN
1	B	155	VAL
1	B	161	LEU
1	B	173	LEU
1	B	189	MSE
1	B	191	MSE
1	B	192	ARG
1	B	196	GLU
1	B	199	PRO
1	B	226	ASP
1	B	228	ASN
1	B	241	LEU
1	B	242	VAL
1	B	243	SER
1	B	245	GLU
1	B	251	LEU
1	B	255	LEU
1	B	267	LEU
1	B	290	ASP
1	B	295	ASP
1	B	302	LEU
1	B	311	ARG
1	B	357	SER
1	B	362	LEU
1	B	382	ASP
1	B	385	VAL
1	B	402	VAL
1	B	408	LYS
1	B	409	VAL
1	B	411	LEU
1	B	414	ILE
1	B	416	ARG

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Mol	Chain	Res	Type
1	B	420	THR
1	B	425	THR
1	B	428	ASP
1	B	430	LYS
1	B	441	THR
1	B	442	MSE
1	B	444	SER
1	B	455	THR
1	B	456	THR
1	B	457	LYS
1	B	474	THR
1	B	483	THR
1	B	485	PHE
1	B	494	LEU
1	B	510	SER
1	B	517	ILE
1	B	523	SER
1	B	531	LEU
1	B	559	LYS
1	B	570	ILE
1	B	575	THR
1	B	590	SER
1	B	593	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	206	GLN
1	A	228	ASN
1	A	279	HIS
1	A	282	GLN
1	A	326	ASN
1	A	329	GLN
1	A	398	ASN
1	A	447	HIS
1	A	481	ASN
1	A	488	ASN
1	A	573	HIS
1	B	65	HIS
1	B	126	ASN
1	B	206	GLN

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Mol	Chain	Res	Type
1	B	228	ASN
1	B	265	HIS
1	B	279	HIS
1	B	329	GLN
1	B	447	HIS
1	B	480	HIS
1	B	481	ASN
1	B	488	ASN
1	B	573	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

Of 6 ligands modelled in this entry, 6 are unknown - 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

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, 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	571/608 (93%)	-0.60	1 (0%)	95	94	28, 44, 66, 80	0
1	B	571/608 (93%)	-0.31	11 (1%)	66	59	28, 49, 83, 98	27 (4%)
All	All	1142/1216 (93%)	-0.45	12 (1%)	80	75	28, 46, 75, 98	27 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	594	GLU	4.2
1	B	406	GLY	4.0
1	B	411	LEU	3.6
1	B	412	ALA	3.4
1	B	464	TRP	2.7
1	B	593	ILE	2.6
1	B	407	ALA	2.6
1	B	592	VAL	2.4
1	B	419	PHE	2.4
1	B	418	ARG	2.4
1	B	460	PHE	2.3
1	A	583	LEU	2.2

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

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UNX	A	608	1/1	0.38	0.58	43,43,43,43	0
2	UNX	B	608	1/1	0.52	0.54	50,50,50,50	0
2	UNX	A	607	1/1	0.62	0.64	43,43,43,43	0
2	UNX	B	607	1/1	0.63	0.58	60,60,60,60	0
2	UNX	A	606	1/1	0.68	0.72	53,53,53,53	0
2	UNX	B	606	1/1	0.71	0.61	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.