Full wwPDB X-ray Structure Validation Report (i)

Sep 30, 2021 – 02:23 PM EDT

PDB ID	:	3MC2
Title	:	Crystal Structure of the Murine Inhibitor of Carbonic Anhydrase
Authors	:	Eckenroth, B.E.; Mason, A.B.; Everse, S.J.
Deposited on	:	2010-03-26
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

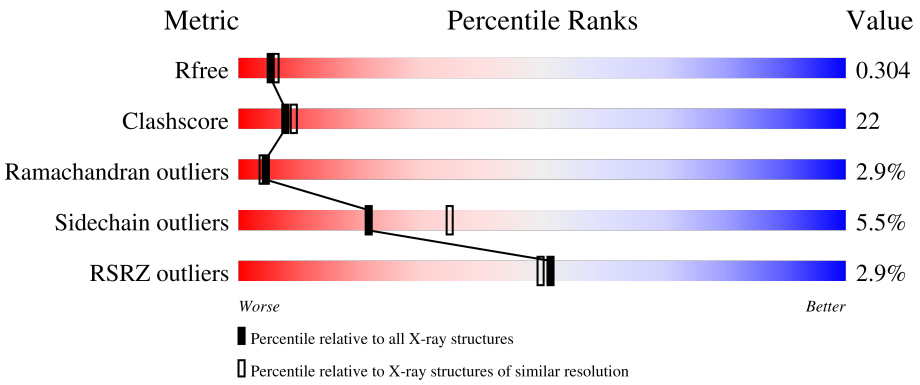
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	687	3% 56% 38%
1	B	687	2% 58% 37%
1	C	687	2% 59% 35%
1	D	687	4% 59% 34%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20772 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 Inhibitor of Carbonic Anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	675	5193	3257	902	986	48	51	0	0
1	B	675	5193	3257	902	986	48	79	0	0
1	C	675	5193	3257	902	986	48	45	0	0
1	D	675	5193	3257	902	986	48	57	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9DBD0
A	-4	HIS	-	expression tag	UNP Q9DBD0
A	-3	HIS	-	expression tag	UNP Q9DBD0
A	-2	HIS	-	expression tag	UNP Q9DBD0
A	-1	HIS	-	expression tag	UNP Q9DBD0
A	0	HIS	-	expression tag	UNP Q9DBD0
A	470	ASP	ASN	engineered mutation	UNP Q9DBD0
A	645	ASP	ASN	engineered mutation	UNP Q9DBD0
B	-5	HIS	-	expression tag	UNP Q9DBD0
B	-4	HIS	-	expression tag	UNP Q9DBD0
B	-3	HIS	-	expression tag	UNP Q9DBD0
B	-2	HIS	-	expression tag	UNP Q9DBD0
B	-1	HIS	-	expression tag	UNP Q9DBD0
B	0	HIS	-	expression tag	UNP Q9DBD0
B	470	ASP	ASN	engineered mutation	UNP Q9DBD0
B	645	ASP	ASN	engineered mutation	UNP Q9DBD0
C	-5	HIS	-	expression tag	UNP Q9DBD0
C	-4	HIS	-	expression tag	UNP Q9DBD0
C	-3	HIS	-	expression tag	UNP Q9DBD0
C	-2	HIS	-	expression tag	UNP Q9DBD0
C	-1	HIS	-	expression tag	UNP Q9DBD0

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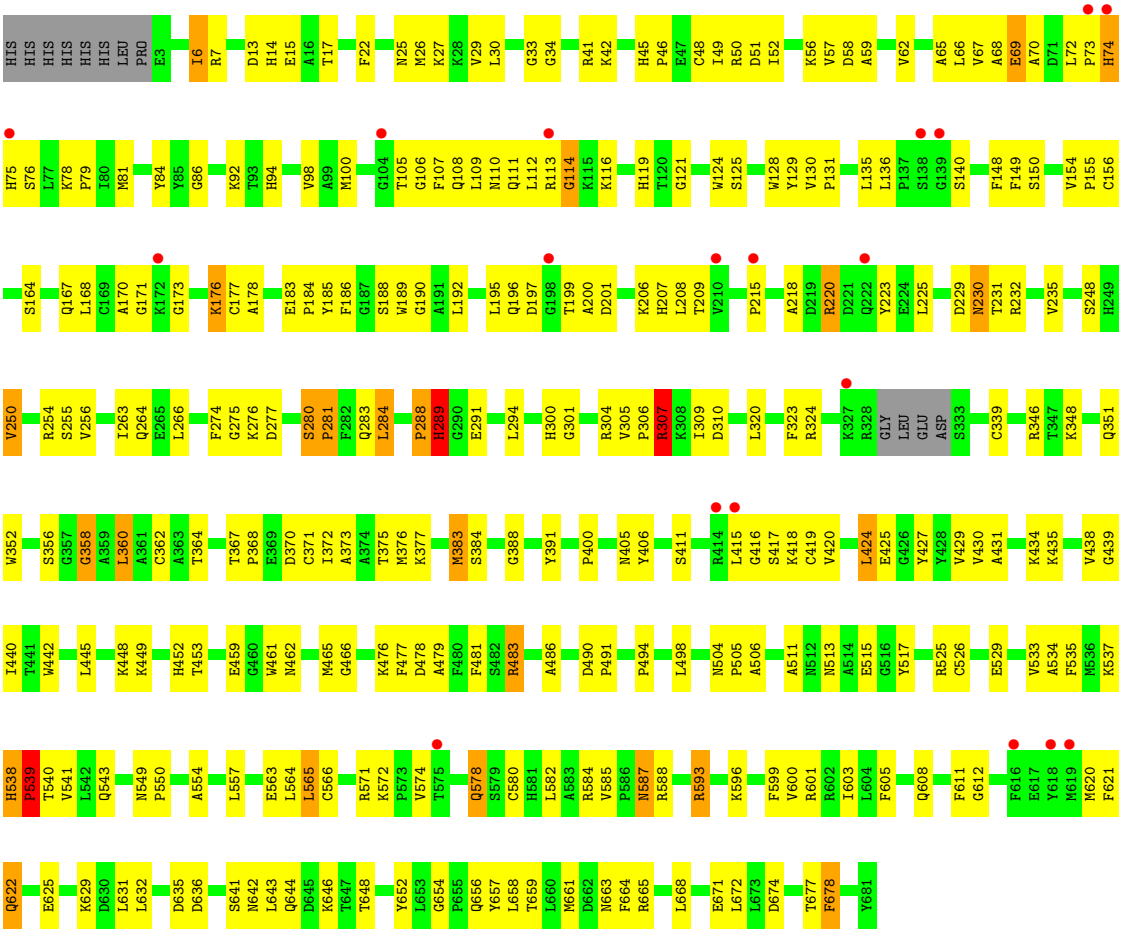
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q9DBD0
C	470	ASP	ASN	engineered mutation	UNP Q9DBD0
C	645	ASP	ASN	engineered mutation	UNP Q9DBD0
D	-5	HIS	-	expression tag	UNP Q9DBD0
D	-4	HIS	-	expression tag	UNP Q9DBD0
D	-3	HIS	-	expression tag	UNP Q9DBD0
D	-2	HIS	-	expression tag	UNP Q9DBD0
D	-1	HIS	-	expression tag	UNP Q9DBD0
D	0	HIS	-	expression tag	UNP Q9DBD0
D	470	ASP	ASN	engineered mutation	UNP Q9DBD0
D	645	ASP	ASN	engineered mutation	UNP Q9DBD0

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.

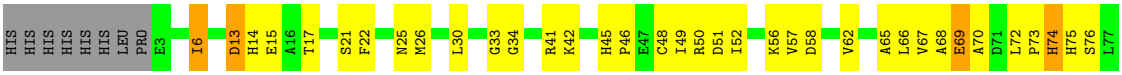
• Molecule 1: Inhibitor of Carbonic Anhydrase

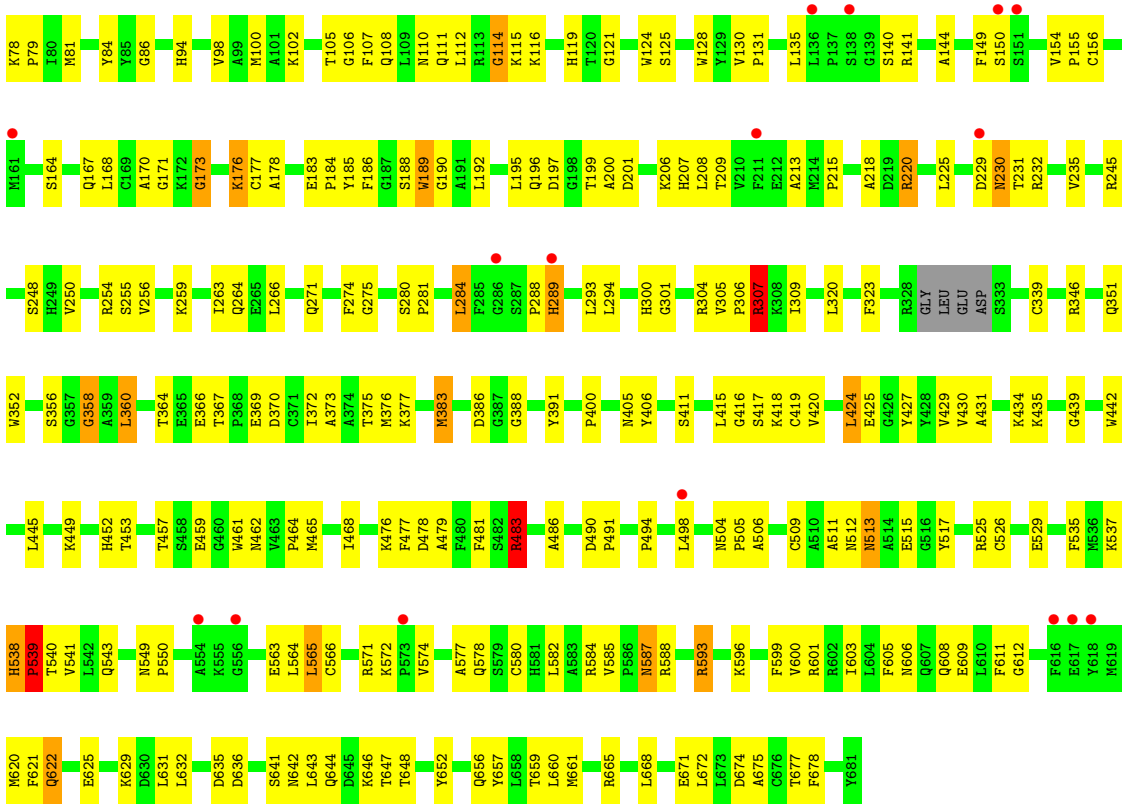
Chain A:



• Molecule 1: Inhibitor of Carbonic Anhydrase

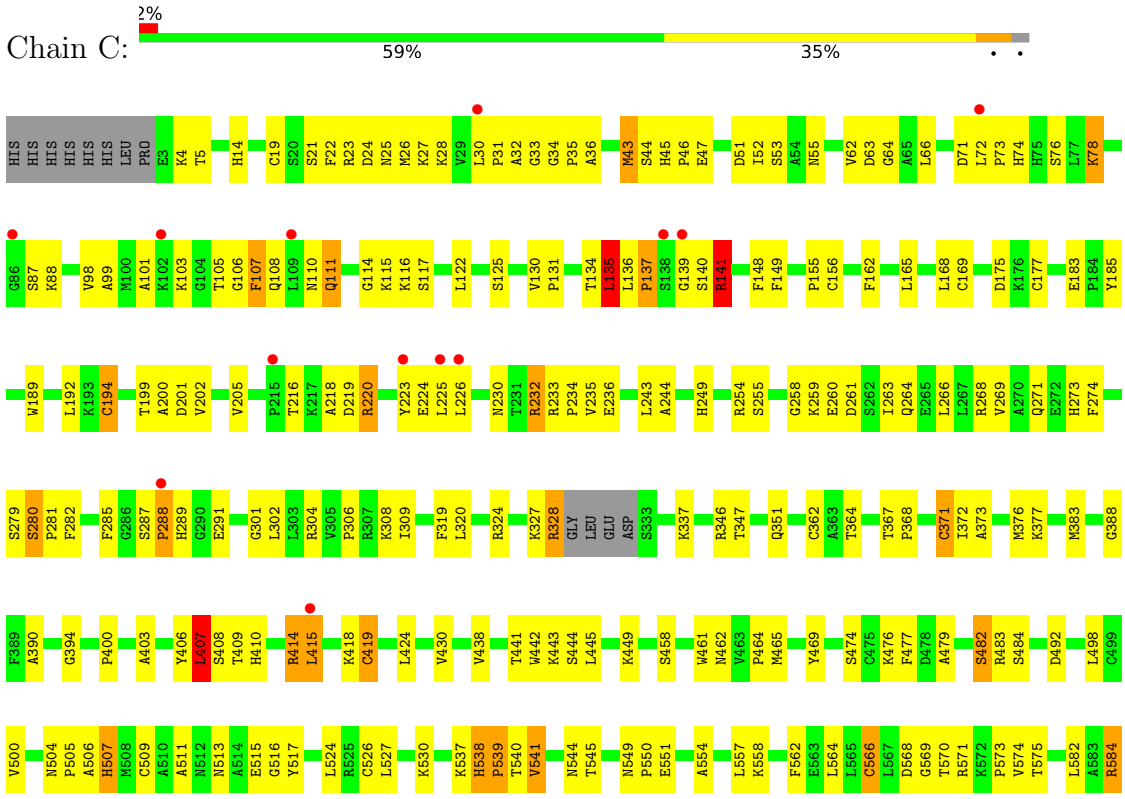
Chain B:

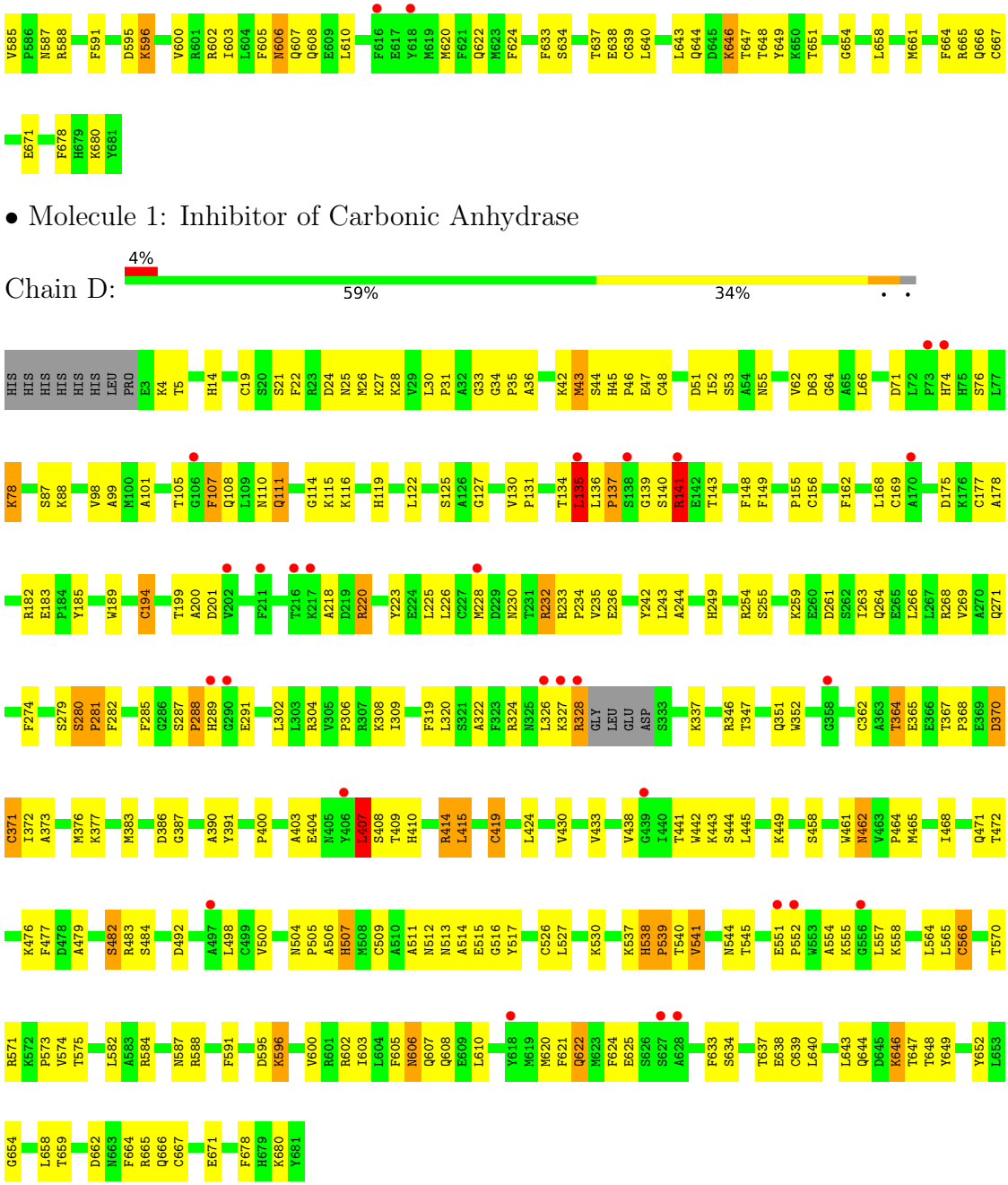




• Molecule 1: Inhibitor of Carbonic Anhydrase

Chain C:




V585 P586 N587 R588 F591 D595 K596 V600 R601 R602 I603 L604 F605 N606 Q607 Q608 E609 L610 F616 E617 Y618 M619 M620 F621 Q622 M623 F624 F633 S634 T637 E638 C639 L640 L643 Q644 D645 K646 T647 T648 Y649 K650 T651 G654 L658 M661 F664 R665 Q666 C667
E671 F678 H679 K680 Y681
• Molecule 1: Inhibitor of Carbonic Anhydrase
Chain D:
4%
59%
34%
HIS HIS HIS HIS HIS HIS LEU PRO E3 K4 T5 H14 C19 S20 S21 F22 R23 D24 N25 M26 K27 K28 V29 L30 P31 A32 G33 G34 P35 A36 K42 M43 S44 H45 P46 E47 C48 D51 I52 S53 A54 N55 V62 D63 G64 A65 L66 D71 L72 P73 H74 H75 S76 L77
K78 S87 K88 V98 A99 M100 A101 T105 G106 F107 Q108 L109 N110 Q111 G114 K115 K116 H119 L122 S125 A126 G127 V130 P131 T134 L135 L136 P137 S138 G139 S140 R141 E142 T143 F148 F149 P155 C156 F162 L168 C169 A170 D175 K176 C177 A178
R182 E183 P184 Y185 W189 C194 T199 A200 D201 V202 F211 T216 K217 A218 D219 R220 Y223 E224 L225 L226 C227 M228 D229 N230 T231 R232 R233 P234 V235 E236 Y242 L243 A244 H249 R254 S255 K259 E260 D261 S262 I263 Q264 E265 L266 L267 R268 V269 A270 Q271
F274 S279 S280 P281 F282 F285 G286 S287 P288 H289 G290 E291 L302 L303 R304 V305 P306 R307 K308 I309 F319 L320 S321 A322 F323 R324 N325 L326 K327 R328 GLY LEU GLU ASP S333 K337 R346 T347 Q351 W352 G358 C362 A363 T364 E365 E366 T367 P368 E369 D370
C371 I372 A373 M376 K377 M383 D386 G387 A390 Y391 P400 A403 E404 N405 Y406 L407 S408 T409 H410 R414 L415 C419 L424 V430 V433 V438 G439 T440 T441 W442 K443 S444 L445 K449 S458 W461 N462 V463 P464 M465 I468 Q471 T472
K476 F477 D478 A479 S482 R483 S484 D492 A497 L498 C499 V500 N504 P505 A506 H507 M508 C509 A510 A511 N512 N513 A514 E515 G516 Y517 C526 L527 K530 K537 H538 P539 T540 V541 N544 T545 E551 P552 W553 A554 K555 G556 L557 K558 L564 L565 C566 T570
R571 K572 P573 V574 T575 L582 A583 R584 N587 R588 F591 D595 K596 V600 R601 R602 I603 L604 F605 N606 Q607 Q608 E609 L610 Y618 M619 M620 F621 Q622 M623 F624 E625 S626 S627 A628 F633 S634 T637 E638 C639 L640 L643 Q644 D645 K646 T647 T648 Y649 Y652 L653
G654 L658 T659 D662 N663 F664 R665 Q666 C667 E671 F678 H679 K680 Y681

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.56Å 136.93Å 155.57Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	19.00 – 2.40 18.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.00-2.40) 93.9 (18.95-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.41Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.239 , 0.301 0.241 , 0.304	Depositor DCC
R_{free} test set	10093 reflections (9.56%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	1 of 105600 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20772	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7286e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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)

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	0.61	4/5312 (0.1%)	1.04	10/7179 (0.1%)
1	B	0.58	4/5312 (0.1%)	0.99	8/7179 (0.1%)
1	C	0.51	3/5312 (0.1%)	0.75	8/7179 (0.1%)
1	D	0.47	3/5312 (0.1%)	0.73	7/7179 (0.1%)
All	All	0.55	14/21248 (0.1%)	0.89	33/28716 (0.1%)

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	1
1	B	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	ARG	CZ-NH1	-14.12	1.14	1.33
1	A	307	ARG	CZ-NH1	-13.47	1.15	1.33
1	A	254	ARG	CZ-NH2	-13.44	1.15	1.33
1	B	307	ARG	CZ-NH2	-12.93	1.16	1.33
1	A	307	ARG	CZ-NH2	-11.93	1.17	1.33
1	A	254	ARG	CZ-NH1	-11.89	1.17	1.33
1	B	254	ARG	CZ-NH2	-11.65	1.18	1.33
1	B	254	ARG	CZ-NH1	-11.44	1.18	1.33
1	C	141	ARG	CZ-NH1	-8.94	1.21	1.33
1	C	141	ARG	CZ-NH2	-8.81	1.21	1.33
1	D	141	ARG	CZ-NH2	-8.73	1.21	1.33
1	C	232	ARG	CD-NE	-6.82	1.34	1.46
1	D	141	ARG	CZ-NH1	-6.81	1.24	1.33
1	D	232	ARG	CD-NE	-6.76	1.34	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	ARG	NE-CZ-NH2	34.14	137.37	120.30
1	B	254	ARG	NE-CZ-NH1	31.73	136.16	120.30
1	B	307	ARG	NE-CZ-NH1	29.80	135.20	120.30
1	A	254	ARG	NE-CZ-NH2	29.11	134.85	120.30
1	B	307	ARG	NH1-CZ-NH2	-23.68	93.36	119.40
1	A	254	ARG	NH1-CZ-NH2	-23.34	93.73	119.40
1	B	254	ARG	NH1-CZ-NH2	-22.94	94.17	119.40
1	A	307	ARG	NH1-CZ-NH2	-22.63	94.51	119.40
1	B	307	ARG	NE-CZ-NH2	22.27	131.44	120.30
1	A	254	ARG	NE-CZ-NH1	20.22	130.41	120.30
1	D	141	ARG	NE-CZ-NH1	18.41	129.51	120.30
1	B	254	ARG	NE-CZ-NH2	18.33	129.46	120.30
1	A	601	ARG	NE-CZ-NH2	-18.13	111.23	120.30
1	A	601	ARG	NE-CZ-NH1	16.09	128.34	120.30
1	C	141	ARG	NE-CZ-NH1	15.79	128.19	120.30
1	C	141	ARG	NE-CZ-NH2	15.62	128.11	120.30
1	A	307	ARG	NE-CZ-NH1	15.38	127.99	120.30
1	D	141	ARG	NH1-CZ-NH2	-14.87	103.05	119.40
1	C	141	ARG	NH1-CZ-NH2	-14.36	103.61	119.40
1	D	141	ARG	NE-CZ-NH2	14.03	127.31	120.30
1	A	304	ARG	NE-CZ-NH1	13.79	127.19	120.30
1	C	602	ARG	NE-CZ-NH1	12.28	126.44	120.30
1	D	602	ARG	NE-CZ-NH2	10.15	125.38	120.30
1	C	602	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	304	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	C	232	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	B	304	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	D	602	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	D	232	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	C	602	ARG	CD-NE-CZ	5.91	131.87	123.60
1	B	601	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	D	602	ARG	CD-NE-CZ	5.43	131.20	123.60
1	C	232	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	652	TYR	Sidechain
1	B	652	TYR	Sidechain

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	5193	0	5024	224	0
1	B	5193	0	5024	210	0
1	C	5193	0	5024	233	0
1	D	5193	0	5024	222	0
All	All	20772	0	20096	884	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 22.

All (884) 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:C:414:ARG:HG2	1:C:415:LEU:H	1.21	1.05
1:D:414:ARG:HG2	1:D:415:LEU:H	1.21	1.03
1:C:558:LYS:HB3	1:C:558:LYS:HZ2	1.22	1.02
1:D:558:LYS:HZ2	1:D:558:LYS:HB3	1.22	1.00
1:A:572:LYS:HE2	1:A:580:CYS:HB2	1.43	0.99
1:B:587:ASN:N	1:B:587:ASN:HD22	1.57	0.98
1:C:218:ALA:HA	1:C:220:ARG:HE	1.27	0.96
1:D:218:ALA:HA	1:D:220:ARG:HE	1.30	0.96
1:A:587:ASN:N	1:A:587:ASN:HD22	1.59	0.96
1:B:572:LYS:HE2	1:B:580:CYS:HB2	1.46	0.95
1:B:112:LEU:HA	1:B:115:LYS:HE2	1.50	0.94
1:B:587:ASN:H	1:B:587:ASN:ND2	1.59	0.93
1:A:587:ASN:H	1:A:587:ASN:ND2	1.61	0.92
1:C:371:CYS:HB3	1:C:383:MET:SD	2.12	0.90
1:C:108:GLN:NE2	1:C:232:ARG:HG3	1.90	0.86
1:D:220:ARG:H	1:D:220:ARG:HD3	1.40	0.85
1:A:416:GLY:C	1:A:418:LYS:H	1.79	0.85
1:C:220:ARG:H	1:C:220:ARG:HD3	1.39	0.85
1:D:371:CYS:HB3	1:D:383:MET:SD	2.17	0.85
1:B:416:GLY:C	1:B:418:LYS:H	1.80	0.85
1:C:441:THR:HG22	1:C:444:SER:OG	1.77	0.84
1:A:587:ASN:HD22	1:A:587:ASN:H	0.88	0.84
1:C:337:LYS:NZ	1:C:337:LYS:HB2	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:PRO:HD2	1:D:647:THR:O	1.79	0.83
1:A:564:LEU:HG	1:A:574:VAL:HA	1.61	0.82
1:B:587:ASN:HD22	1:B:587:ASN:H	0.84	0.81
1:D:558:LYS:HB3	1:D:558:LYS:NZ	1.96	0.81
1:D:337:LYS:HB2	1:D:337:LYS:NZ	1.95	0.80
1:C:558:LYS:HB3	1:C:558:LYS:NZ	1.97	0.80
1:C:400:PRO:HD2	1:C:647:THR:O	1.82	0.79
1:A:442:TRP:HA	1:A:445:LEU:HD11	1.65	0.78
1:B:564:LEU:HG	1:B:574:VAL:HA	1.65	0.78
1:C:108:GLN:HE22	1:C:232:ARG:HG3	1.48	0.78
1:D:441:THR:H	1:D:444:SER:HB2	1.49	0.78
1:C:103:LYS:HA	1:C:224:GLU:HG2	1.64	0.77
1:B:442:TRP:HA	1:B:445:LEU:HD11	1.67	0.77
1:D:541:VAL:CG1	1:D:574:VAL:HG21	2.14	0.77
1:A:644:GLN:HA	1:A:644:GLN:HE21	1.50	0.77
1:B:406:TYR:OH	1:B:588:ARG:HG3	1.85	0.76
1:B:656:GLN:O	1:B:659:THR:HG22	1.84	0.76
1:C:14:HIS:ND1	1:C:289:HIS:HB3	2.00	0.76
1:B:70:ALA:HB1	1:B:75:HIS:O	1.87	0.75
1:C:5:THR:HG23	1:C:36:ALA:HB3	1.68	0.75
1:A:171:GLY:HA3	1:A:176:LYS:HA	1.69	0.75
1:C:216:THR:OG1	1:C:219:ASP:HB2	1.87	0.74
1:D:14:HIS:ND1	1:D:289:HIS:HB3	2.01	0.74
1:A:665:ARG:HA	1:A:668:LEU:HD12	1.69	0.74
1:A:70:ALA:HB1	1:A:75:HIS:O	1.88	0.74
1:B:644:GLN:HE21	1:B:644:GLN:HA	1.51	0.74
1:C:441:THR:H	1:C:444:SER:HB2	1.53	0.74
1:D:441:THR:HG22	1:D:444:SER:OG	1.86	0.74
1:D:108:GLN:HB2	1:D:111:GLN:HE22	1.53	0.74
1:C:541:VAL:CG1	1:C:574:VAL:HG21	2.18	0.73
1:C:108:GLN:HB2	1:C:111:GLN:HE22	1.53	0.73
1:A:280:SER:OG	1:A:281:PRO:HD3	1.88	0.73
1:B:171:GLY:HA3	1:B:176:LYS:HA	1.71	0.73
1:C:328:ARG:C	1:C:328:ARG:HE	1.91	0.73
1:A:110:ASN:CG	1:A:230:ASN:HD21	1.92	0.73
1:C:259:LYS:O	1:C:263:ILE:HG13	1.89	0.72
1:A:27:LYS:NZ	1:D:659:THR:HG23	2.03	0.72
1:B:110:ASN:CG	1:B:230:ASN:HD21	1.93	0.72
1:D:328:ARG:HE	1:D:328:ARG:C	1.91	0.72
1:A:656:GLN:O	1:A:659:THR:HG22	1.88	0.72
1:B:30:LEU:HD11	1:B:33:GLY:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:HD11	1:A:33:GLY:O	1.88	0.72
1:B:372:ILE:O	1:B:376:MET:HG3	1.90	0.72
1:D:88:LYS:HE3	1:D:88:LYS:HA	1.72	0.72
1:C:279:SER:OG	1:C:281:PRO:HD2	1.88	0.72
1:D:367:THR:HG22	1:D:511:ALA:HB3	1.72	0.72
1:D:43:MET:HB2	1:D:47:GLU:OE1	1.88	0.72
1:D:368:PRO:O	1:D:372:ILE:HG13	1.89	0.72
1:C:414:ARG:HG2	1:C:415:LEU:N	2.03	0.71
1:B:72:LEU:HB3	1:B:73:PRO:HD2	1.73	0.71
1:A:168:LEU:HD23	1:A:200:ALA:HB2	1.73	0.71
1:D:654:GLY:O	1:D:658:LEU:HB2	1.90	0.71
1:A:406:TYR:OH	1:A:588:ARG:HG3	1.91	0.70
1:D:337:LYS:HB2	1:D:337:LYS:HZ2	1.56	0.70
1:A:307:ARG:HG3	1:A:671:GLU:OE2	1.90	0.70
1:C:88:LYS:HE3	1:C:88:LYS:HA	1.74	0.70
1:D:414:ARG:HG2	1:D:415:LEU:N	2.03	0.70
1:C:654:GLY:O	1:C:658:LEU:HB2	1.91	0.70
1:D:110:ASN:HB2	1:D:230:ASN:HD21	1.56	0.70
1:B:427:TYR:HB2	1:B:538:HIS:HB2	1.72	0.70
1:A:72:LEU:HB3	1:A:73:PRO:HD2	1.74	0.70
1:B:307:ARG:HG3	1:B:671:GLU:OE2	1.91	0.70
1:D:279:SER:OG	1:D:281:PRO:HD2	1.91	0.70
1:B:74:HIS:O	1:B:74:HIS:ND1	2.25	0.69
1:C:110:ASN:HB2	1:C:230:ASN:HD21	1.57	0.69
1:B:665:ARG:HA	1:B:668:LEU:HD12	1.74	0.69
1:B:405:ASN:OD1	1:B:424:LEU:HB2	1.92	0.69
1:A:605:PHE:HZ	1:A:642:ASN:OD1	1.75	0.69
1:B:168:LEU:HD23	1:B:200:ALA:HB2	1.75	0.69
1:B:352:TRP:CE2	1:B:360:LEU:HD22	2.28	0.69
1:C:407:LEU:HD21	1:C:410:HIS:HB2	1.75	0.69
1:B:105:THR:HB	1:B:107:PHE:CE2	2.27	0.69
1:A:105:THR:HB	1:A:107:PHE:CE2	2.28	0.69
1:D:5:THR:HG23	1:D:36:ALA:HB3	1.74	0.69
1:A:427:TYR:HB2	1:A:538:HIS:HB2	1.73	0.68
1:A:440:ILE:HA	1:A:448:LYS:HE2	1.75	0.68
1:B:644:GLN:HA	1:B:644:GLN:NE2	2.08	0.68
1:C:19:CYS:O	1:C:22:PHE:HB3	1.93	0.68
1:A:405:ASN:OD1	1:A:424:LEU:HB2	1.93	0.68
1:B:425:GLU:O	1:B:584:ARG:HD3	1.93	0.68
1:A:277:ASP:HA	1:A:283:GLN:HE22	1.59	0.68
1:A:459:GLU:HG3	1:A:537:LYS:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:PHE:CD2	1:B:621:PHE:HB3	2.28	0.68
1:C:98:VAL:HB	1:C:225:LEU:HD11	1.76	0.68
1:A:178:ALA:H	1:A:183:GLU:HB2	1.59	0.67
1:B:605:PHE:HZ	1:B:642:ASN:OD1	1.76	0.67
1:C:368:PRO:O	1:C:372:ILE:HG13	1.94	0.67
1:D:98:VAL:HB	1:D:225:LEU:HD11	1.77	0.67
1:A:644:GLN:HA	1:A:644:GLN:NE2	2.09	0.67
1:C:224:GLU:HG3	1:C:232:ARG:HH21	1.58	0.67
1:D:4:LYS:O	1:D:35:PRO:HA	1.94	0.67
1:A:372:ILE:O	1:A:376:MET:HG3	1.95	0.67
1:C:271:GLN:NE2	1:C:302:LEU:H	1.93	0.67
1:C:458:SER:HA	1:C:462:ASN:HB2	1.76	0.66
1:B:351:GLN:HE21	1:B:621:PHE:HE1	1.43	0.66
1:C:500:VAL:CG1	1:C:516:GLY:HA3	2.25	0.66
1:B:73:PRO:O	1:B:74:HIS:HB3	1.96	0.66
1:D:259:LYS:O	1:D:263:ILE:HG13	1.95	0.66
1:A:70:ALA:HA	1:A:75:HIS:HB3	1.76	0.66
1:A:351:GLN:HE21	1:A:621:PHE:HE1	1.43	0.66
1:B:459:GLU:HG3	1:B:537:LYS:HB3	1.77	0.66
1:C:4:LYS:O	1:C:35:PRO:HA	1.95	0.66
1:D:407:LEU:HD21	1:D:410:HIS:HB2	1.77	0.66
1:B:70:ALA:HA	1:B:75:HIS:HB3	1.76	0.66
1:D:134:THR:HG22	1:D:134:THR:O	1.96	0.66
1:C:271:GLN:HE22	1:C:302:LEU:H	1.41	0.65
1:B:178:ALA:H	1:B:183:GLU:HB2	1.61	0.65
1:B:306:PRO:HD3	1:B:678:PHE:CD1	2.31	0.65
1:C:108:GLN:CD	1:C:232:ARG:HG3	2.16	0.65
1:A:425:GLU:O	1:A:584:ARG:HD3	1.96	0.65
1:C:43:MET:HB2	1:C:47:GLU:OE1	1.96	0.65
1:B:41:ARG:HG3	1:B:42:LYS:N	2.11	0.65
1:C:122:LEU:HB3	1:C:156:CYS:HB2	1.78	0.65
1:A:352:TRP:CE2	1:A:360:LEU:HD22	2.32	0.65
1:B:70:ALA:CB	1:B:75:HIS:O	2.45	0.65
1:C:306:PRO:HG2	1:C:309:ILE:CG2	2.26	0.65
1:C:367:THR:HG22	1:C:511:ALA:HB3	1.79	0.65
1:C:418:LYS:NZ	1:C:418:LYS:HB3	2.11	0.65
1:A:416:GLY:C	1:A:418:LYS:N	2.48	0.64
1:A:622:GLN:HB3	1:A:625:GLU:HB3	1.78	0.64
1:B:45:HIS:ND1	1:B:62:VAL:HG12	2.12	0.64
1:B:416:GLY:C	1:B:418:LYS:N	2.48	0.64
1:A:611:PHE:CD2	1:A:621:PHE:HB3	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:PRO:O	1:D:309:ILE:HG22	1.97	0.64
1:D:458:SER:HA	1:D:462:ASN:HB2	1.79	0.64
1:A:306:PRO:HD3	1:A:678:PHE:CD1	2.32	0.64
1:B:622:GLN:HB3	1:B:625:GLU:HB3	1.78	0.64
1:A:400:PRO:HB2	1:A:643:LEU:CD1	2.28	0.64
1:A:74:HIS:O	1:A:74:HIS:ND1	2.30	0.64
1:D:271:GLN:NE2	1:D:302:LEU:H	1.96	0.64
1:D:111:GLN:H	1:D:111:GLN:NE2	1.96	0.63
1:A:70:ALA:CB	1:A:75:HIS:O	2.46	0.63
1:C:415:LEU:HD11	1:C:419:CYS:HB2	1.79	0.63
1:C:337:LYS:HB2	1:C:337:LYS:HZ2	1.63	0.63
1:B:442:TRP:HB2	1:B:565:LEU:HD22	1.80	0.63
1:D:19:CYS:O	1:D:22:PHE:HB3	1.98	0.63
1:D:271:GLN:HE22	1:D:302:LEU:H	1.45	0.63
1:B:400:PRO:HB2	1:B:643:LEU:CD1	2.29	0.63
1:A:73:PRO:O	1:A:74:HIS:HB3	1.99	0.63
1:B:611:PHE:HB3	1:B:621:PHE:O	1.98	0.63
1:C:407:LEU:HD11	1:C:410:HIS:HA	1.79	0.63
1:A:65:ALA:HB2	1:A:125:SER:HB3	1.79	0.62
1:D:122:LEU:HB3	1:D:156:CYS:HB2	1.81	0.62
1:C:134:THR:O	1:C:134:THR:HG22	1.99	0.62
1:C:108:GLN:H	1:C:111:GLN:NE2	1.97	0.62
1:A:665:ARG:HH21	1:A:677:THR:HG21	1.65	0.62
1:C:106:GLY:HA2	1:C:232:ARG:NH1	2.15	0.62
1:C:409:THR:O	1:C:410:HIS:HB3	2.00	0.62
1:A:416:GLY:O	1:A:418:LYS:N	2.33	0.61
1:A:442:TRP:HB2	1:A:565:LEU:HD22	1.81	0.61
1:B:599:PHE:O	1:B:603:ILE:HG12	2.01	0.61
1:D:500:VAL:CG1	1:D:516:GLY:HA3	2.29	0.61
1:A:596:LYS:O	1:A:600:VAL:HG23	2.00	0.61
1:B:186:PHE:H	1:B:190:GLY:HA3	1.63	0.61
1:A:629:LYS:HD3	1:A:635:ASP:OD1	2.01	0.61
1:A:30:LEU:HG	1:A:34:GLY:HA3	1.82	0.61
1:D:407:LEU:HD11	1:D:410:HIS:HA	1.82	0.61
1:B:517:TYR:CG	1:B:526:CYS:HB2	2.35	0.61
1:B:30:LEU:HG	1:B:34:GLY:HA3	1.82	0.60
1:C:45:HIS:ND1	1:C:62:VAL:HG12	2.16	0.60
1:A:207:HIS:CE1	1:A:208:LEU:HG	2.36	0.60
1:C:218:ALA:HA	1:C:220:ARG:NE	2.09	0.60
1:C:573:PRO:HB2	1:C:575:THR:HG22	1.83	0.60
1:D:306:PRO:HG2	1:D:309:ILE:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:SER:OG	1:A:206:LYS:HG2	2.01	0.60
1:B:173:GLY:O	1:B:176:LYS:HG2	2.01	0.60
1:A:27:LYS:HZ3	1:D:659:THR:HG23	1.66	0.60
1:B:367:THR:HG22	1:B:511:ALA:HB3	1.83	0.60
1:A:51:ASP:HB3	1:A:56:LYS:HB2	1.84	0.60
1:A:170:ALA:O	1:A:184:PRO:HG2	2.02	0.60
1:A:504:ASN:HB2	1:A:505:PRO:HD2	1.84	0.60
1:B:505:PRO:O	1:B:506:ALA:HB3	2.02	0.60
1:B:168:LEU:HG	1:B:199:THR:HG22	1.83	0.60
1:B:416:GLY:O	1:B:418:LYS:N	2.35	0.60
1:D:605:PHE:O	1:D:608:GLN:HG2	2.02	0.60
1:A:611:PHE:HB3	1:A:621:PHE:O	2.02	0.60
1:A:186:PHE:H	1:A:190:GLY:HA3	1.66	0.59
1:A:663:ASN:HB3	1:C:23:ARG:NH1	2.17	0.59
1:D:573:PRO:HB2	1:D:575:THR:HG22	1.83	0.59
1:A:45:HIS:ND1	1:A:62:VAL:HG12	2.16	0.59
1:B:188:SER:OG	1:B:206:LYS:HG2	2.01	0.59
1:D:45:HIS:ND1	1:D:62:VAL:HG12	2.17	0.59
1:C:21:SER:O	1:C:25:ASN:ND2	2.35	0.59
1:A:41:ARG:HG3	1:A:42:LYS:N	2.17	0.59
1:D:409:THR:O	1:D:410:HIS:HB3	2.02	0.59
1:D:449:LYS:HE3	1:D:483:ARG:HH21	1.66	0.59
1:B:65:ALA:HB2	1:B:125:SER:HB3	1.84	0.59
1:B:207:HIS:CE1	1:B:208:LEU:HG	2.38	0.59
1:B:587:ASN:N	1:B:587:ASN:ND2	2.32	0.59
1:C:44:SER:HB2	1:C:46:PRO:HD2	1.83	0.59
1:C:605:PHE:O	1:C:608:GLN:HG2	2.03	0.59
1:A:517:TYR:CG	1:A:526:CYS:HB2	2.37	0.59
1:D:108:GLN:H	1:D:111:GLN:NE2	2.00	0.59
1:A:674:ASP:HA	1:A:677:THR:OG1	2.03	0.59
1:B:596:LYS:O	1:B:600:VAL:HG23	2.02	0.59
1:C:111:GLN:NE2	1:C:111:GLN:H	2.00	0.59
1:D:449:LYS:HE3	1:D:483:ARG:NH2	2.18	0.59
1:A:116:LYS:HB3	1:A:200:ALA:HA	1.84	0.58
1:B:665:ARG:HH21	1:B:677:THR:HG21	1.68	0.58
1:B:79:PRO:O	1:B:305:VAL:HG21	2.02	0.58
1:C:443:LYS:NZ	1:C:443:LYS:HB3	2.18	0.58
1:C:527:LEU:O	1:C:527:LEU:HD23	2.03	0.58
1:C:634:SER:HB2	1:C:637:THR:OG1	2.03	0.58
1:A:427:TYR:CE1	1:A:587:ASN:HA	2.39	0.58
1:B:170:ALA:O	1:B:184:PRO:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:SER:HB2	1:D:637:THR:OG1	2.02	0.58
1:B:48:CYS:O	1:B:52:ILE:HG13	2.04	0.58
1:C:484:SER:HA	1:C:498:LEU:HD12	1.86	0.58
1:A:352:TRP:HB2	1:A:621:PHE:CZ	2.39	0.58
1:D:606:ASN:N	1:D:606:ASN:HD22	2.02	0.58
1:C:504:ASN:HB3	1:C:507:HIS:CG	2.38	0.58
1:D:44:SER:HB2	1:D:46:PRO:HD2	1.85	0.58
1:D:606:ASN:N	1:D:606:ASN:ND2	2.51	0.58
1:A:136:LEU:HD23	1:A:136:LEU:H	1.69	0.57
1:B:504:ASN:HB2	1:B:505:PRO:HD2	1.86	0.57
1:C:268:ARG:HE	1:C:269:VAL:CG1	2.16	0.57
1:D:21:SER:O	1:D:25:ASN:ND2	2.37	0.57
1:D:415:LEU:HD11	1:D:419:CYS:HB2	1.86	0.57
1:C:337:LYS:HB2	1:C:337:LYS:HZ3	1.70	0.57
1:A:48:CYS:O	1:A:52:ILE:HG13	2.04	0.57
1:A:427:TYR:HE1	1:A:587:ASN:HA	1.69	0.57
1:D:596:LYS:O	1:D:600:VAL:HG23	2.05	0.57
1:A:461:TRP:O	1:A:465:MET:HB2	2.04	0.57
1:C:596:LYS:HB2	1:C:596:LYS:NZ	2.18	0.57
1:C:596:LYS:O	1:C:600:VAL:HG23	2.04	0.57
1:A:599:PHE:O	1:A:603:ILE:HG12	2.05	0.57
1:B:116:LYS:HB3	1:B:200:ALA:HA	1.86	0.57
1:C:346:ARG:HH21	1:C:364:THR:HG22	1.69	0.57
1:D:105:THR:HB	1:D:107:PHE:CE1	2.40	0.57
1:D:430:VAL:HA	1:D:582:LEU:HD13	1.87	0.57
1:A:108:GLN:H	1:A:111:GLN:HB2	1.70	0.57
1:B:405:ASN:HB2	1:B:641:SER:OG	2.05	0.57
1:B:465:MET:HE2	1:B:465:MET:HA	1.86	0.57
1:A:665:ARG:NH2	1:A:677:THR:HG21	2.20	0.57
1:B:57:VAL:HG12	1:B:58:ASP:H	1.70	0.57
1:D:346:ARG:HH21	1:D:364:THR:HG22	1.69	0.57
1:A:320:LEU:HA	1:A:323:PHE:HB3	1.86	0.56
1:B:352:TRP:HB2	1:B:621:PHE:CZ	2.40	0.56
1:B:665:ARG:NH2	1:B:677:THR:HG21	2.20	0.56
1:C:140:SER:O	1:C:141:ARG:HB2	2.05	0.56
1:C:233:ARG:HG2	1:C:234:PRO:HD2	1.87	0.56
1:C:306:PRO:O	1:C:309:ILE:HG22	2.06	0.56
1:C:566:CYS:SG	1:C:570:THR:HB	2.44	0.56
1:D:140:SER:O	1:D:141:ARG:CB	2.53	0.56
1:A:57:VAL:HG12	1:A:58:ASP:H	1.68	0.56
1:A:538:HIS:HD2	1:A:539:PRO:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ALA:HB3	1:B:185:TYR:HE2	1.69	0.56
1:D:433:VAL:HG11	1:D:565:LEU:HD11	1.87	0.56
1:D:558:LYS:HZ2	1:D:558:LYS:CB	2.08	0.56
1:B:538:HIS:HD2	1:B:539:PRO:HD2	1.70	0.56
1:C:140:SER:O	1:C:141:ARG:CB	2.53	0.56
1:C:415:LEU:HB3	1:C:638:GLU:CB	2.35	0.56
1:A:168:LEU:HG	1:A:199:THR:HG22	1.87	0.56
1:A:415:LEU:HD23	1:A:415:LEU:H	1.71	0.56
1:C:268:ARG:HE	1:C:269:VAL:HG13	1.68	0.56
1:C:678:PHE:O	1:C:680:LYS:HD2	2.05	0.56
1:B:427:TYR:CE1	1:B:587:ASN:HA	2.40	0.56
1:B:674:ASP:HA	1:B:677:THR:OG1	2.05	0.56
1:C:666:GLN:H	1:C:666:GLN:NE2	2.04	0.56
1:D:414:ARG:CG	1:D:415:LEU:H	2.05	0.56
1:A:445:LEU:HB3	1:A:481:PHE:HE2	1.70	0.56
1:D:189:TRP:CE2	1:D:291:GLU:HB3	2.40	0.56
1:C:517:TYR:CG	1:C:526:CYS:HB2	2.41	0.56
1:C:280:SER:O	1:C:281:PRO:C	2.44	0.55
1:D:666:GLN:H	1:D:666:GLN:NE2	2.04	0.55
1:A:27:LYS:HZ2	1:D:659:THR:HG23	1.70	0.55
1:A:554:ALA:HA	1:A:557:LEU:HD13	1.87	0.55
1:D:527:LEU:HD23	1:D:527:LEU:O	2.06	0.55
1:A:543:GLN:HE22	1:A:636:ASP:HB3	1.71	0.55
1:B:108:GLN:H	1:B:111:GLN:HB2	1.72	0.55
1:B:543:GLN:HE22	1:B:636:ASP:HB3	1.72	0.55
1:B:442:TRP:H	1:B:565:LEU:HD21	1.72	0.55
1:C:415:LEU:HB3	1:C:638:GLU:HG3	1.87	0.55
1:D:268:ARG:HE	1:D:269:VAL:CG1	2.19	0.55
1:A:674:ASP:HA	1:A:677:THR:HG1	1.71	0.55
1:D:403:ALA:HB1	1:D:424:LEU:HD23	1.88	0.55
1:D:541:VAL:HG13	1:D:574:VAL:HG21	1.88	0.55
1:D:554:ALA:O	1:D:557:LEU:HD13	2.06	0.55
1:C:189:TRP:CE2	1:C:291:GLU:HB3	2.42	0.55
1:A:505:PRO:O	1:A:506:ALA:HB3	2.07	0.55
1:B:46:PRO:HG3	1:B:66:LEU:HD22	1.87	0.55
1:B:427:TYR:HE1	1:B:587:ASN:HA	1.72	0.55
1:B:51:ASP:HB3	1:B:56:LYS:HB2	1.88	0.55
1:C:449:LYS:HE3	1:C:483:ARG:NH2	2.22	0.55
1:C:541:VAL:HG13	1:C:574:VAL:HG21	1.89	0.55
1:B:400:PRO:C	1:B:643:LEU:HD11	2.27	0.55
1:C:409:THR:O	1:C:410:HIS:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:LEU:HB3	1:D:638:GLU:HG3	1.88	0.54
1:D:218:ALA:HA	1:D:220:ARG:NE	2.12	0.54
1:D:407:LEU:HG	1:D:408:SER:N	2.22	0.54
1:A:79:PRO:O	1:A:305:VAL:HG21	2.07	0.54
1:B:121:GLY:HA2	1:B:155:PRO:HD2	1.89	0.54
1:B:400:PRO:HB2	1:B:643:LEU:HD11	1.89	0.54
1:C:441:THR:HG23	1:C:444:SER:H	1.71	0.54
1:D:415:LEU:HB3	1:D:638:GLU:CB	2.38	0.54
1:D:424:LEU:HG	1:D:587:ASN:HD22	1.73	0.54
1:C:103:LYS:HA	1:C:224:GLU:CG	2.34	0.54
1:D:280:SER:O	1:D:281:PRO:C	2.45	0.54
1:D:504:ASN:HB3	1:D:507:HIS:CG	2.43	0.54
1:A:429:VAL:HG12	1:A:582:LEU:HD12	1.88	0.54
1:A:465:MET:HA	1:A:465:MET:HE2	1.90	0.54
1:C:407:LEU:HG	1:C:408:SER:N	2.23	0.54
1:D:564:LEU:O	1:D:571:ARG:HA	2.07	0.54
1:C:105:THR:HB	1:C:107:PHE:CE1	2.42	0.54
1:C:554:ALA:O	1:C:557:LEU:HD13	2.07	0.54
1:D:233:ARG:HG2	1:D:234:PRO:HD2	1.89	0.54
1:D:538:HIS:O	1:D:540:THR:N	2.41	0.54
1:C:346:ARG:NE	1:C:362:CYS:HB2	2.23	0.54
1:B:445:LEU:HB3	1:B:481:PHE:HE2	1.72	0.54
1:C:424:LEU:HG	1:C:587:ASN:HD22	1.73	0.54
1:D:610:LEU:O	1:D:620:MET:HE1	2.08	0.53
1:A:442:TRP:H	1:A:565:LEU:HD21	1.74	0.53
1:B:164:SER:HA	1:B:167:GLN:HE21	1.73	0.53
1:B:192:LEU:HD23	1:B:192:LEU:O	2.08	0.53
1:B:435:LYS:HG3	1:B:563:GLU:OE2	2.08	0.53
1:C:347:THR:O	1:C:351:GLN:HG3	2.08	0.53
1:B:196:GLN:HE22	1:B:215:PRO:HD3	1.73	0.53
1:C:108:GLN:OE1	1:C:232:ARG:HG3	2.08	0.53
1:A:405:ASN:HB2	1:A:641:SER:OG	2.08	0.53
1:A:277:ASP:HA	1:A:283:GLN:NE2	2.22	0.53
1:A:367:THR:HG22	1:A:511:ALA:HB3	1.91	0.53
1:B:306:PRO:O	1:B:309:ILE:HG22	2.07	0.53
1:C:414:ARG:O	1:C:415:LEU:HB2	2.09	0.53
1:C:414:ARG:CG	1:C:415:LEU:H	2.05	0.53
1:C:136:LEU:H	1:C:136:LEU:HD23	1.73	0.53
1:C:407:LEU:HD21	1:C:410:HIS:CB	2.38	0.53
1:D:443:LYS:NZ	1:D:443:LYS:HB3	2.24	0.53
1:C:103:LYS:CA	1:C:224:GLU:HG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:GLN:NE2	1:C:304:ARG:HD2	2.23	0.53
1:D:99:ALA:HB3	1:D:226:LEU:HB2	1.91	0.53
1:D:35:PRO:HB2	1:D:266:LEU:HD12	1.91	0.53
1:D:372:ILE:O	1:D:376:MET:HG3	2.09	0.53
1:A:170:ALA:HB3	1:A:185:TYR:HE2	1.73	0.53
1:D:678:PHE:O	1:D:680:LYS:HD2	2.09	0.53
1:B:429:VAL:HG12	1:B:582:LEU:HD12	1.90	0.52
1:C:538:HIS:HB3	1:C:539:PRO:CD	2.39	0.52
1:C:538:HIS:O	1:C:540:THR:N	2.41	0.52
1:C:558:LYS:HZ2	1:C:558:LYS:CB	2.08	0.52
1:D:140:SER:O	1:D:141:ARG:HB2	2.08	0.52
1:A:435:LYS:HG3	1:A:563:GLU:OE2	2.10	0.52
1:A:515:GLU:HG3	1:A:517:TYR:H	1.74	0.52
1:A:538:HIS:O	1:A:539:PRO:C	2.48	0.52
1:C:403:ALA:HB1	1:C:424:LEU:HD23	1.90	0.52
1:C:540:THR:O	1:C:544:ASN:ND2	2.43	0.52
1:C:588:ARG:NH1	1:C:633:PHE:HA	2.24	0.52
1:D:441:THR:H	1:D:444:SER:CB	2.21	0.52
1:B:320:LEU:HA	1:B:323:PHE:HB3	1.91	0.52
1:B:538:HIS:O	1:B:539:PRO:C	2.48	0.52
1:D:414:ARG:O	1:D:415:LEU:HB2	2.09	0.52
1:A:400:PRO:HB2	1:A:643:LEU:HD13	1.90	0.52
1:D:424:LEU:HD11	1:D:587:ASN:ND2	2.25	0.52
1:D:517:TYR:CG	1:D:526:CYS:HB2	2.45	0.52
1:A:188:SER:O	1:A:209:THR:HG21	2.10	0.52
1:C:185:TYR:CD1	1:C:194:CYS:HB2	2.44	0.52
1:C:449:LYS:HE3	1:C:483:ARG:HH21	1.75	0.52
1:C:606:ASN:N	1:C:606:ASN:HD22	2.08	0.52
1:D:136:LEU:HB2	1:D:139:GLY:O	2.10	0.52
1:B:415:LEU:H	1:B:415:LEU:HD23	1.75	0.52
1:B:629:LYS:HD3	1:B:635:ASP:OD1	2.10	0.52
1:C:390:ALA:HB1	1:C:591:PHE:CZ	2.44	0.52
1:C:441:THR:H	1:C:444:SER:CB	2.22	0.52
1:D:268:ARG:HE	1:D:269:VAL:HG13	1.73	0.52
1:C:509:CYS:N	1:C:515:GLU:OE1	2.39	0.52
1:D:484:SER:HA	1:D:498:LEU:HD12	1.91	0.51
1:B:459:GLU:CD	1:B:459:GLU:H	2.13	0.51
1:C:346:ARG:NE	1:C:362:CYS:CB	2.73	0.51
1:D:347:THR:O	1:D:351:GLN:HG3	2.10	0.51
1:C:63:ASP:HB3	1:C:66:LEU:HD13	1.92	0.51
1:C:78:LYS:HB2	1:C:78:LYS:NZ	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:ASN:N	1:C:606:ASN:ND2	2.58	0.51
1:A:196:GLN:HE22	1:A:215:PRO:HD3	1.75	0.51
1:A:400:PRO:HB2	1:A:643:LEU:HD11	1.91	0.51
1:A:400:PRO:C	1:A:643:LEU:HD11	2.31	0.51
1:B:188:SER:O	1:B:209:THR:HG21	2.11	0.51
1:C:430:VAL:HA	1:C:582:LEU:HD13	1.91	0.51
1:D:409:THR:O	1:D:410:HIS:CB	2.58	0.51
1:C:135:LEU:O	1:C:135:LEU:HD12	2.11	0.51
1:D:130:VAL:HB	1:D:131:PRO:HD3	1.93	0.51
1:D:373:ALA:O	1:D:377:LYS:HG3	2.11	0.51
1:B:461:TRP:O	1:B:465:MET:HB2	2.10	0.51
1:B:525:ARG:O	1:B:529:GLU:HG2	2.10	0.51
1:D:407:LEU:HD21	1:D:410:HIS:CB	2.40	0.51
1:A:86:GLY:H	1:A:300:HIS:CD2	2.29	0.51
1:B:453:THR:HG23	1:B:535:PHE:O	2.10	0.51
1:C:88:LYS:HA	1:C:88:LYS:CE	2.39	0.51
1:C:320:LEU:O	1:C:324:ARG:HG2	2.11	0.51
1:B:73:PRO:O	1:B:74:HIS:CB	2.59	0.51
1:C:588:ARG:HH11	1:C:633:PHE:HA	1.76	0.51
1:A:164:SER:HA	1:A:167:GLN:HE21	1.75	0.50
1:A:225:LEU:HG	1:A:235:VAL:HA	1.93	0.50
1:B:106:GLY:HA2	1:B:232:ARG:CZ	2.40	0.50
1:D:538:HIS:HB3	1:D:539:PRO:CD	2.42	0.50
1:A:427:TYR:CD2	1:A:537:LYS:HB2	2.46	0.50
1:C:52:ILE:O	1:C:254:ARG:HD3	2.12	0.50
1:C:564:LEU:O	1:C:571:ARG:HA	2.10	0.50
1:A:17:THR:HG22	1:D:471:GLN:HA	1.93	0.50
1:A:229:ASP:O	1:A:231:THR:N	2.44	0.50
1:D:140:SER:O	1:D:141:ARG:HG3	2.11	0.50
1:A:459:GLU:H	1:A:459:GLU:CD	2.15	0.50
1:B:218:ALA:HA	1:B:220:ARG:NE	2.27	0.50
1:B:476:LYS:NZ	1:B:476:LYS:HB2	2.26	0.50
1:B:674:ASP:HA	1:B:677:THR:HG1	1.76	0.50
1:D:88:LYS:HA	1:D:88:LYS:CE	2.40	0.50
1:A:121:GLY:HA2	1:A:155:PRO:HD2	1.93	0.50
1:B:86:GLY:H	1:B:300:HIS:CD2	2.30	0.50
1:C:101:ALA:O	1:C:223:TYR:HB3	2.11	0.50
1:C:136:LEU:HB2	1:C:139:GLY:O	2.11	0.50
1:D:105:THR:HB	1:D:107:PHE:CZ	2.47	0.50
1:A:25:ASN:HB3	1:A:274:PHE:CZ	2.46	0.50
1:C:306:PRO:HG2	1:C:309:ILE:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LEU:HD11	1:C:587:ASN:ND2	2.27	0.50
1:C:664:PHE:CD2	1:C:667:CYS:HB2	2.47	0.50
1:D:461:TRP:O	1:D:464:PRO:HD2	2.12	0.50
1:C:35:PRO:HB2	1:C:266:LEU:HD12	1.94	0.50
1:A:155:PRO:O	1:A:156:CYS:HB2	2.12	0.49
1:D:135:LEU:HD12	1:D:135:LEU:O	2.12	0.49
1:A:373:ALA:O	1:A:377:LYS:HG3	2.11	0.49
1:A:525:ARG:O	1:A:529:GLU:HG2	2.12	0.49
1:B:388:GLY:HA3	1:B:462:ASN:HD21	1.78	0.49
1:C:545:THR:HG22	1:C:557:LEU:HB3	1.95	0.49
1:D:168:LEU:HD21	1:D:200:ALA:HB2	1.94	0.49
1:D:477:PHE:C	1:D:479:ALA:H	2.16	0.49
1:B:15:GLU:HG2	1:B:294:LEU:HD23	1.94	0.49
1:B:427:TYR:CD2	1:B:537:LYS:HB2	2.47	0.49
1:D:346:ARG:NE	1:D:362:CYS:CB	2.76	0.49
1:A:306:PRO:O	1:A:309:ILE:HG22	2.11	0.49
1:A:543:GLN:NE2	1:A:636:ASP:HB3	2.28	0.49
1:A:631:LEU:O	1:A:632:LEU:HB2	2.12	0.49
1:B:229:ASP:O	1:B:231:THR:N	2.46	0.49
1:B:606:ASN:O	1:B:609:GLU:HB3	2.12	0.49
1:C:116:LYS:HB2	1:C:201:ASP:OD1	2.12	0.49
1:C:136:LEU:HD23	1:C:136:LEU:N	2.28	0.49
1:A:106:GLY:HA2	1:A:232:ARG:CZ	2.42	0.49
1:B:13:ASP:O	1:B:17:THR:HG23	2.11	0.49
1:C:469:TYR:HD2	1:C:474:SER:O	1.95	0.49
1:D:588:ARG:NH1	1:D:633:PHE:HA	2.27	0.49
1:C:103:LYS:HG3	1:C:224:GLU:OE2	2.11	0.49
1:C:388:GLY:HA2	1:C:661:MET:HE1	1.95	0.49
1:C:130:VAL:HB	1:C:131:PRO:HD3	1.95	0.49
1:D:62:VAL:O	1:D:249:HIS:HB3	2.13	0.49
1:A:383:MET:HE2	1:A:384:SER:O	2.13	0.49
1:B:65:ALA:O	1:B:68:ALA:HB3	2.13	0.49
1:D:45:HIS:N	1:D:46:PRO:CD	2.76	0.49
1:D:136:LEU:HD23	1:D:136:LEU:H	1.76	0.49
1:D:648:THR:HG22	1:D:649:TYR:N	2.28	0.49
1:A:13:ASP:O	1:A:17:THR:HG23	2.12	0.49
1:A:70:ALA:CA	1:A:75:HIS:O	2.61	0.48
1:B:25:ASN:HB3	1:B:274:PHE:CZ	2.48	0.48
1:B:155:PRO:O	1:B:156:CYS:HB2	2.13	0.48
1:B:274:PHE:O	1:B:284:LEU:HB2	2.13	0.48
1:B:373:ALA:O	1:B:377:LYS:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:GLN:NE2	1:B:636:ASP:HB3	2.27	0.48
1:D:264:GLN:NE2	1:D:304:ARG:HD2	2.28	0.48
1:D:390:ALA:HB1	1:D:591:PHE:CZ	2.47	0.48
1:A:15:GLU:HG2	1:A:294:LEU:HD23	1.95	0.48
1:A:452:HIS:HB2	1:A:486:ALA:HA	1.94	0.48
1:A:644:GLN:HE21	1:A:644:GLN:CA	2.20	0.48
1:D:136:LEU:HD23	1:D:136:LEU:N	2.28	0.48
1:D:185:TYR:CD1	1:D:194:CYS:HB2	2.48	0.48
1:D:346:ARG:NE	1:D:362:CYS:HB2	2.28	0.48
1:C:346:ARG:HB2	1:C:364:THR:HB	1.95	0.48
1:C:610:LEU:O	1:C:620:MET:HE1	2.13	0.48
1:A:67:VAL:HG12	1:A:67:VAL:O	2.13	0.48
1:A:431:ALA:HB2	1:A:582:LEU:HD11	1.96	0.48
1:B:218:ALA:C	1:B:220:ARG:H	2.16	0.48
1:B:400:PRO:HB2	1:B:643:LEU:HD13	1.94	0.48
1:C:603:ILE:O	1:C:607:GLN:HG2	2.14	0.48
1:C:624:PHE:CZ	1:C:640:LEU:HG	2.48	0.48
1:A:608:GLN:O	1:A:612:GLY:HA3	2.14	0.48
1:D:438:VAL:HA	1:D:571:ARG:HH12	1.79	0.48
1:C:99:ALA:HB3	1:C:226:LEU:HB2	1.96	0.48
1:C:477:PHE:C	1:C:479:ALA:H	2.17	0.48
1:D:48:CYS:O	1:D:52:ILE:HG13	2.13	0.48
1:A:65:ALA:O	1:A:68:ALA:HB3	2.14	0.48
1:A:73:PRO:O	1:A:74:HIS:CB	2.62	0.48
1:A:218:ALA:C	1:A:220:ARG:H	2.17	0.48
1:B:68:ALA:C	1:B:69:GLU:OE2	2.51	0.48
1:C:538:HIS:HB3	1:C:539:PRO:HD2	1.95	0.48
1:C:498:LEU:O	1:C:530:LYS:HD2	2.14	0.47
1:D:287:SER:HA	1:D:288:PRO:HD3	1.75	0.47
1:D:304:ARG:HB3	1:D:304:ARG:NH1	2.29	0.47
1:A:69:GLU:N	1:A:69:GLU:OE2	2.47	0.47
1:B:225:LEU:HG	1:B:235:VAL:HA	1.95	0.47
1:B:229:ASP:O	1:B:231:THR:HG23	2.14	0.47
1:D:545:THR:HG22	1:D:557:LEU:HB3	1.96	0.47
1:A:49:ILE:HD11	1:A:62:VAL:HG21	1.96	0.47
1:A:81:MET:O	1:A:250:VAL:HG12	2.14	0.47
1:A:587:ASN:N	1:A:587:ASN:ND2	2.33	0.47
1:A:274:PHE:O	1:A:284:LEU:HB2	2.15	0.47
1:A:445:LEU:HB3	1:A:481:PHE:CE2	2.48	0.47
1:A:608:GLN:O	1:A:612:GLY:N	2.47	0.47
1:B:367:THR:O	1:B:370:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:SER:O	1:B:25:ASN:ND2	2.25	0.47
1:B:538:HIS:CD2	1:B:539:PRO:HD2	2.49	0.47
1:B:605:PHE:CZ	1:B:642:ASN:OD1	2.62	0.47
1:C:648:THR:HG22	1:C:649:TYR:N	2.30	0.47
1:D:116:LYS:HB2	1:D:201:ASP:OD1	2.15	0.47
1:D:136:LEU:O	1:D:136:LEU:HG	2.14	0.47
1:D:235:VAL:HG23	1:D:236:GLU:N	2.30	0.47
1:B:259:LYS:O	1:B:263:ILE:HG13	2.14	0.47
1:B:293:LEU:O	1:B:294:LEU:HB2	2.14	0.47
1:D:28:LYS:HB2	1:D:28:LYS:NZ	2.30	0.47
1:A:218:ALA:HA	1:A:220:ARG:NE	2.30	0.47
1:D:63:ASP:HB2	1:D:249:HIS:CE1	2.50	0.47
1:D:261:ASP:OD2	1:D:261:ASP:N	2.47	0.47
1:D:324:ARG:O	1:D:328:ARG:HB3	2.15	0.47
1:A:557:LEU:HD12	1:A:557:LEU:N	2.30	0.47
1:C:45:HIS:HB2	1:C:46:PRO:HD3	1.96	0.47
1:D:407:LEU:HD21	1:D:410:HIS:CA	2.45	0.47
1:B:70:ALA:CA	1:B:75:HIS:O	2.63	0.47
1:C:309:ILE:HG23	1:C:309:ILE:O	2.15	0.47
1:C:458:SER:HB3	1:C:585:VAL:HG11	1.97	0.47
1:A:59:ALA:HB2	1:A:263:ILE:HD13	1.97	0.47
1:A:476:LYS:HB2	1:A:476:LYS:NZ	2.30	0.47
1:C:461:TRP:O	1:C:464:PRO:HD2	2.15	0.47
1:D:175:ASP:OD1	1:D:182:ARG:HB3	2.15	0.47
1:A:391:TYR:CE1	1:A:661:MET:HB2	2.50	0.46
1:A:442:TRP:HA	1:A:445:LEU:CD1	2.42	0.46
1:B:81:MET:SD	1:B:264:GLN:NE2	2.88	0.46
1:B:391:TYR:CE1	1:B:661:MET:HB2	2.50	0.46
1:C:643:LEU:O	1:C:644:GLN:HB2	2.14	0.46
1:D:140:SER:O	1:D:141:ARG:CG	2.63	0.46
1:D:175:ASP:O	1:D:183:GLU:HG2	2.15	0.46
1:D:320:LEU:O	1:D:324:ARG:HG2	2.15	0.46
1:A:155:PRO:HB3	1:A:178:ALA:O	2.15	0.46
1:B:424:LEU:HD13	1:B:425:GLU:N	2.29	0.46
1:D:63:ASP:HB3	1:D:66:LEU:HD13	1.98	0.46
1:D:309:ILE:HG23	1:D:309:ILE:O	2.14	0.46
1:A:229:ASP:O	1:A:231:THR:HG23	2.15	0.46
1:A:388:GLY:HA3	1:A:462:ASN:HD21	1.80	0.46
1:B:155:PRO:HB3	1:B:178:ALA:O	2.16	0.46
1:D:624:PHE:CZ	1:D:640:LEU:HG	2.49	0.46
1:B:209:THR:HG22	1:B:209:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ASP:OD2	1:C:261:ASP:N	2.47	0.46
1:D:115:LYS:O	1:D:149:PHE:HB3	2.15	0.46
1:D:551:GLU:HA	1:D:552:PRO:HD3	1.74	0.46
1:B:517:TYR:CZ	1:B:526:CYS:HA	2.50	0.46
1:B:631:LEU:O	1:B:632:LEU:HB2	2.16	0.46
1:C:235:VAL:HG23	1:C:236:GLU:N	2.31	0.46
1:C:274:PHE:HB3	1:C:282:PHE:O	2.14	0.46
1:D:274:PHE:HB3	1:D:282:PHE:O	2.14	0.46
1:C:24:ASP:O	1:C:28:LYS:HG3	2.16	0.46
1:C:136:LEU:HG	1:C:136:LEU:O	2.15	0.46
1:C:438:VAL:HA	1:C:571:ARG:HH12	1.80	0.46
1:D:101:ALA:O	1:D:223:TYR:HB3	2.14	0.46
1:A:46:PRO:HG3	1:A:66:LEU:HD22	1.96	0.46
1:A:367:THR:O	1:A:370:ASP:HB2	2.16	0.46
1:B:464:PRO:O	1:B:468:ILE:HD13	2.15	0.46
1:C:30:LEU:N	1:C:31:PRO:HD3	2.30	0.46
1:C:45:HIS:N	1:C:46:PRO:CD	2.79	0.46
1:D:408:SER:OG	1:D:415:LEU:HD13	2.16	0.46
1:A:116:LYS:O	1:A:201:ASP:N	2.48	0.46
1:C:125:SER:HB3	1:C:319:PHE:HZ	1.80	0.46
1:C:505:PRO:O	1:C:506:ALA:HB3	2.15	0.46
1:B:445:LEU:HB3	1:B:481:PHE:CE2	2.50	0.46
1:C:666:GLN:H	1:C:666:GLN:CD	2.19	0.46
1:D:122:LEU:HD22	1:D:156:CYS:O	2.16	0.46
1:A:45:HIS:O	1:A:49:ILE:HG12	2.16	0.46
1:A:585:VAL:HG12	1:A:657:TYR:CE1	2.51	0.46
1:B:46:PRO:O	1:B:50:ARG:HG3	2.16	0.46
1:C:72:LEU:H	1:C:72:LEU:HD22	1.81	0.46
1:C:105:THR:HB	1:C:107:PHE:CZ	2.51	0.46
1:C:407:LEU:HD23	1:C:408:SER:O	2.16	0.46
1:A:124:TRP:O	1:A:128:TRP:HB3	2.16	0.45
1:A:192:LEU:HD23	1:A:192:LEU:O	2.15	0.45
1:B:442:TRP:N	1:B:565:LEU:HD21	2.30	0.45
1:C:287:SER:HA	1:C:288:PRO:HD3	1.74	0.45
1:C:324:ARG:O	1:C:328:ARG:HB3	2.17	0.45
1:D:280:SER:H	1:D:281:PRO:HD2	1.80	0.45
1:D:566:CYS:SG	1:D:570:THR:HB	2.56	0.45
1:A:6:ILE:HD13	1:A:266:LEU:HD22	1.97	0.45
1:B:346:ARG:NH2	1:B:364:THR:HG22	2.30	0.45
1:A:346:ARG:NH2	1:A:364:THR:HG22	2.31	0.45
1:A:442:TRP:N	1:A:565:LEU:HD21	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:PHE:CZ	1:A:642:ASN:OD1	2.62	0.45
1:B:176:LYS:HB2	1:B:176:LYS:NZ	2.31	0.45
1:C:280:SER:H	1:C:281:PRO:CD	2.30	0.45
1:C:304:ARG:NH1	1:C:304:ARG:HB3	2.31	0.45
1:D:53:SER:C	1:D:55:ASN:H	2.19	0.45
1:A:256:VAL:O	1:A:256:VAL:HG13	2.16	0.45
1:A:339:CYS:HB3	1:A:383:MET:HG2	1.96	0.45
1:C:407:LEU:HD21	1:C:410:HIS:CA	2.45	0.45
1:D:52:ILE:O	1:D:254:ARG:HD3	2.17	0.45
1:D:280:SER:H	1:D:281:PRO:CD	2.30	0.45
1:D:306:PRO:HG2	1:D:309:ILE:HG21	1.98	0.45
1:A:22:PHE:O	1:A:26:MET:HG2	2.17	0.45
1:B:69:GLU:OE2	1:B:69:GLU:N	2.49	0.45
1:B:452:HIS:HB2	1:B:486:ALA:HA	1.97	0.45
1:C:5:THR:HG23	1:C:36:ALA:CB	2.44	0.45
1:C:243:LEU:O	1:C:244:ALA:HB2	2.17	0.45
1:D:243:LEU:O	1:D:244:ALA:HB2	2.17	0.45
1:B:49:ILE:HD11	1:B:62:VAL:HG21	1.99	0.45
1:C:584:ARG:O	1:C:584:ARG:NH1	2.50	0.45
1:C:646:LYS:HD2	1:C:651:THR:O	2.17	0.45
1:A:150:SER:O	1:A:164:SER:HB3	2.17	0.45
1:A:415:LEU:HD23	1:A:415:LEU:N	2.31	0.45
1:A:538:HIS:CD2	1:A:539:PRO:HD2	2.50	0.45
1:B:116:LYS:O	1:B:200:ALA:HB1	2.17	0.45
1:B:420:VAL:HG13	1:B:605:PHE:CE1	2.51	0.45
1:C:279:SER:OG	1:C:280:SER:N	2.45	0.45
1:D:606:ASN:ND2	1:D:606:ASN:H	2.15	0.45
1:A:375:THR:O	1:A:593:ARG:NH1	2.50	0.45
1:C:372:ILE:O	1:C:376:MET:HG3	2.17	0.45
1:D:509:CYS:N	1:D:515:GLU:OE1	2.45	0.45
1:D:588:ARG:HH11	1:D:633:PHE:HA	1.81	0.45
1:A:116:LYS:O	1:A:200:ALA:HB1	2.16	0.45
1:B:430:VAL:HB	1:B:564:LEU:HD22	1.98	0.45
1:C:373:ALA:O	1:C:377:LYS:HG3	2.17	0.45
1:D:424:LEU:CG	1:D:587:ASN:HD22	2.30	0.45
1:D:538:HIS:HB3	1:D:539:PRO:HD2	1.99	0.45
1:D:78:LYS:HB2	1:D:78:LYS:NZ	2.31	0.45
1:D:441:THR:HG23	1:D:444:SER:H	1.81	0.45
1:D:505:PRO:O	1:D:506:ALA:HB3	2.16	0.45
1:A:420:VAL:HG13	1:A:605:PHE:CE1	2.52	0.44
1:A:453:THR:HG23	1:A:535:PHE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:TRP:O	1:B:128:TRP:HB3	2.17	0.44
1:B:339:CYS:HB3	1:B:383:MET:HG2	1.98	0.44
1:B:375:THR:O	1:B:593:ARG:NH1	2.50	0.44
1:B:515:GLU:HG3	1:B:517:TYR:H	1.81	0.44
1:C:406:TYR:HD2	1:C:637:THR:HA	1.82	0.44
1:A:68:ALA:C	1:A:69:GLU:OE2	2.55	0.44
1:B:6:ILE:HD13	1:B:266:LEU:HD22	1.99	0.44
1:B:256:VAL:HG13	1:B:256:VAL:O	2.17	0.44
1:C:280:SER:H	1:C:281:PRO:HD2	1.82	0.44
1:C:415:LEU:HB3	1:C:638:GLU:CG	2.47	0.44
1:C:568:ASP:OD1	1:C:569:GLY:N	2.50	0.44
1:D:643:LEU:O	1:D:644:GLN:HB2	2.18	0.44
1:A:125:SER:HA	1:A:129:TYR:HB2	1.99	0.44
1:A:440:ILE:HG23	1:A:448:LYS:CD	2.47	0.44
1:B:449:LYS:HB3	1:B:498:LEU:HD11	1.99	0.44
1:D:22:PHE:CZ	1:D:266:LEU:HD21	2.52	0.44
1:A:7:ARG:O	1:A:57:VAL:HG12	2.17	0.44
1:A:209:THR:O	1:A:209:THR:HG22	2.17	0.44
1:A:415:LEU:HD12	1:A:419:CYS:HB2	1.98	0.44
1:B:100:MET:HB3	1:B:195:LEU:CD2	2.47	0.44
1:C:34:GLY:HA3	1:C:35:PRO:HD2	1.85	0.44
1:A:92:LYS:HG3	1:A:94:HIS:CE1	2.52	0.44
1:A:465:MET:HE1	1:A:481:PHE:HE1	1.82	0.44
1:C:25:ASN:HA	1:C:28:LYS:HE3	1.99	0.44
1:C:28:LYS:HB2	1:C:28:LYS:NZ	2.33	0.44
1:C:464:PRO:HB2	1:C:465:MET:HE3	1.99	0.44
1:C:596:LYS:HB2	1:C:596:LYS:HZ1	1.82	0.44
1:D:346:ARG:HB2	1:D:364:THR:HB	1.99	0.44
1:D:541:VAL:HG11	1:D:574:VAL:HG21	1.97	0.44
1:A:478:ASP:HB2	1:A:494:PRO:HD2	2.00	0.44
1:B:431:ALA:HB2	1:B:582:LEU:HD11	1.99	0.44
1:A:70:ALA:O	1:A:76:SER:HA	2.18	0.44
1:D:28:LYS:HB2	1:D:28:LYS:HZ2	1.82	0.44
1:D:155:PRO:O	1:D:156:CYS:HB2	2.18	0.44
1:D:461:TRP:CD2	1:D:465:MET:HG3	2.53	0.44
1:B:45:HIS:CG	1:B:62:VAL:HG12	2.53	0.44
1:B:141:ARG:HB2	1:B:144:ALA:HB2	2.00	0.44
1:B:540:THR:HG22	1:B:543:GLN:OE1	2.18	0.44
1:C:367:THR:HB	1:C:368:PRO:CD	2.48	0.44
1:D:498:LEU:O	1:D:530:LYS:HD2	2.18	0.44
1:A:113:ARG:HA	1:A:148:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:THR:OG1	1:D:370:ASP:OD1	2.34	0.43
1:B:105:THR:HB	1:B:107:PHE:CD2	2.53	0.43
1:B:400:PRO:HD2	1:B:647:THR:O	2.18	0.43
1:C:461:TRP:CD2	1:C:465:MET:HG3	2.53	0.43
1:D:44:SER:CB	1:D:46:PRO:HD2	2.48	0.43
1:A:46:PRO:O	1:A:50:ARG:HG3	2.19	0.43
1:A:81:MET:SD	1:A:264:GLN:NE2	2.91	0.43
1:A:100:MET:HB3	1:A:195:LEU:CD2	2.48	0.43
1:C:63:ASP:HB2	1:C:249:HIS:CE1	2.54	0.43
1:D:42:LYS:HB3	1:D:47:GLU:OE2	2.18	0.43
1:B:477:PHE:C	1:B:479:ALA:H	2.21	0.43
1:C:328:ARG:C	1:C:328:ARG:NE	2.68	0.43
1:C:549:ASN:HA	1:C:550:PRO:HD3	1.85	0.43
1:D:666:GLN:H	1:D:666:GLN:CD	2.21	0.43
1:A:45:HIS:O	1:A:48:CYS:HB2	2.18	0.43
1:B:356:SER:C	1:B:358:GLY:H	2.22	0.43
1:B:442:TRP:HA	1:B:445:LEU:CD1	2.44	0.43
1:D:169:CYS:HA	1:D:185:TYR:HD2	1.84	0.43
1:D:664:PHE:CD2	1:D:667:CYS:HB2	2.53	0.43
1:A:30:LEU:CG	1:A:34:GLY:HA3	2.48	0.43
1:A:45:HIS:CG	1:A:62:VAL:HG12	2.52	0.43
1:A:98:VAL:HB	1:A:225:LEU:HD22	2.01	0.43
1:A:114:GLY:HA2	1:A:149:PHE:HA	1.99	0.43
1:A:188:SER:C	1:A:209:THR:HG21	2.39	0.43
1:A:424:LEU:HD13	1:A:425:GLU:N	2.33	0.43
1:B:70:ALA:O	1:B:76:SER:HA	2.19	0.43
1:B:130:VAL:HB	1:B:131:PRO:HD3	2.01	0.43
1:B:164:SER:HA	1:B:167:GLN:NE2	2.33	0.43
1:B:643:LEU:O	1:B:644:GLN:HB2	2.18	0.43
1:C:31:PRO:C	1:C:33:GLY:N	2.71	0.43
1:D:24:ASP:O	1:D:28:LYS:HG3	2.18	0.43
1:D:322:ALA:O	1:D:326:LEU:HD13	2.19	0.43
1:D:415:LEU:HB3	1:D:638:GLU:CG	2.49	0.43
1:B:430:VAL:HG11	1:B:577:ALA:HB1	1.99	0.43
1:C:117:SER:OG	1:C:202:VAL:HB	2.18	0.43
1:C:169:CYS:HA	1:C:185:TYR:HD2	1.83	0.43
1:C:175:ASP:O	1:C:183:GLU:HG2	2.19	0.43
1:C:285:PHE:HZ	1:C:302:LEU:CD1	2.32	0.43
1:C:564:LEU:HD21	1:C:574:VAL:HG23	2.01	0.43
1:A:549:ASN:HA	1:A:550:PRO:HD3	1.89	0.43
1:B:465:MET:HE1	1:B:481:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG23	1:A:30:LEU:N	2.33	0.43
1:B:585:VAL:HG12	1:B:657:TYR:CE1	2.53	0.43
1:A:195:LEU:HB3	1:A:223:TYR:CE2	2.54	0.43
1:B:45:HIS:O	1:B:48:CYS:HB2	2.19	0.43
1:B:45:HIS:O	1:B:49:ILE:HG12	2.19	0.43
1:B:366:GLU:O	1:B:512:ASN:HB3	2.18	0.43
1:C:122:LEU:CB	1:C:156:CYS:HB2	2.47	0.43
1:C:328:ARG:NE	1:C:328:ARG:O	2.50	0.43
1:C:441:THR:HG23	1:C:443:LYS:N	2.34	0.43
1:D:441:THR:N	1:D:444:SER:HB2	2.25	0.43
1:D:540:THR:O	1:D:544:ASN:ND2	2.52	0.43
1:A:119:HIS:CG	1:A:154:VAL:HG22	2.54	0.42
1:A:276:LYS:HE2	1:A:300:HIS:CE1	2.54	0.42
1:A:348:LYS:O	1:A:348:LYS:HG2	2.19	0.42
1:D:27:LYS:O	1:D:31:PRO:HB3	2.19	0.42
1:A:352:TRP:O	1:A:352:TRP:CD1	2.72	0.42
1:A:540:THR:HG22	1:A:543:GLN:OE1	2.19	0.42
1:A:654:GLY:O	1:A:658:LEU:HB2	2.19	0.42
1:B:505:PRO:O	1:B:506:ALA:CB	2.66	0.42
1:D:125:SER:HB3	1:D:319:PHE:HZ	1.84	0.42
1:A:356:SER:C	1:A:358:GLY:H	2.22	0.42
1:B:114:GLY:HA2	1:B:149:PHE:HA	2.00	0.42
1:B:346:ARG:NH2	1:B:364:THR:CG2	2.82	0.42
1:B:352:TRP:CD1	1:B:352:TRP:O	2.73	0.42
1:B:415:LEU:HD12	1:B:419:CYS:HB2	2.01	0.42
1:C:168:LEU:HD21	1:C:200:ALA:HB2	2.01	0.42
1:C:424:LEU:CG	1:C:587:ASN:HD22	2.32	0.42
1:D:134:THR:O	1:D:134:THR:CG2	2.66	0.42
1:A:320:LEU:O	1:A:324:ARG:HG3	2.19	0.42
1:B:22:PHE:O	1:B:26:MET:HG2	2.19	0.42
1:B:102:LYS:H	1:B:102:LYS:HD3	1.84	0.42
1:B:483:ARG:HE	1:B:483:ARG:HB3	1.37	0.42
1:C:442:TRP:CE3	1:C:445:LEU:HD11	2.55	0.42
1:C:27:LYS:O	1:C:31:PRO:HB3	2.19	0.42
1:C:273:HIS:HB3	1:C:274:PHE:CE1	2.55	0.42
1:C:541:VAL:HG21	1:C:562:PHE:CD2	2.54	0.42
1:C:564:LEU:HG	1:C:574:VAL:HA	2.00	0.42
1:D:28:LYS:NZ	1:D:28:LYS:CB	2.82	0.42
1:A:84:TYR:CE1	1:A:301:GLY:HA3	2.55	0.42
1:A:130:VAL:HB	1:A:131:PRO:HD3	2.02	0.42
1:C:108:GLN:H	1:C:111:GLN:HE21	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:VAL:CA	1:C:582:LEU:HD13	2.50	0.42
1:D:643:LEU:HB3	1:D:646:LYS:O	2.19	0.42
1:A:291:GLU:HA	1:A:291:GLU:OE1	2.19	0.42
1:C:192:LEU:HG	1:C:205:VAL:HG11	2.01	0.42
1:D:407:LEU:HD23	1:D:408:SER:O	2.19	0.42
1:D:464:PRO:HB2	1:D:465:MET:HE3	2.01	0.42
1:A:434:LYS:O	1:A:571:ARG:NH2	2.52	0.42
1:A:449:LYS:HB3	1:A:498:LEU:HD11	2.02	0.42
1:B:67:VAL:HG12	1:B:67:VAL:O	2.19	0.42
1:B:435:LYS:HG3	1:B:563:GLU:CD	2.39	0.42
1:C:418:LYS:HB3	1:C:418:LYS:HZ2	1.81	0.42
1:D:45:HIS:HB2	1:D:46:PRO:HD3	2.00	0.42
1:D:285:PHE:HZ	1:D:302:LEU:HD12	1.85	0.42
1:A:483:ARG:HE	1:A:483:ARG:HB3	1.41	0.42
1:B:549:ASN:HA	1:B:550:PRO:HD3	1.86	0.42
1:B:608:GLN:O	1:B:612:GLY:HA3	2.18	0.42
1:D:143:THR:HG23	1:D:162:PHE:HE2	1.85	0.42
1:D:228:MET:HE3	1:D:228:MET:HA	2.02	0.42
1:D:442:TRP:CE3	1:D:445:LEU:HD11	2.55	0.42
1:A:13:ASP:OD1	1:A:41:ARG:NH1	2.49	0.42
1:C:285:PHE:HZ	1:C:302:LEU:HD12	1.85	0.42
1:D:119:HIS:HD2	1:D:127:GLY:O	2.03	0.42
1:A:459:GLU:CG	1:A:537:LYS:HB3	2.46	0.41
1:B:188:SER:C	1:B:209:THR:HG21	2.41	0.41
1:B:309:ILE:HB	1:B:675:ALA:HB1	2.01	0.41
1:C:53:SER:C	1:C:55:ASN:H	2.23	0.41
1:C:115:LYS:O	1:C:149:PHE:HB3	2.19	0.41
1:C:137:PRO:HD3	1:C:148:PHE:HD1	1.85	0.41
1:C:549:ASN:C	1:C:551:GLU:H	2.23	0.41
1:D:76:SER:O	1:D:255:SER:N	2.29	0.41
1:A:541:VAL:HG11	1:A:574:VAL:HB	2.02	0.41
1:B:478:ASP:HB2	1:B:494:PRO:HD2	2.02	0.41
1:B:541:VAL:HG11	1:B:574:VAL:HB	2.00	0.41
1:B:644:GLN:HE21	1:B:644:GLN:CA	2.20	0.41
1:D:25:ASN:HD22	1:D:25:ASN:H	1.68	0.41
1:B:84:TYR:CE1	1:B:301:GLY:HA3	2.56	0.41
1:B:189:TRP:CE2	1:B:213:ALA:HB2	2.55	0.41
1:B:476:LYS:O	1:B:479:ALA:HB3	2.21	0.41
1:C:301:GLY:C	1:C:302:LEU:HD12	2.41	0.41
1:D:108:GLN:HE22	1:D:232:ARG:N	2.18	0.41
1:D:468:ILE:O	1:D:472:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:THR:HB	1:B:369:GLU:OE1	2.21	0.41
1:C:406:TYR:C	1:C:638:GLU:HG2	2.40	0.41
1:D:31:PRO:C	1:D:33:GLY:N	2.72	0.41
1:D:130:VAL:HG12	1:D:243:LEU:HD23	2.01	0.41
1:D:352:TRP:HB2	1:D:621:PHE:CE2	2.56	0.41
1:D:30:LEU:N	1:D:31:PRO:HD3	2.35	0.41
1:D:587:ASN:O	1:D:652:TYR:OH	2.36	0.41
1:A:105:THR:HB	1:A:107:PHE:CD2	2.55	0.41
1:A:310:ASP:OD2	1:A:377:LYS:NZ	2.40	0.41
1:B:70:ALA:HA	1:B:75:HIS:CB	2.49	0.41
1:C:76:SER:O	1:C:255:SER:N	2.27	0.41
1:C:308:LYS:HD3	1:C:671:GLU:HB2	2.03	0.41
1:C:394:GLY:HA3	1:C:649:TYR:CG	2.55	0.41
1:D:178:ALA:HB3	1:D:183:GLU:HB2	2.01	0.41
1:D:404:GLU:HB3	1:D:588:ARG:O	2.20	0.41
1:A:45:HIS:N	1:A:46:PRO:CD	2.83	0.41
1:A:155:PRO:O	1:A:156:CYS:CB	2.69	0.41
1:A:438:VAL:HG23	1:A:438:VAL:O	2.21	0.41
1:A:477:PHE:C	1:A:479:ALA:H	2.24	0.41
1:B:94:HIS:CD2	1:B:245:ARG:NH2	2.89	0.41
1:C:122:LEU:HD22	1:C:156:CYS:O	2.21	0.41
1:C:254:ARG:HB2	1:C:258:GLY:HA3	2.02	0.41
1:D:122:LEU:CB	1:D:156:CYS:HB2	2.49	0.41
1:D:308:LYS:HD3	1:D:671:GLU:HB2	2.03	0.41
1:D:337:LYS:HB2	1:D:337:LYS:HZ3	1.81	0.41
1:D:441:THR:HG23	1:D:443:LYS:H	1.86	0.41
1:A:430:VAL:HB	1:A:564:LEU:HD22	2.02	0.41
1:A:533:VAL:HG12	1:A:534:ALA:N	2.35	0.41
1:A:622:GLN:HE21	1:A:622:GLN:HB2	1.63	0.41
1:B:111:GLN:N	1:B:111:GLN:OE1	2.54	0.41
1:B:434:LYS:O	1:B:571:ARG:NH2	2.53	0.41
1:B:657:TYR:O	1:B:660:LEU:HB3	2.21	0.41
1:C:28:LYS:HB2	1:C:28:LYS:HZ2	1.84	0.41
1:C:111:GLN:H	1:C:111:GLN:CD	2.24	0.41
1:C:155:PRO:O	1:C:156:CYS:HB2	2.21	0.41
1:C:524:LEU:CD2	1:C:544:ASN:HD22	2.33	0.41
1:D:226:LEU:N	1:D:226:LEU:HD12	2.36	0.41
1:D:242:TYR:HD1	1:D:244:ALA:N	2.18	0.41
1:D:328:ARG:O	1:D:328:ARG:NE	2.53	0.41
1:A:109:LEU:O	1:A:112:LEU:HD12	2.21	0.41
1:A:288:PRO:HG2	1:A:289:HIS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:PRO:O	1:A:371:CYS:HB2	2.21	0.41
1:A:466:GLY:HA2	1:A:664:PHE:CD2	2.56	0.41
1:A:476:LYS:O	1:A:479:ALA:HB3	2.21	0.41
1:B:386:ASP:OD1	1:B:457:THR:HA	2.21	0.41
1:D:391:TYR:OH	1:D:662:ASP:OD1	2.33	0.41
1:D:603:ILE:O	1:D:607:GLN:HG2	2.20	0.41
1:A:72:LEU:HB3	1:A:73:PRO:CD	2.49	0.41
1:C:31:PRO:O	1:C:32:ALA:C	2.59	0.41
1:D:512:ASN:OD1	1:D:514:ALA:HB3	2.21	0.41
1:A:490:ASP:HA	1:A:491:PRO:HD3	1.98	0.40
1:B:72:LEU:HB3	1:B:73:PRO:CD	2.47	0.40
1:B:98:VAL:HB	1:B:225:LEU:HD22	2.03	0.40
1:B:116:LYS:O	1:B:201:ASP:N	2.51	0.40
1:B:490:ASP:HA	1:B:491:PRO:HD3	1.95	0.40
1:C:418:LYS:HB3	1:C:418:LYS:HZ3	1.84	0.40
1:D:386:ASP:CG	1:D:387:GLY:N	2.74	0.40
1:B:30:LEU:CG	1:B:34:GLY:HA3	2.50	0.40
1:C:168:LEU:HD11	1:C:199:THR:O	2.22	0.40
1:C:260:GLU:H	1:C:260:GLU:CD	2.24	0.40
1:C:624:PHE:CE1	1:C:640:LEU:HG	2.57	0.40
1:D:34:GLY:HA3	1:D:35:PRO:HD2	1.86	0.40
1:A:113:ARG:HA	1:A:148:PHE:HZ	1.85	0.40
1:B:271:GLN:NE2	1:B:301:GLY:HA3	2.36	0.40
1:C:108:GLN:HE22	1:C:232:ARG:CG	2.27	0.40
1:C:162:PHE:HB2	1:C:165:LEU:HD12	2.03	0.40
1:D:365:GLU:HB2	1:D:371:CYS:SG	2.62	0.40
1:D:564:LEU:HG	1:D:574:VAL:HA	2.03	0.40
1:A:517:TYR:CZ	1:A:526:CYS:HA	2.56	0.40
1:B:352:TRP:CE3	1:B:632:LEU:HD13	2.57	0.40
1:B:420:VAL:O	1:B:641:SER:HA	2.22	0.40
1:C:441:THR:CG2	1:C:444:SER:H	2.34	0.40
1:D:168:LEU:HD11	1:D:199:THR:O	2.21	0.40
1:D:441:THR:HG23	1:D:443:LYS:N	2.36	0.40
1:D:622:GLN:HB2	1:D:625:GLU:HB3	2.04	0.40
1:A:578:GLN:HE21	1:A:578:GLN:HB3	1.64	0.40
1:B:119:HIS:CD2	1:B:154:VAL:HG22	2.57	0.40
1:B:150:SER:O	1:B:164:SER:HB3	2.22	0.40
1:C:337:LYS:NZ	1:C:337:LYS:CB	2.74	0.40
1:C:644:GLN:OE1	1:C:644:GLN:HA	2.21	0.40
1:D:137:PRO:HD3	1:D:148:PHE:HD1	1.86	0.40
1:D:644:GLN:OE1	1:D:644:GLN:HA	2.21	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	671/687 (98%)	578 (86%)	74 (11%)	19 (3%)	5 4
1	B	671/687 (98%)	574 (86%)	78 (12%)	19 (3%)	5 4
1	C	671/687 (98%)	568 (85%)	83 (12%)	20 (3%)	4 3
1	D	671/687 (98%)	563 (84%)	87 (13%)	21 (3%)	4 3
All	All	2684/2748 (98%)	2283 (85%)	322 (12%)	79 (3%)	4 4

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	280	SER
1	A	289	HIS
1	A	539	PRO
1	A	620	MET
1	B	230	ASN
1	B	280	SER
1	B	289	HIS
1	B	539	PRO
1	B	620	MET
1	C	141	ARG
1	C	280	SER
1	C	665	ARG
1	D	141	ARG
1	D	280	SER
1	D	665	ARG
1	A	140	SER
1	A	275	GLY
1	A	288	PRO
1	A	307	ARG

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Mol	Chain	Res	Type
1	A	417	SER
1	B	140	SER
1	B	288	PRO
1	B	307	ARG
1	B	417	SER
1	C	646	LYS
1	D	646	LYS
1	A	114	GLY
1	A	281	PRO
1	A	513	ASN
1	B	114	GLY
1	B	275	GLY
1	B	281	PRO
1	C	537	LYS
1	C	538	HIS
1	D	407	LEU
1	A	439	GLY
1	A	646	LYS
1	B	411	SER
1	B	439	GLY
1	B	513	ASN
1	B	646	LYS
1	C	87	SER
1	C	107	PHE
1	C	407	LEU
1	C	414	ARG
1	C	482	SER
1	D	87	SER
1	D	414	ARG
1	D	537	LYS
1	D	538	HIS
1	A	358	GLY
1	A	411	SER
1	A	678	PHE
1	B	358	GLY
1	C	135	LEU
1	C	513	ASN
1	D	135	LEU
1	D	415	LEU
1	D	462	ASN
1	D	482	SER
1	B	483	ARG

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Mol	Chain	Res	Type
1	C	114	GLY
1	C	288	PRO
1	C	415	LEU
1	D	107	PHE
1	D	114	GLY
1	D	513	ASN
1	D	539	PRO
1	C	73	PRO
1	C	539	PRO
1	D	288	PRO
1	B	173	GLY
1	C	64	GLY
1	D	64	GLY
1	D	137	PRO
1	C	137	PRO
1	D	281	PRO
1	A	173	GLY

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	563/574 (98%)	532 (94%)	31 (6%)	21	35
1	B	563/574 (98%)	530 (94%)	33 (6%)	19	32
1	C	563/574 (98%)	535 (95%)	28 (5%)	24	40
1	D	563/574 (98%)	532 (94%)	31 (6%)	21	35
All	All	2252/2296 (98%)	2129 (94%)	123 (6%)	21	35

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	14	HIS
1	A	69	GLU
1	A	74	HIS

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Mol	Chain	Res	Type
1	A	78	LYS
1	A	135	LEU
1	A	176	LYS
1	A	177	CYS
1	A	189	TRP
1	A	197	ASP
1	A	220	ARG
1	A	248	SER
1	A	250	VAL
1	A	255	SER
1	A	284	LEU
1	A	289	HIS
1	A	360	LEU
1	A	362	CYS
1	A	383	MET
1	A	424	LEU
1	A	483	ARG
1	A	538	HIS
1	A	539	PRO
1	A	565	LEU
1	A	566	CYS
1	A	578	GLN
1	A	587	ASN
1	A	593	ARG
1	A	622	GLN
1	A	648	THR
1	A	672	LEU
1	B	6	ILE
1	B	13	ASP
1	B	14	HIS
1	B	69	GLU
1	B	74	HIS
1	B	78	LYS
1	B	135	LEU
1	B	176	LYS
1	B	177	CYS
1	B	189	TRP
1	B	197	ASP
1	B	220	ARG
1	B	248	SER
1	B	250	VAL
1	B	255	SER

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Mol	Chain	Res	Type
1	B	284	LEU
1	B	289	HIS
1	B	360	LEU
1	B	383	MET
1	B	424	LEU
1	B	483	ARG
1	B	509	CYS
1	B	513	ASN
1	B	538	HIS
1	B	539	PRO
1	B	565	LEU
1	B	566	CYS
1	B	578	GLN
1	B	587	ASN
1	B	593	ARG
1	B	622	GLN
1	B	648	THR
1	B	672	LEU
1	C	26	MET
1	C	43	MET
1	C	51	ASP
1	C	71	ASP
1	C	74	HIS
1	C	78	LYS
1	C	111	GLN
1	C	135	LEU
1	C	177	CYS
1	C	194	CYS
1	C	220	ARG
1	C	327	LYS
1	C	328	ARG
1	C	371	CYS
1	C	407	LEU
1	C	419	CYS
1	C	476	LYS
1	C	482	SER
1	C	492	ASP
1	C	507	HIS
1	C	541	VAL
1	C	566	CYS
1	C	584	ARG
1	C	595	ASP

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Mol	Chain	Res	Type
1	C	596	LYS
1	C	606	ASN
1	C	622	GLN
1	C	639	CYS
1	D	26	MET
1	D	43	MET
1	D	51	ASP
1	D	71	ASP
1	D	74	HIS
1	D	78	LYS
1	D	111	GLN
1	D	135	LEU
1	D	177	CYS
1	D	194	CYS
1	D	220	ARG
1	D	327	LYS
1	D	328	ARG
1	D	364	THR
1	D	370	ASP
1	D	371	CYS
1	D	407	LEU
1	D	419	CYS
1	D	476	LYS
1	D	482	SER
1	D	492	ASP
1	D	507	HIS
1	D	541	VAL
1	D	555	LYS
1	D	566	CYS
1	D	584	ARG
1	D	595	ASP
1	D	596	LYS
1	D	606	ASN
1	D	622	GLN
1	D	639	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	110	ASN
1	A	167	GLN

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Mol	Chain	Res	Type
1	A	207	HIS
1	A	230	ASN
1	A	300	HIS
1	A	334	GLN
1	A	351	GLN
1	A	421	ASN
1	A	462	ASN
1	A	578	GLN
1	A	587	ASN
1	A	622	GLN
1	A	642	ASN
1	A	644	GLN
1	A	656	GLN
1	A	663	ASN
1	A	666	GLN
1	B	55	ASN
1	B	110	ASN
1	B	167	GLN
1	B	207	HIS
1	B	230	ASN
1	B	300	HIS
1	B	334	GLN
1	B	351	GLN
1	B	421	ASN
1	B	462	ASN
1	B	587	ASN
1	B	606	ASN
1	B	622	GLN
1	B	644	GLN
1	B	656	GLN
1	B	663	ASN
1	B	666	GLN
1	C	111	GLN
1	C	167	GLN
1	C	230	ASN
1	C	249	HIS
1	C	264	GLN
1	C	271	GLN
1	C	283	GLN
1	C	405	ASN
1	C	518	HIS
1	C	544	ASN

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Mol	Chain	Res	Type
1	C	578	GLN
1	C	587	ASN
1	C	606	ASN
1	C	614	ASN
1	C	622	GLN
1	C	663	ASN
1	C	679	HIS
1	D	111	GLN
1	D	119	HIS
1	D	167	GLN
1	D	230	ASN
1	D	249	HIS
1	D	264	GLN
1	D	271	GLN
1	D	283	GLN
1	D	405	ASN
1	D	518	HIS
1	D	544	ASN
1	D	578	GLN
1	D	587	ASN
1	D	606	ASN
1	D	608	GLN
1	D	614	ASN
1	D	622	GLN
1	D	663	ASN
1	D	679	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	675/687 (98%)	-0.14	19 (2%)	53	51	15, 64, 105, 116	18 (2%)
1	B	675/687 (98%)	0.03	16 (2%)	59	57	19, 79, 112, 128	25 (3%)
1	C	675/687 (98%)	-0.10	15 (2%)	62	60	36, 68, 109, 125	16 (2%)
1	D	675/687 (98%)	0.15	27 (4%)	38	37	48, 83, 114, 134	19 (2%)
All	All	2700/2748 (98%)	-0.01	77 (2%)	51	50	15, 74, 110, 134	78 (2%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	PRO	6.8
1	D	290	GLY	6.1
1	D	326	LEU	5.9
1	D	618	TYR	5.1
1	D	170	ALA	5.1
1	D	138	SER	4.8
1	D	289	HIS	4.8
1	A	138	SER	4.8
1	C	72	LEU	4.3
1	C	139	GLY	4.1
1	C	138	SER	4.0
1	D	556	GLY	3.8
1	B	618	TYR	3.7
1	A	73	PRO	3.7
1	B	556	GLY	3.5
1	A	327	LYS	3.4
1	D	628	ALA	3.4
1	B	286	GLY	3.3
1	C	109	LEU	3.3
1	D	327	LYS	3.2
1	D	141	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	415	LEU	3.1
1	B	554	ALA	3.1
1	A	618	TYR	3.0
1	D	135	LEU	3.0
1	A	74	HIS	2.8
1	D	439	GLY	2.8
1	D	211	PHE	2.8
1	B	161	MET	2.8
1	D	627	SER	2.8
1	A	575	THR	2.8
1	C	226	LEU	2.7
1	D	358	GLY	2.7
1	A	172	LYS	2.6
1	C	102	LYS	2.6
1	D	217	LYS	2.6
1	D	202	VAL	2.5
1	A	113	ARG	2.5
1	B	136	LEU	2.5
1	C	86	GLY	2.4
1	B	211	PHE	2.4
1	B	138	SER	2.4
1	A	198	GLY	2.3
1	A	210	VAL	2.3
1	B	616	PHE	2.3
1	A	104	GLY	2.3
1	C	30	LEU	2.3
1	C	415	LEU	2.3
1	D	106	GLY	2.3
1	A	215	PRO	2.3
1	C	288	PRO	2.3
1	D	216	THR	2.3
1	D	74	HIS	2.2
1	A	414	ARG	2.2
1	C	223	TYR	2.2
1	D	497	ALA	2.2
1	D	228	MET	2.2
1	A	616	PHE	2.2
1	D	73	PRO	2.2
1	B	229	ASP	2.2
1	D	551	GLU	2.2
1	B	289	HIS	2.1
1	B	617	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	618	TYR	2.1
1	D	552	PRO	2.1
1	B	150	SER	2.1
1	C	225	LEU	2.1
1	A	75	HIS	2.1
1	B	498	LEU	2.0
1	A	139	GLY	2.0
1	D	328	ARG	2.0
1	A	222	GLN	2.0
1	B	151	SER	2.0
1	D	406	TYR	2.0
1	B	573	PRO	2.0
1	C	616	PHE	2.0
1	A	619	MET	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.