Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 03:20 PM EST

PDB ID	:	4FPB
Title	:	Crystal Structure of Recombinant Human Hexokinase Type I with 1,5-Anhydroglucitol 6-Phosphate
Authors	:	Shen, L.; Honzatko, R.B.
Deposited on	:	2012-06-21
Resolution	:	3.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

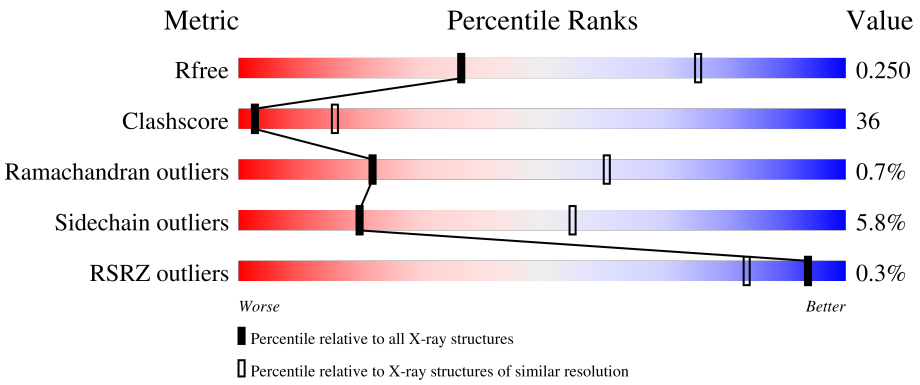
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	917	49% 45% • •
1	B	917	49% 46% • •

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
5	CIT	A	1007	-	-	-	X

2 Entry composition (i)

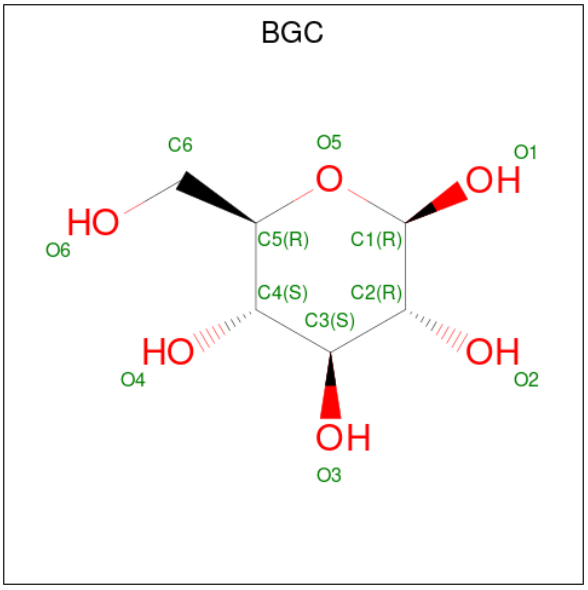
There are 6 unique types of molecules in this entry. The entry contains 14395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hexokinase-1.

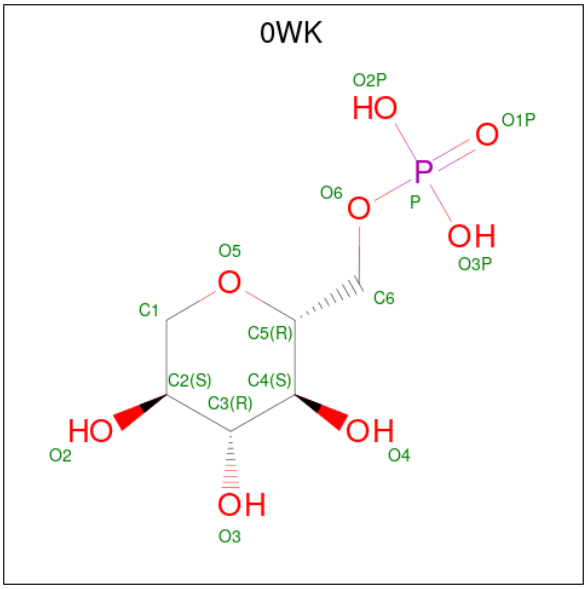
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	899	7032	4407	1240	1332	53	0	0	0
1	B	899	7032	4407	1240	1332	53	0	0	0

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0
2	A	1	12	6	6	0	0
2	B	1	12	6	6	0	0
2	B	1	12	6	6	0	0

- Molecule 3 is 1,5-anhydro-6-O-phosphono-D-glucitol (three-letter code: 0WK) (formula: $C_6H_{13}O_8P$).

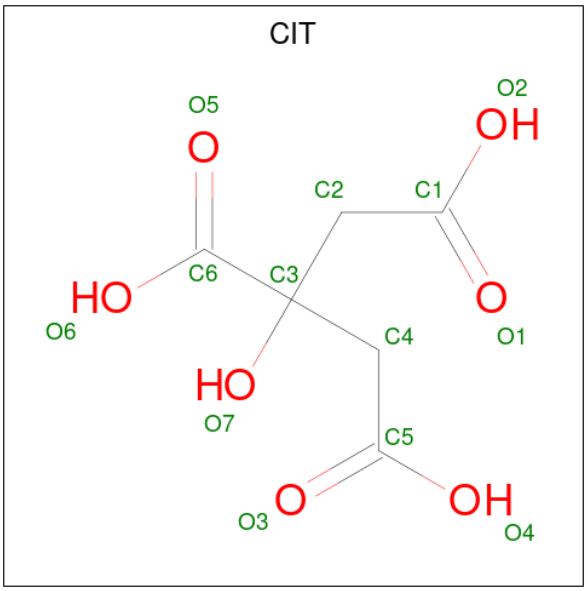


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	15	6	8	1	0	0
			Total	C	O	P		
3	A	1	15	6	8	1	0	0
			Total	C	O	P		
3	B	1	15	6	8	1	0	0
			Total	C	O	P		
3	B	1	15	6	8	1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0
			Total	Na		
4	B	2	2	2	0	0

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 6 7	0	0
5	B	1	Total C O 13 6 7	0	0

- Molecule 6 is water.

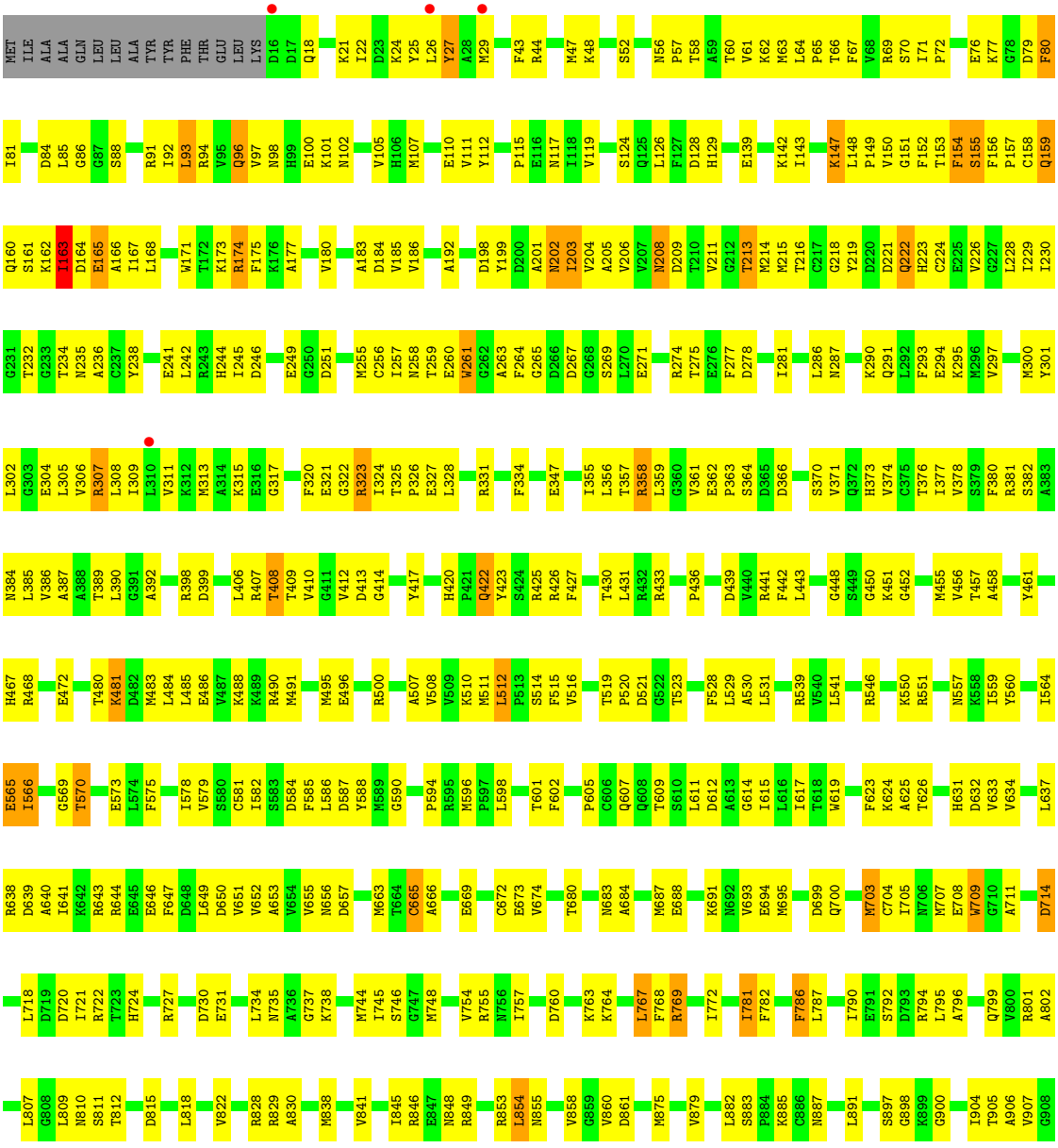
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	94	Total O 94 94	0	0
6	B	99	Total O 99 99	0	0

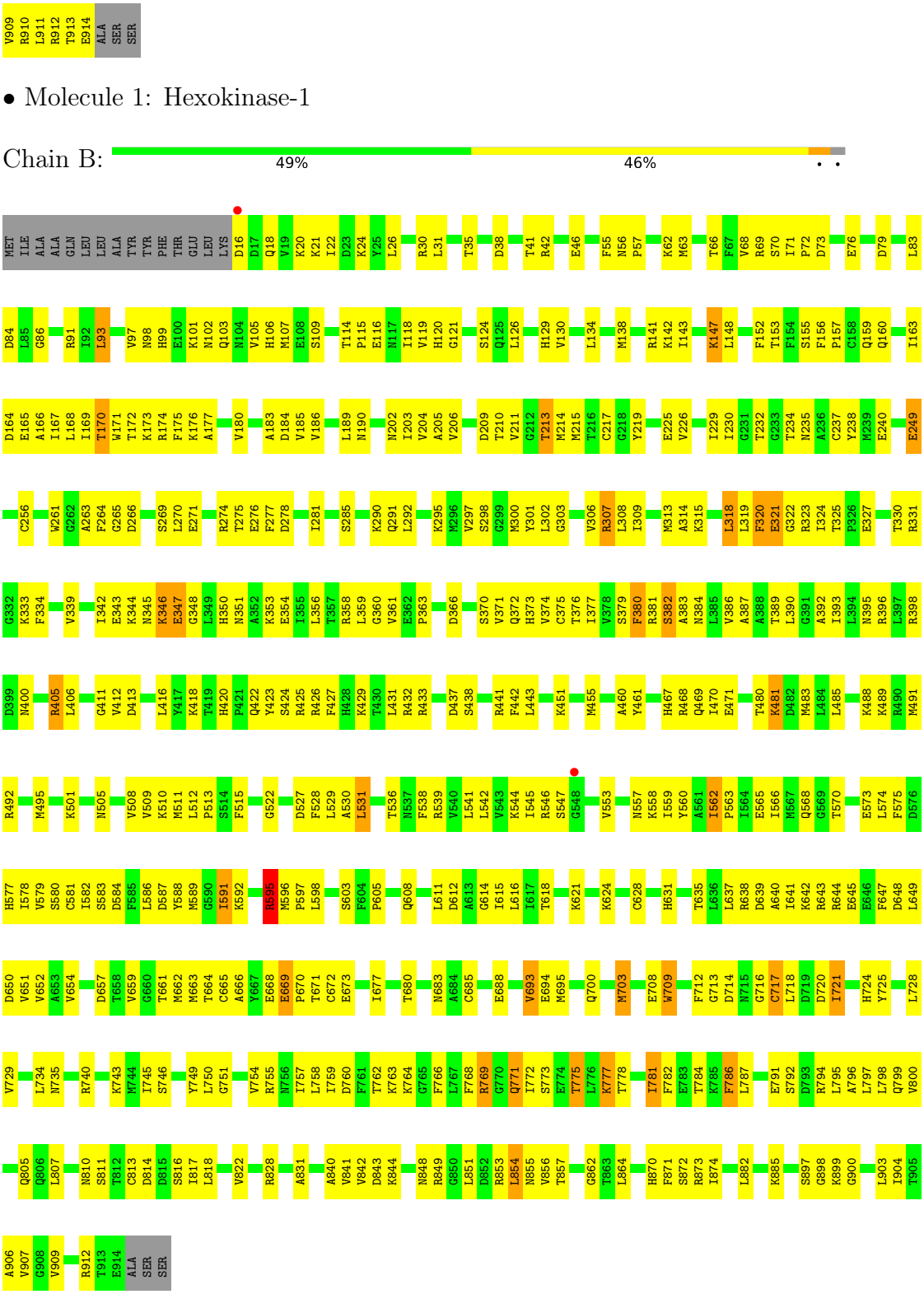
3 Residue-property plots (i)

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: Hexokinase-1

Chain A:




V909 R910 L911 R912 T913 E914 ALA SER SER
• Molecule 1: Hexokinase-1
Chain B:
49%
46%
MET ILE ALA ALA GLN LEU LEU ALA TYR TYR PHE THR GLU LEU LYS D16 D17 Q18 V19 K20 K21 I22 D23 K24 Y25 L26 R30 L31 T35 D38 T41 R42 E46 F55 N56 P57 K62 M63 T66 F67 V68 R69 S70 I71 P72 D73 E76 D79 L83
D84 L85 G86 R91 I92 L93 V97 N98 H99 E100 K101 N102 Q103 N104 V105 H106 M107 E108 S109 T114 P115 E116 N117 I118 V119 H120 G121 S124 Q125 L126 H129 V130 L134 M138 R141 K142 I143 K147 L148 F152 T153 F154 S155 F156 P157 C158 Q159 Q160 I163
D164 E165 A166 I167 L168 I169 T170 W171 T172 K173 R174 F175 K176 A177 V180 A183 D184 V185 V186 L189 N190 N202 I203 V204 A205 V206 D209 T210 V211 G212 T213 M214 M215 T216 C217 G218 Y219 E225 V226 I229 I230 G231 T232 G233 T234 N235 A236 C237 Y238 M239 E240 E249
C256 W261 G262 A263 F264 G265 D266 S269 L270 E271 R274 T275 E276 F277 D278 I281 S285 K290 Q291 L292 K295 M296 V297 S298 G299 M300 Y301 L302 G303 V306 R307 L308 I309 M313 A314 K315 L318 L319 F320 E321 G322 R323 I324 T325 P326 E327 T330 R331
G332 K333 F334 V339 I342 E343 K344 N345 K346 E347 G348 L349 H350 N351 A352 K353 E354 I355 L356 T357 R358 L359 G360 V361 E362 P363 D366 S370 V371 Q372 H373 V374 C375 T376 I377 V378 S379 F380 R381 S382 A383 N384 L385 V386 A387 A388 T389 L390 G391 A392 I393 L394 N395 R396 L397 R398
D399 N400 R405 L406 G411 V412 D413 L416 Y417 K418 T419 H420 P421 Q422 Y423 S424 R425 R426 F427 H428 K429 T430 L431 R432 R433 D437 S438 R441 F442 L443 K451 M455 A460 Y461 H467 R468 Q469 I470 E471 T480 K481 D482 M483 L484 L485 K488 K489 R490 M491
R492 M495 K501 N505 V508 V509 K510 M511 L512 P513 S514 F515 G522 D527 F528 L529 A530 L531 T536 N537 F538 R539 V540 L541 L542 V543 K544 I545 R546 S547 G548 V553 N557 K558 I559 Y560 A561 I562 P563 I564 E565 I566 M567 Q568 G569 T570 E573 L574 F575 D576
H577 I578 V579 S580 C581 I582 S583 D584 F585 L586 D587 Y588 M589 G590 I591 K592 R595 M596 P597 L598 S603 F604 P605 Q608 L611 D612 A613 G614 I615 L616 I617 T618 K621 K624 C628 H631 T635 L636 L637 R638 D639 A640 I641 K642 R643 R644 E645 E646 F647 D648 L649
D650 V651 V652 A653 V654 D657 T658 V659 G660 T661 M662 M663 T664 C665 A666 Y667 E668 E669 P670 T671 C672 E673 I677 T680 N683 A684 C685 E688 V693 E694 M695 Q700 M703 E708 W709 F712 G713 D714 N715 G716 C717 L718 D719 D720 I721 H724 Y725 L728
V729 L734 N735 R740 K743 M744 I745 S746 Y749 L750 G751 V754 R755 N756 I757 L758 I759 D760 F761 T762 K763 K764 G765 F766 L767 F768 R769 G770 Q771 I772 S773 E774 T775 L776 K777 T778 I781 F782 E783 T784 K785 F786 L787 E791 S792 D793 R794 L795 A796 L797 L798 Q799 V800
Q805 L806 L807 N810 S811 T812 C813 D814 D815 S816 I817 L818 V822 R828 A831 A840 V841 V842 D843 K844 N848 R849 G850 L851 D852 R853 L854 N855 V856 T857 G862 T863 L864 H870 F871 S872 R873 I874 L882 K885 S897 G898 K899 G900 L903 I904 T905
A906 V907 G908 V909 R912 T913 E914 ALA SER SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.72Å 121.21Å 120.79Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	46.24 – 3.00 46.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	82.7 (46.24-3.00) 82.7 (46.24-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.229 , 0.256 0.225 , 0.250	Depositor DCC
R_{free} test set	1955 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	71.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 19.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14395	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: 0WK, BGC, NA, CIT

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	0.36	1/7138 (0.0%)	0.49	1/9606 (0.0%)
1	B	0.35	2/7138 (0.0%)	0.51	2/9606 (0.0%)
All	All	0.35	3/14276 (0.0%)	0.50	3/19212 (0.0%)

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	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	ARG	CZ-NH2	14.91	1.52	1.33
1	B	595	ARG	CZ-NH2	12.36	1.49	1.33
1	B	595	ARG	CZ-NH1	9.11	1.44	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	595	ARG	NE-CZ-NH1	-11.74	114.43	120.30
1	A	323	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	B	595	ARG	NE-CZ-NH2	5.73	123.16	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	PHE	Peptide
1	B	595	ARG	Sidechain
1	B	668	GLU	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	7032	0	7090	521	0
1	B	7032	0	7090	508	0
2	A	24	0	24	4	0
2	B	24	0	24	4	0
3	A	30	0	22	2	0
3	B	30	0	22	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	13	0	5	1	0
5	B	13	0	5	4	0
6	A	94	0	0	10	0
6	B	99	0	0	25	0
All	All	14395	0	14282	1025	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 36.

All (1025) 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:B:319:LEU:HB3	1:B:320:PHE:CE1	1.36	1.56
1:A:320:PHE:CZ	1:A:361:VAL:HG21	1.64	1.31
1:A:570:THR:CG2	1:A:573:GLU:HG3	1.58	1.31
1:A:520:PRO:HD3	1:A:663:MET:CE	1.65	1.25
1:B:319:LEU:CB	1:B:320:PHE:CE1	2.25	1.20
1:A:162:LYS:O	1:A:163:ILE:HG22	1.42	1.20
1:B:319:LEU:HB3	1:B:320:PHE:CD1	1.78	1.18
1:A:93:LEU:N	1:A:93:LEU:HD23	1.64	1.12
1:B:319:LEU:C	1:B:320:PHE:HD1	1.50	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ALA:O	1:A:510:LYS:HE2	1.50	1.10
1:B:320:PHE:HB3	1:B:323:ARG:HH21	1.14	1.10
1:B:346:LYS:HG3	1:B:347:GLU:OE2	1.52	1.10
1:B:541:LEU:HD23	1:B:557:ASN:HB3	1.34	1.10
1:A:380:PHE:CD2	1:A:426:ARG:HD3	1.87	1.09
1:A:160:GLN:HG2	1:A:165:GLU:O	1.52	1.08
1:B:320:PHE:HD1	1:B:320:PHE:N	1.49	1.08
1:A:663:MET:HG3	1:A:904:ILE:HD11	1.12	1.07
1:B:536:THR:HG22	6:B:1160:HOH:O	1.51	1.07
1:B:169:ILE:HG22	1:B:170:THR:HG22	1.10	1.07
1:B:319:LEU:C	1:B:320:PHE:CD1	2.28	1.07
1:B:854:LEU:HD12	1:B:855:ASN:N	1.69	1.06
1:A:570:THR:HG23	1:A:573:GLU:HG3	1.09	1.06
1:A:480:THR:HG23	1:A:483:MET:HE3	1.38	1.05
1:A:663:MET:HG3	1:A:904:ILE:CD1	1.86	1.05
1:A:520:PRO:HD3	1:A:663:MET:HE1	1.40	1.04
1:A:786:PHE:CE2	1:A:790:ILE:HD11	1.94	1.03
1:B:320:PHE:HB3	1:B:323:ARG:NH2	1.74	1.02
1:B:319:LEU:CB	1:B:320:PHE:HE1	1.64	1.01
1:B:870:HIS:CD2	1:B:873:ARG:HH21	1.78	1.01
1:A:380:PHE:HD2	1:A:426:ARG:HD3	1.20	1.01
1:B:344:LYS:O	1:B:348:GLY:CA	2.11	0.99
1:B:522:GLY:HA3	6:B:1195:HOH:O	1.64	0.98
1:B:320:PHE:HD2	1:B:361:VAL:HB	1.24	0.98
1:A:570:THR:HG23	1:A:573:GLU:CG	1.93	0.98
1:A:564:ILE:HG13	1:A:565:GLU:N	1.76	0.97
1:B:115:PRO:HD2	1:B:118:ILE:HD12	1.48	0.96
1:B:853:ARG:HB3	1:B:853:ARG:HH11	1.28	0.96
1:B:160:GLN:HG2	1:B:165:GLU:O	1.64	0.95
1:B:760:ASP:O	1:B:764:LYS:HG2	1.65	0.95
1:B:853:ARG:HB3	1:B:853:ARG:NH1	1.82	0.95
1:B:320:PHE:CD2	1:B:361:VAL:HB	2.01	0.95
1:B:425:ARG:HH22	5:B:1007:CIT:H22	1.29	0.95
1:A:380:PHE:HE2	1:A:426:ARG:HG2	1.28	0.95
1:A:290:LYS:O	1:A:295:LYS:HE3	1.67	0.94
1:A:422:GLN:OE1	1:A:422:GLN:HA	1.66	0.94
1:B:320:PHE:CD1	1:B:320:PHE:N	2.25	0.93
1:A:663:MET:CG	1:A:904:ILE:HD11	1.99	0.93
1:A:320:PHE:CE2	1:A:361:VAL:HG21	2.03	0.92
1:A:203:ILE:N	1:A:203:ILE:CD1	2.32	0.92
1:A:174:ARG:HG3	1:A:174:ARG:HH11	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PHE:CZ	1:A:361:VAL:CG2	2.51	0.92
1:A:486:GLU:HG2	6:A:1119:HOH:O	1.69	0.91
1:A:510:LYS:HB3	1:A:512:LEU:CD1	2.00	0.91
1:A:431:LEU:HD23	1:A:442:PHE:HZ	1.35	0.91
1:A:510:LYS:HB3	1:A:512:LEU:HD11	1.49	0.91
1:A:162:LYS:O	1:A:163:ILE:CG2	2.19	0.90
1:A:520:PRO:HD3	1:A:663:MET:HE3	1.51	0.90
1:B:101:LYS:O	1:B:103:GLN:HG3	1.71	0.90
1:A:760:ASP:OD2	1:A:764:LYS:HE2	1.72	0.90
1:A:564:ILE:HG13	1:A:565:GLU:H	1.32	0.90
1:A:714:ASP:OD2	1:A:738:LYS:HA	1.72	0.89
1:B:313:MET:HE2	1:B:318:LEU:HD12	1.52	0.89
1:B:762:THR:CG2	1:B:772:ILE:HD13	2.03	0.88
1:B:771:GLN:HE21	1:B:771:GLN:C	1.77	0.88
1:A:44:ARG:HG2	1:A:392:ALA:HB1	1.56	0.88
1:A:570:THR:HG21	1:A:573:GLU:HG3	1.54	0.88
1:B:420:HIS:HD2	1:B:423:TYR:H	1.22	0.87
1:B:426:ARG:HH21	5:B:1007:CIT:H41	1.38	0.87
1:B:346:LYS:CG	1:B:347:GLU:OE2	2.22	0.87
1:A:219:TYR:HD2	1:A:451:LYS:HD3	1.37	0.87
1:B:297:VAL:HA	1:B:382:SER:HB2	1.55	0.87
1:A:203:ILE:N	1:A:203:ILE:HD12	1.89	0.86
1:B:173:LYS:HE2	2:B:1001:BGC:O5	1.75	0.86
1:A:97:VAL:HG22	1:A:105:VAL:HA	1.56	0.86
1:B:344:LYS:O	1:B:348:GLY:N	2.09	0.85
1:B:844:LYS:NZ	1:B:848:ASN:HD21	1.74	0.85
1:B:545:ILE:O	1:B:546:ARG:HD3	1.74	0.85
1:A:93:LEU:N	1:A:93:LEU:CD2	2.39	0.85
1:A:795:LEU:HD11	1:A:799:GLN:HG2	1.58	0.85
1:A:62:LYS:HB3	1:A:64:LEU:CD2	2.06	0.85
1:B:319:LEU:CB	1:B:320:PHE:CD1	2.53	0.85
1:B:266:ASP:OD1	1:B:292:LEU:HG	1.75	0.84
1:B:320:PHE:CB	1:B:323:ARG:NH2	2.39	0.84
1:B:870:HIS:HD2	1:B:873:ARG:HH21	1.23	0.84
1:A:900:GLY:O	1:A:904:ILE:HG12	1.78	0.83
1:B:390:LEU:HD12	1:B:390:LEU:O	1.78	0.83
1:B:189:LEU:HD23	1:B:203:ILE:HD11	1.59	0.83
1:B:347:GLU:HB2	1:B:351:ASN:ND2	1.93	0.83
1:A:174:ARG:HG3	1:A:174:ARG:NH1	1.89	0.83
1:B:315:LYS:HG2	1:B:324:ILE:CD1	2.09	0.82
1:B:480:THR:HG23	1:B:483:MET:CE	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD23	1:A:93:LEU:H	1.42	0.82
1:A:174:ARG:NH2	1:A:300:MET:HG3	1.93	0.82
1:B:265:GLY:HA2	1:B:269:SER:HB3	1.62	0.81
1:A:422:GLN:HG3	1:A:426:ARG:NH2	1.95	0.81
1:A:612:ASP:O	1:A:634:VAL:HG21	1.81	0.81
1:B:98:ASN:O	1:B:103:GLN:O	1.97	0.81
1:B:313:MET:CE	1:B:318:LEU:HD12	2.10	0.81
1:B:356:LEU:HD11	1:B:371:VAL:HG21	1.63	0.81
1:B:390:LEU:HD23	1:B:427:PHE:HZ	1.45	0.81
1:A:520:PRO:CD	1:A:663:MET:CE	2.55	0.81
1:A:202:ASN:C	1:A:203:ILE:HD12	2.02	0.81
1:A:174:ARG:HH11	1:A:174:ARG:CG	1.94	0.80
1:A:174:ARG:HH22	1:A:300:MET:HG3	1.44	0.80
1:B:118:ILE:HD13	1:B:129:HIS:CD2	2.17	0.80
1:B:230:ILE:HD11	1:B:386:VAL:HG11	1.64	0.80
1:B:320:PHE:HE2	1:B:361:VAL:HG21	1.46	0.80
1:B:545:ILE:C	1:B:546:ARG:HD3	2.02	0.80
1:B:541:LEU:HD23	1:B:557:ASN:CB	2.11	0.80
1:A:163:ILE:HD13	1:A:163:ILE:O	1.82	0.80
1:A:66:THR:HG22	1:A:256:CYS:O	1.81	0.80
1:A:315:LYS:HA	1:A:324:ILE:HD11	1.64	0.80
1:A:86:GLY:HA3	1:A:155:SER:OG	1.82	0.79
1:B:762:THR:HG21	1:B:772:ILE:HD13	1.63	0.79
1:A:361:VAL:O	1:A:363:PRO:HD3	1.83	0.79
1:A:422:GLN:HG3	1:A:425:ARG:HH21	1.48	0.78
1:A:380:PHE:CE2	1:A:426:ARG:HG2	2.17	0.78
1:B:782:PHE:HD1	1:B:786:PHE:CE1	2.02	0.78
1:A:229:ILE:HD12	3:A:1002:0WK:H7	1.65	0.78
1:B:563:PRO:HD2	1:B:566:ILE:HD12	1.64	0.78
1:B:680:THR:O	1:B:746:SER:HB2	1.84	0.78
1:B:771:GLN:HE21	1:B:771:GLN:CA	1.96	0.78
1:A:422:GLN:HB3	1:A:426:ARG:CZ	2.14	0.78
1:A:156:PHE:HZ	1:A:175:PHE:CD2	2.02	0.78
1:B:870:HIS:CD2	1:B:873:ARG:NH2	2.51	0.78
1:A:422:GLN:OE1	1:A:422:GLN:CA	2.32	0.78
1:A:58:THR:OG1	1:B:799:GLN:NE2	2.17	0.77
1:B:320:PHE:CA	1:B:323:ARG:NH2	2.46	0.77
1:A:62:LYS:HB3	1:A:64:LEU:HD21	1.64	0.77
1:B:169:ILE:HG22	1:B:170:THR:CG2	2.05	0.77
1:B:189:LEU:HD23	1:B:203:ILE:CD1	2.13	0.77
1:A:66:THR:CG2	1:A:256:CYS:O	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ASP:O	1:A:587:ASP:HB2	1.84	0.77
1:B:169:ILE:CG2	1:B:170:THR:HG22	2.05	0.77
1:B:854:LEU:HD12	1:B:855:ASN:H	1.48	0.77
1:A:208:ASN:HD22	1:A:209:ASP:N	1.82	0.77
1:B:382:SER:OG	1:B:423:TYR:HE2	1.67	0.77
1:B:565:GLU:HG2	1:B:566:ILE:H	1.49	0.77
1:B:318:LEU:O	1:B:319:LEU:HD23	1.85	0.77
1:A:66:THR:HG21	1:A:256:CYS:HB3	1.67	0.76
1:A:324:ILE:HG23	1:A:328:LEU:HD23	1.65	0.76
1:A:911:LEU:O	1:A:914:GLU:HB3	1.84	0.76
1:B:595:ARG:NE	1:B:648:ASP:OD2	2.18	0.76
1:B:844:LYS:HZ3	1:B:848:ASN:HD21	1.33	0.76
1:A:202:ASN:C	1:A:202:ASN:OD1	2.23	0.76
1:A:219:TYR:CD2	1:A:451:LYS:HD3	2.20	0.76
1:A:166:ALA:HB3	1:A:185:VAL:CG2	2.15	0.76
1:A:57:PRO:HG2	1:B:799:GLN:HE21	1.51	0.75
1:A:390:LEU:O	1:A:390:LEU:HD12	1.86	0.75
1:B:66:THR:HG22	1:B:256:CYS:O	1.85	0.75
1:B:455:MET:HE2	1:B:455:MET:HA	1.69	0.75
1:A:85:LEU:O	1:A:155:SER:CB	2.35	0.74
1:B:204:VAL:HG12	1:B:460:ALA:HB1	1.69	0.74
1:B:101:LYS:O	1:B:103:GLN:CG	2.35	0.74
1:B:347:GLU:CB	1:B:351:ASN:ND2	2.50	0.74
1:A:218:GLY:HA2	1:A:221:ASP:O	1.87	0.74
1:A:380:PHE:HE2	1:A:426:ARG:CG	2.01	0.74
1:A:520:PRO:CD	1:A:663:MET:HE1	2.17	0.74
1:B:405:ARG:HB3	1:B:405:ARG:HH11	1.51	0.74
1:A:422:GLN:HB3	1:A:426:ARG:NH1	2.03	0.73
1:A:245:ILE:HD13	1:A:257:ILE:HD11	1.69	0.73
1:A:480:THR:HG23	1:A:483:MET:CE	2.17	0.73
1:A:575:PHE:O	1:A:579:VAL:HG23	1.88	0.73
1:A:94:ARG:NE	1:A:96:GLN:OE1	2.22	0.73
1:A:105:VAL:HG21	1:A:219:TYR:HE2	1.53	0.73
1:A:320:PHE:CE1	1:A:361:VAL:CG2	2.71	0.73
1:A:472:GLU:OE1	6:A:1118:HOH:O	2.07	0.73
1:B:664:THR:HG23	1:B:899:LYS:HB3	1.71	0.73
1:A:290:LYS:O	1:A:295:LYS:CE	2.36	0.72
1:A:320:PHE:CE1	1:A:361:VAL:HG21	2.23	0.72
1:A:480:THR:OG1	1:A:483:MET:HG3	1.89	0.72
1:A:222:GLN:N	1:A:222:GLN:OE1	2.22	0.72
1:B:265:GLY:O	1:B:292:LEU:HD12	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLN:CG	1:A:426:ARG:NH2	2.53	0.72
1:B:522:GLY:CA	6:B:1195:HOH:O	2.27	0.72
1:A:93:LEU:CD1	1:A:450:GLY:HA3	2.19	0.72
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.23	0.72
1:A:93:LEU:HD11	1:A:450:GLY:HA3	1.71	0.72
1:B:390:LEU:HD23	1:B:427:PHE:CZ	2.24	0.71
1:A:507:ALA:O	1:A:510:LYS:CE	2.36	0.71
1:A:85:LEU:O	1:A:155:SER:HB2	1.91	0.71
1:A:691:LYS:HA	1:A:699:ASP:HB2	1.72	0.71
1:A:105:VAL:HG21	1:A:219:TYR:CE2	2.26	0.71
1:A:154:PHE:HA	1:A:155:SER:CB	2.20	0.70
1:A:640:ALA:HA	1:A:643:ARG:HE	1.56	0.70
1:A:26:LEU:HD22	1:A:29:MET:CE	2.20	0.70
1:B:320:PHE:CE2	1:B:361:VAL:HG21	2.26	0.70
1:A:119:VAL:HG13	1:A:175:PHE:CD1	2.27	0.70
1:B:531:LEU:HD11	1:B:582:ILE:HD12	1.73	0.70
1:B:635:THR:HG22	1:B:639:ASP:OD2	1.91	0.69
1:B:657:ASP:OD2	1:B:677:ILE:HD13	1.93	0.69
1:B:315:LYS:HG2	1:B:324:ILE:HD11	1.74	0.69
1:A:235:ASN:HA	1:A:261:TRP:NE1	2.08	0.69
1:A:721:ILE:C	1:A:721:ILE:HD12	2.13	0.69
1:B:56:ASN:N	1:B:57:PRO:HD2	2.08	0.69
1:B:320:PHE:HA	1:B:323:ARG:NH2	2.06	0.69
1:B:771:GLN:HE21	1:B:772:ILE:N	1.90	0.69
1:A:221:ASP:C	1:A:222:GLN:OE1	2.31	0.69
1:B:382:SER:OG	1:B:423:TYR:CE2	2.47	0.68
1:B:529:LEU:HD11	1:B:586:LEU:HD21	1.74	0.68
1:B:347:GLU:HB2	1:B:351:ASN:HD21	1.56	0.68
1:B:597:PRO:HA	1:B:650:ASP:O	1.93	0.68
1:B:441:ARG:NH2	1:B:443:LEU:HD13	2.08	0.68
1:B:579:VAL:HG11	1:B:641:ILE:HA	1.76	0.68
1:B:578:ILE:O	1:B:582:ILE:HG12	1.94	0.68
1:B:118:ILE:HD13	1:B:129:HIS:HD2	1.57	0.68
1:B:166:ALA:HB3	1:B:185:VAL:HG22	1.76	0.67
1:A:420:HIS:CD2	1:A:423:TYR:HB2	2.30	0.67
1:A:854:LEU:HD12	1:A:855:ASN:N	2.09	0.67
1:A:72:PRO:HD3	1:A:215:MET:CE	2.25	0.67
1:A:91:ARG:HH11	1:A:91:ARG:HB2	1.59	0.67
1:A:291:GLN:O	1:A:295:LYS:HG3	1.95	0.67
1:B:347:GLU:N	1:B:347:GLU:CD	2.47	0.67
1:B:624:LYS:HD2	1:B:734:LEU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:VAL:HG11	1:A:334:PHE:CE2	2.29	0.67
1:B:319:LEU:HB3	1:B:320:PHE:HE1	0.87	0.67
1:A:62:LYS:CB	1:A:64:LEU:HD21	2.25	0.67
1:B:230:ILE:HG22	1:B:416:LEU:HD23	1.76	0.66
1:B:469:GLN:NE2	1:B:766:PHE:HZ	1.93	0.66
1:A:184:ASP:OD1	1:A:186:VAL:HB	1.95	0.66
1:B:530:ALA:HB3	1:B:541:LEU:HB2	1.76	0.66
1:B:771:GLN:CA	1:B:771:GLN:NE2	2.56	0.66
1:B:319:LEU:CA	1:B:320:PHE:HD1	2.07	0.66
1:A:139:GLU:HA	1:A:139:GLU:OE1	1.96	0.66
1:A:520:PRO:CD	1:A:663:MET:HE3	2.22	0.66
1:B:539:ARG:CZ	1:B:559:ILE:HD11	2.25	0.66
1:B:382:SER:HG	1:B:423:TYR:HE2	1.43	0.66
1:A:44:ARG:HG2	1:A:392:ALA:CB	2.25	0.66
1:A:168:LEU:CD2	1:A:180:VAL:HG12	2.25	0.66
1:B:666:ALA:HA	1:B:672:CYS:HB3	1.78	0.66
1:A:159:GLN:HB3	1:A:167:ILE:HB	1.77	0.65
1:A:168:LEU:HD23	1:A:180:VAL:HG12	1.78	0.65
1:A:529:LEU:HD11	1:A:586:LEU:HD21	1.77	0.65
1:A:566:ILE:HD13	1:A:566:ILE:H	1.60	0.65
1:A:769:ARG:NH2	1:A:812:THR:HG23	2.11	0.65
1:B:346:LYS:CB	1:B:347:GLU:OE2	2.45	0.65
1:B:769:ARG:NH2	1:B:810:ASN:O	2.30	0.65
1:B:814:ASP:O	6:B:1178:HOH:O	2.15	0.65
1:A:56:ASN:N	1:A:57:PRO:HD2	2.12	0.65
1:A:222:GLN:O	1:A:223:HIS:CG	2.50	0.65
1:B:565:GLU:HG2	1:B:566:ILE:N	2.11	0.65
1:A:162:LYS:HB3	1:A:164:ASP:HB3	1.79	0.65
1:A:347:GLU:HA	1:A:347:GLU:OE2	1.97	0.65
1:A:441:ARG:NH2	1:A:443:LEU:HD13	2.12	0.65
1:A:566:ILE:CD1	1:A:566:ILE:N	2.60	0.65
1:A:62:LYS:HB3	1:A:64:LEU:HD23	1.77	0.65
1:A:154:PHE:HA	1:A:155:SER:HB2	1.79	0.64
1:B:471:GLU:CG	6:B:1129:HOH:O	2.45	0.64
1:A:412:VAL:HG12	1:A:413:ASP:N	2.12	0.64
1:A:691:LYS:HB3	6:A:1132:HOH:O	1.96	0.64
1:B:79:ASP:HB3	1:B:148:LEU:HD22	1.79	0.64
1:A:376:THR:O	1:A:380:PHE:HB2	1.97	0.64
1:A:587:ASP:O	1:A:590:GLY:N	2.28	0.64
1:B:628:CYS:O	1:B:631:HIS:HB2	1.96	0.64
1:A:311:VAL:HG22	1:A:328:LEU:HG	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HB2	1:A:91:ARG:NH1	2.13	0.64
1:A:98:ASN:CG	1:A:101:LYS:HD3	2.18	0.64
1:A:221:ASP:OD1	1:A:222:GLN:O	2.16	0.64
1:B:97:VAL:HG21	1:B:455:MET:HE1	1.79	0.64
1:B:121:GLY:O	1:B:177:ALA:HA	1.98	0.64
1:B:342:ILE:O	1:B:372:GLN:HG3	1.97	0.64
1:A:100:GLU:HA	1:A:100:GLU:OE1	1.97	0.64
1:A:163:ILE:CD1	1:A:205:ALA:HB1	2.27	0.64
1:A:530:ALA:O	1:A:531:LEU:HD12	1.98	0.64
1:A:624:LYS:HE3	1:A:734:LEU:HD22	1.78	0.64
1:B:344:LYS:O	1:B:348:GLY:HA2	1.98	0.64
1:A:94:ARG:NH1	1:A:143:ILE:HG21	2.13	0.63
1:A:302:LEU:O	1:A:306:VAL:HG23	1.97	0.63
1:A:570:THR:CG2	1:A:573:GLU:CG	2.55	0.63
1:A:680:THR:O	1:A:746:SER:HB2	1.97	0.63
1:A:875:MET:O	1:A:879:VAL:HG23	1.98	0.63
1:B:164:ASP:HB3	1:B:204:VAL:O	1.99	0.63
1:B:649:LEU:O	1:B:649:LEU:HD12	1.98	0.63
1:B:762:THR:HG22	1:B:772:ILE:HD13	1.80	0.63
1:B:141:ARG:O	1:B:143:ILE:HG23	1.99	0.63
1:A:208:ASN:HD22	1:A:209:ASP:H	1.45	0.63
1:A:209:ASP:OD1	1:A:229:ILE:HG13	1.99	0.63
1:A:829:ARG:HD2	6:A:1101:HOH:O	1.98	0.63
1:B:501:LYS:CB	1:B:695:MET:SD	2.87	0.63
1:A:24:LYS:O	1:A:27:TYR:HB3	1.99	0.63
1:A:665:CYS:SG	1:A:891:LEU:HD23	2.39	0.62
1:A:786:PHE:CZ	1:A:790:ILE:HG13	2.34	0.62
1:B:587:ASP:OD1	1:B:592:LYS:HD2	1.98	0.62
1:B:772:ILE:CG2	1:B:777:LYS:HD2	2.29	0.62
1:A:98:ASN:OD1	1:A:100:GLU:HB2	2.00	0.62
1:A:234:THR:HG22	1:A:294:GLU:HG3	1.81	0.62
1:A:101:LYS:HD2	1:A:101:LYS:N	2.15	0.62
1:A:98:ASN:OD1	1:A:101:LYS:HD3	1.99	0.62
1:A:325:THR:HB	1:A:326:PRO:HD2	1.80	0.62
1:A:380:PHE:CE2	1:A:426:ARG:CG	2.80	0.62
1:B:451:LYS:O	1:B:455:MET:HG2	1.99	0.62
1:B:471:GLU:HG3	6:B:1129:HOH:O	2.00	0.62
1:A:818:LEU:O	1:A:822:VAL:HG23	2.00	0.62
1:B:26:LEU:HD11	1:B:374:VAL:HG13	1.82	0.62
1:B:354:GLU:O	1:B:358:ARG:HG3	2.00	0.62
1:B:663:MET:HG3	1:B:904:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG21	1:B:455:MET:CE	2.30	0.62
1:A:644:ARG:NH1	1:A:646:GLU:OE2	2.33	0.61
1:A:640:ALA:HB2	1:A:643:ARG:HH21	1.65	0.61
1:B:797:LEU:HD21	1:B:817:ILE:CD1	2.30	0.61
1:B:35:THR:O	1:B:38:ASP:HB3	2.00	0.61
1:B:786:PHE:CE2	1:B:807:LEU:HD11	2.35	0.61
1:B:91:ARG:HB2	1:B:91:ARG:NH1	2.15	0.61
1:B:79:ASP:HB3	1:B:148:LEU:CD2	2.31	0.61
1:A:828:ARG:HD3	6:A:1183:HOH:O	2.01	0.61
1:B:527:ASP:OD2	1:B:544:LYS:HE2	2.00	0.61
1:B:800:VAL:HG12	1:B:816:SER:HB3	1.83	0.61
1:A:745:ILE:HA	1:A:830:ALA:HB1	1.82	0.61
1:B:165:GLU:HG3	1:B:184:ASP:OD2	2.01	0.61
1:B:380:PHE:CE2	1:B:426:ARG:HD3	2.36	0.61
1:A:578:ILE:O	1:A:582:ILE:HG13	2.01	0.60
1:A:277:PHE:CE1	1:A:309:ILE:HA	2.35	0.60
1:B:539:ARG:HH11	1:B:557:ASN:ND2	1.99	0.60
1:B:638:ARG:O	1:B:642:LYS:HG3	2.01	0.60
1:A:79:ASP:O	1:A:148:LEU:HD22	2.01	0.60
1:A:598:LEU:HD22	1:A:651:VAL:HG22	1.83	0.60
1:A:760:ASP:O	1:A:764:LYS:HG3	2.00	0.60
1:B:163:ILE:HG22	6:B:1153:HOH:O	2.02	0.60
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.37	0.60
1:A:566:ILE:HD13	1:A:566:ILE:N	2.15	0.60
1:B:21:LYS:NZ	1:B:21:LYS:HB3	2.17	0.60
1:B:538:PHE:CD2	1:B:562:ILE:HD11	2.36	0.60
1:B:583:SER:HB2	1:B:647:PHE:HE2	1.66	0.60
1:A:564:ILE:HA	6:A:1164:HOH:O	2.00	0.60
1:A:433:ARG:O	1:A:436:PRO:HD3	2.02	0.60
1:B:105:VAL:HG11	1:B:451:LYS:HG3	1.84	0.60
1:B:106:HIS:ND1	1:B:107:MET:N	2.50	0.60
1:B:420:HIS:CD2	1:B:423:TYR:HB2	2.37	0.60
1:B:483:MET:HG3	6:B:1168:HOH:O	2.01	0.60
1:B:291:GLN:OE1	1:B:291:GLN:HA	2.02	0.60
1:B:319:LEU:CA	1:B:320:PHE:CD1	2.83	0.60
1:B:412:VAL:HG12	1:B:413:ASP:N	2.17	0.60
1:B:71:ILE:HA	1:B:215:MET:SD	2.42	0.59
1:B:320:PHE:HB3	1:B:323:ARG:CZ	2.32	0.59
1:B:232:THR:O	1:B:298:SER:HB2	2.03	0.59
1:B:853:ARG:HH11	1:B:853:ARG:CB	2.08	0.59
1:A:748:MET:O	1:A:748:MET:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:LEU:HD12	1:B:649:LEU:C	2.22	0.59
1:A:166:ALA:HB3	1:A:185:VAL:HG22	1.83	0.59
1:A:420:HIS:HD2	1:A:423:TYR:HB2	1.65	0.59
1:B:20:LYS:HG3	1:B:24:LYS:HE3	1.83	0.59
1:B:743:LYS:HA	1:B:749:TYR:CD2	2.37	0.59
1:A:162:LYS:O	1:A:163:ILE:CB	2.51	0.59
1:A:579:VAL:HG21	1:A:640:ALA:CB	2.31	0.59
1:B:105:VAL:HG21	1:B:219:TYR:CE2	2.37	0.59
1:B:480:THR:HG23	1:B:483:MET:HE2	1.83	0.59
1:B:644:ARG:O	1:B:645:GLU:HB2	2.02	0.59
1:A:384:ASN:O	1:A:387:ALA:HB3	2.03	0.59
1:B:485:LEU:HD23	1:B:882:LEU:HD22	1.85	0.59
1:A:26:LEU:HD22	1:A:29:MET:HE2	1.83	0.59
1:A:91:ARG:HH11	1:A:91:ARG:CB	2.16	0.59
1:A:767:LEU:HB3	1:A:768:PHE:CD2	2.37	0.59
1:B:652:VAL:HG21	1:B:909:VAL:HG23	1.82	0.59
1:A:422:GLN:CG	1:A:426:ARG:CZ	2.81	0.59
1:B:171:TRP:HB3	1:B:175:PHE:O	2.02	0.59
1:A:297:VAL:HG12	1:A:297:VAL:O	2.03	0.58
1:A:422:GLN:CB	1:A:426:ARG:NH1	2.66	0.58
1:A:665:CYS:SG	1:A:672:CYS:SG	3.00	0.58
1:A:65:PRO:HA	1:A:257:ILE:HD13	1.85	0.58
1:A:218:GLY:HA2	1:A:224:CYS:HB3	1.85	0.58
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.11	0.58
1:A:735:ASN:HB2	1:A:738:LYS:HE3	1.86	0.58
1:B:152:PHE:HB3	1:B:206:VAL:HG22	1.84	0.58
1:B:347:GLU:OE2	1:B:347:GLU:N	2.35	0.58
1:A:422:GLN:CB	1:A:426:ARG:CZ	2.80	0.58
1:B:295:LYS:HA	1:B:301:TYR:CD2	2.38	0.58
1:B:771:GLN:NE2	1:B:772:ILE:N	2.50	0.58
1:B:786:PHE:CD1	1:B:786:PHE:C	2.76	0.58
1:A:126:LEU:O	1:A:129:HIS:HB3	2.02	0.58
1:A:516:VAL:HG21	1:A:904:ILE:HD12	1.85	0.58
1:A:528:PHE:CE2	1:A:906:ALA:HA	2.38	0.58
1:B:420:HIS:HD2	1:B:423:TYR:N	1.96	0.58
1:B:420:HIS:CD2	1:B:423:TYR:H	2.11	0.58
1:A:198:ASP:O	1:A:198:ASP:OD2	2.22	0.58
1:B:659:VAL:HA	1:B:685:CYS:SG	2.44	0.58
1:B:429:LYS:HE3	1:B:433:ARG:NH1	2.19	0.58
1:B:73:ASP:OD1	1:B:76:GLU:OE2	2.22	0.58
1:A:323:ARG:NH2	1:A:362:GLU:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASP:O	1:A:652:VAL:HG23	2.04	0.57
1:A:769:ARG:NH2	1:A:815:ASP:OD2	2.37	0.57
1:B:538:PHE:CB	1:B:562:ILE:CD1	2.82	0.57
1:B:615:ILE:HA	1:B:631:HIS:O	2.03	0.57
1:B:26:LEU:HD12	1:B:377:ILE:CD1	2.34	0.57
1:B:66:THR:HG23	1:B:68:VAL:H	1.69	0.57
1:B:184:ASP:OD1	1:B:186:VAL:HG23	2.05	0.57
1:B:320:PHE:CD2	1:B:361:VAL:CB	2.82	0.57
1:A:80:PHE:CE2	1:A:458:ALA:HA	2.39	0.57
1:A:306:VAL:HG11	1:A:334:PHE:HE2	1.69	0.57
1:A:320:PHE:CG	1:A:361:VAL:HB	2.38	0.57
1:A:688:GLU:OE1	1:A:848:ASN:ND2	2.37	0.57
1:A:380:PHE:CE2	1:A:426:ARG:HD3	2.39	0.57
1:A:422:GLN:HG3	1:A:426:ARG:CZ	2.34	0.57
1:B:528:PHE:CZ	1:B:906:ALA:HB2	2.40	0.57
1:B:616:LEU:HD11	1:B:618:THR:O	2.04	0.57
1:B:714:ASP:OD1	1:B:740:ARG:HG2	2.04	0.57
1:A:222:GLN:O	1:A:223:HIS:ND1	2.37	0.57
1:B:541:LEU:HD13	1:B:898:GLY:CA	2.35	0.57
1:A:160:GLN:CG	1:A:165:GLU:O	2.40	0.57
1:A:381:ARG:O	1:A:382:SER:C	2.43	0.57
1:A:786:PHE:CZ	1:A:790:ILE:HD11	2.40	0.57
1:B:66:THR:HG21	1:B:256:CYS:HB3	1.85	0.57
1:B:666:ALA:HA	1:B:669:GLU:O	2.05	0.57
1:A:44:ARG:HA	1:A:47:MET:HE2	1.87	0.56
1:A:530:ALA:HB3	1:A:541:LEU:HB2	1.87	0.56
1:A:786:PHE:C	1:A:786:PHE:CD1	2.78	0.56
1:A:92:ILE:C	1:A:93:LEU:HD23	2.22	0.56
1:A:541:LEU:HD22	1:A:898:GLY:HA3	1.87	0.56
1:B:320:PHE:CB	1:B:323:ARG:CZ	2.83	0.56
1:B:320:PHE:CB	1:B:323:ARG:HH21	1.97	0.56
1:A:72:PRO:HG3	1:A:455:MET:HB3	1.87	0.56
1:A:198:ASP:OD2	1:A:198:ASP:C	2.44	0.56
1:B:541:LEU:HD13	1:B:898:GLY:HA3	1.87	0.56
1:B:688:GLU:OE2	1:B:844:LYS:NZ	2.37	0.56
1:A:204:VAL:HG21	1:A:461:TYR:HD1	1.71	0.56
1:A:531:LEU:O	1:A:601:THR:HB	2.06	0.56
1:B:488:LYS:HG3	1:B:840:ALA:HB2	1.87	0.56
1:B:673:GLU:CD	1:B:849:ARG:HH22	2.08	0.56
1:A:373:HIS:CD2	1:A:377:ILE:HD11	2.41	0.56
1:B:575:PHE:O	1:B:579:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:ARG:NH2	1:B:874:ILE:HD13	2.21	0.56
1:A:656:ASN:ND2	2:A:1003:BGC:O3	2.38	0.56
1:A:845:ILE:HG22	1:A:854:LEU:HD21	1.88	0.56
1:B:302:LEU:O	1:B:306:VAL:HG23	2.06	0.56
1:B:320:PHE:O	1:B:323:ARG:HG3	2.05	0.56
1:A:297:VAL:HG13	1:A:382:SER:OG	2.06	0.56
1:B:772:ILE:HG21	1:B:777:LYS:HD2	1.88	0.56
1:A:203:ILE:N	1:A:203:ILE:HD13	2.18	0.55
1:A:309:ILE:O	1:A:313:MET:HG3	2.06	0.55
1:A:325:THR:HB	1:A:326:PRO:CD	2.36	0.55
1:A:579:VAL:HG21	1:A:640:ALA:HB3	1.87	0.55
1:B:210:THR:OG1	1:B:237:CYS:HB3	2.06	0.55
1:B:431:LEU:CD2	1:B:442:PHE:HZ	2.20	0.55
1:A:374:VAL:HA	1:A:377:ILE:HD12	1.88	0.55
1:B:309:ILE:O	1:B:313:MET:HG3	2.06	0.55
1:B:405:ARG:HB3	1:B:405:ARG:NH1	2.20	0.55
1:A:213:THR:HG22	1:A:214:MET:N	2.21	0.55
1:A:115:PRO:HB2	1:A:117:ASN:ND2	2.22	0.55
1:A:64:LEU:HD13	1:A:158:CYS:O	2.06	0.55
1:A:320:PHE:O	1:A:323:ARG:HG3	2.06	0.55
1:A:413:ASP:OD2	1:A:448:GLY:HA2	2.07	0.55
1:A:588:TYR:CE2	1:B:331:ARG:HD2	2.42	0.55
1:B:134:LEU:O	1:B:138:MET:HG3	2.06	0.55
1:B:652:VAL:HG21	1:B:909:VAL:CG2	2.37	0.55
1:B:671:THR:OG1	1:B:857:THR:HG23	2.05	0.55
1:A:167:ILE:HA	1:A:183:ALA:O	2.06	0.55
1:A:222:GLN:O	1:A:223:HIS:CB	2.54	0.55
1:B:320:PHE:O	1:B:321:GLU:HB2	2.06	0.55
1:B:718:LEU:HB2	6:B:1102:HOH:O	2.05	0.55
1:A:912:ARG:C	1:A:914:GLU:H	2.10	0.55
1:B:595:ARG:HG3	1:B:649:LEU:HA	1.88	0.55
1:B:800:VAL:CG1	1:B:816:SER:HB3	2.36	0.55
1:A:245:ILE:CD1	1:A:257:ILE:HD11	2.37	0.55
1:A:425:ARG:HH22	1:A:426:ARG:HE	1.55	0.55
1:A:546:ARG:O	1:A:551:ARG:HA	2.06	0.55
1:A:794:ARG:HH21	1:B:794:ARG:NH2	2.05	0.55
1:A:152:PHE:HB3	1:A:206:VAL:HG22	1.89	0.55
1:A:171:TRP:CZ2	1:A:177:ALA:HB3	2.42	0.55
1:A:297:VAL:O	1:A:297:VAL:CG1	2.55	0.55
1:B:93:LEU:HD12	1:B:93:LEU:N	2.21	0.55
1:B:596:MET:O	1:B:649:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:O	1:B:348:GLY:HA3	2.03	0.54
1:B:429:LYS:HE3	1:B:433:ARG:HH12	1.72	0.54
1:B:605:PRO:HB3	1:B:708:GLU:HG3	1.89	0.54
1:B:553:VAL:HG12	1:B:553:VAL:O	2.06	0.54
1:A:323:ARG:NH2	1:A:362:GLU:HB2	2.21	0.54
1:A:657:ASP:OD2	2:A:1003:BGC:H6C1	2.07	0.54
1:B:565:GLU:CG	1:B:566:ILE:N	2.69	0.54
1:B:754:VAL:HA	1:B:757:ILE:HD12	1.89	0.54
1:A:320:PHE:HZ	1:A:356:LEU:HD22	1.73	0.54
1:A:673:GLU:OE1	1:A:849:ARG:NH2	2.37	0.54
1:B:120:HIS:HA	1:B:176:LYS:O	2.08	0.54
1:B:347:GLU:HB3	1:B:351:ASN:ND2	2.22	0.54
1:B:393:ILE:O	1:B:396:ARG:HB3	2.07	0.54
1:B:587:ASP:OD1	1:B:592:LYS:CD	2.55	0.54
1:B:688:GLU:HA	1:B:688:GLU:OE1	2.08	0.54
1:B:775:THR:O	1:B:778:THR:N	2.36	0.54
1:B:786:PHE:CD2	1:B:807:LEU:HD11	2.42	0.54
1:B:86:GLY:HA3	1:B:155:SER:OG	2.08	0.54
1:B:26:LEU:HD12	1:B:377:ILE:HD12	1.89	0.54
1:B:320:PHE:O	1:B:323:ARG:CZ	2.55	0.54
1:B:644:ARG:HA	1:B:644:ARG:HH11	1.72	0.54
1:B:813:CYS:HB2	6:B:1132:HOH:O	2.06	0.54
1:A:25:TYR:HE2	1:A:313:MET:HG2	1.73	0.54
1:A:564:ILE:CG1	1:A:565:GLU:N	2.61	0.54
1:B:374:VAL:HA	1:B:377:ILE:HD12	1.88	0.54
1:A:110:GLU:HG3	1:A:111:VAL:H	1.72	0.54
1:A:693:VAL:O	1:A:695:MET:N	2.40	0.54
1:B:171:TRP:CZ2	1:B:180:VAL:HG11	2.42	0.54
1:B:380:PHE:CD2	1:B:426:ARG:HD3	2.43	0.54
1:B:508:VAL:O	6:B:1109:HOH:O	2.18	0.54
1:A:578:ILE:HG22	1:A:582:ILE:HD11	1.90	0.53
1:A:721:ILE:C	1:A:721:ILE:CD1	2.76	0.53
1:B:771:GLN:NE2	1:B:771:GLN:HA	2.22	0.53
1:A:327:GLU:OE1	1:A:327:GLU:N	2.40	0.53
1:A:514:SER:OG	1:A:704:CYS:O	2.24	0.53
1:B:56:ASN:N	1:B:57:PRO:CD	2.71	0.53
1:A:163:ILE:HD13	1:A:205:ALA:HB1	1.89	0.53
1:A:560:TYR:CD2	1:A:581:CYS:HB3	2.43	0.53
1:B:209:ASP:OD2	2:B:1001:BGC:H6C1	2.09	0.53
1:B:495:MET:HB3	1:B:511:MET:HE2	1.90	0.53
1:B:204:VAL:HG11	1:B:461:TYR:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:PHE:HB3	1:B:562:ILE:CD1	2.39	0.53
1:B:616:LEU:HD11	1:B:618:THR:C	2.29	0.53
1:B:854:LEU:HD12	1:B:854:LEU:C	2.27	0.53
1:B:18:GLN:HE21	1:B:366:ASP:HB3	1.74	0.53
1:B:513:PRO:HB2	1:B:703:MET:CE	2.38	0.53
1:B:522:GLY:O	1:B:547:SER:HB2	2.09	0.53
1:B:587:ASP:CG	1:B:592:LYS:HD2	2.29	0.53
1:A:69:ARG:O	1:A:70:SER:HB3	2.09	0.53
1:A:274:ARG:HG2	1:A:274:ARG:HH11	1.73	0.53
1:A:320:PHE:CE1	1:A:361:VAL:HG23	2.44	0.53
1:B:307:ARG:HG2	1:B:307:ARG:HH11	1.73	0.53
1:B:631:HIS:HE1	6:B:1174:HOH:O	1.91	0.53
1:B:640:ALA:HA	1:B:643:ARG:HE	1.73	0.53
1:A:58:THR:CG2	6:B:1184:HOH:O	2.56	0.53
1:A:485:LEU:HD23	1:A:882:LEU:HD22	1.90	0.53
1:A:605:PRO:HD3	2:A:1003:BGC:O2	2.09	0.53
1:B:93:LEU:HG	1:B:109:SER:CB	2.38	0.53
1:B:271:GLU:OE2	1:B:274:ARG:HD3	2.08	0.53
1:A:86:GLY:HA2	1:A:175:PHE:CE2	2.44	0.53
1:B:654:VAL:HG13	1:B:654:VAL:O	2.08	0.53
1:A:165:GLU:HA	1:A:186:VAL:HG21	1.91	0.53
1:A:539:ARG:CZ	1:A:559:ILE:HD11	2.39	0.53
1:B:303:GLY:HA2	1:B:339:VAL:HG21	1.90	0.53
1:A:84:ASP:HA	1:A:153:THR:HB	1.90	0.53
1:B:501:LYS:HB2	1:B:695:MET:SD	2.47	0.53
1:B:718:LEU:HD22	1:B:721:ILE:HD11	1.90	0.52
1:B:55:PHE:C	1:B:57:PRO:HD2	2.30	0.52
1:B:93:LEU:HG	1:B:109:SER:HB2	1.91	0.52
1:B:441:ARG:HH21	1:B:443:LEU:HD13	1.73	0.52
1:B:66:THR:CG2	1:B:256:CYS:HB3	2.40	0.52
1:B:330:THR:HB	1:B:333:LYS:HG3	1.92	0.52
1:A:786:PHE:CD1	1:A:787:LEU:N	2.77	0.52
1:A:883:SER:HA	6:A:1103:HOH:O	2.09	0.52
1:B:361:VAL:O	1:B:363:PRO:HD3	2.09	0.52
1:B:579:VAL:HG13	1:B:641:ILE:HG12	1.92	0.52
1:A:601:THR:HA	1:A:655:VAL:O	2.10	0.52
1:B:163:ILE:HG13	1:B:205:ALA:HB1	1.90	0.52
1:A:306:VAL:O	1:A:309:ILE:N	2.43	0.52
1:A:398:ARG:NH1	1:A:398:ARG:HB3	2.24	0.52
1:A:693:VAL:C	1:A:695:MET:H	2.13	0.52
1:B:16:ASP:O	1:B:20:LYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ALA:O	1:B:322:GLY:HA2	2.10	0.52
1:A:93:LEU:HD12	1:A:450:GLY:HA3	1.91	0.52
1:A:154:PHE:CA	1:A:155:SER:CB	2.87	0.52
1:A:275:THR:N	1:A:278:ASP:OD2	2.27	0.52
1:A:611:LEU:HG	1:A:653:ALA:CB	2.40	0.52
1:B:387:ALA:HA	1:B:427:PHE:HE1	1.75	0.52
1:A:110:GLU:HG3	1:A:111:VAL:N	2.25	0.52
1:A:317:GLY:HA2	1:A:322:GLY:CA	2.40	0.52
1:A:356:LEU:O	1:A:359:LEU:HB2	2.10	0.52
1:A:490:ARG:NH2	1:A:720:ASP:OD2	2.32	0.52
1:B:98:ASN:ND2	1:B:101:LYS:HD2	2.24	0.52
1:B:321:GLU:HB2	1:B:323:ARG:NH1	2.25	0.52
1:A:452:GLY:O	1:A:456:VAL:HG23	2.09	0.51
1:A:80:PHE:CD1	1:A:80:PHE:N	2.78	0.51
1:A:361:VAL:O	1:A:363:PRO:CD	2.55	0.51
1:A:380:PHE:CD2	1:A:426:ARG:CD	2.78	0.51
1:B:768:PHE:HE1	1:B:811:SER:HB3	1.75	0.51
1:A:72:PRO:HD3	1:A:215:MET:SD	2.50	0.51
1:A:480:THR:O	1:A:481:LYS:C	2.48	0.51
1:A:512:LEU:CD1	1:A:512:LEU:N	2.73	0.51
1:B:480:THR:HG23	1:B:483:MET:HE3	1.91	0.51
1:A:520:PRO:HD3	1:A:663:MET:SD	2.49	0.51
1:A:523:THR:OG1	1:A:910:ARG:NH1	2.42	0.51
1:A:277:PHE:CZ	1:A:309:ILE:HA	2.46	0.51
1:B:327:GLU:O	1:B:333:LYS:HG3	2.10	0.51
1:A:235:ASN:HA	1:A:261:TRP:CD1	2.46	0.51
1:A:529:LEU:CD1	1:A:586:LEU:HD21	2.40	0.51
1:B:189:LEU:O	1:B:190:ASN:C	2.48	0.51
1:B:306:VAL:O	1:B:308:LEU:N	2.44	0.51
1:B:318:LEU:O	1:B:319:LEU:CD2	2.58	0.51
1:B:538:PHE:HB3	1:B:562:ILE:HD12	1.93	0.51
1:A:86:GLY:CA	1:A:155:SER:OG	2.57	0.50
1:B:560:TYR:CD2	1:B:581:CYS:HB3	2.46	0.50
1:A:500:ARG:HG2	1:A:500:ARG:HH11	1.76	0.50
1:A:845:ILE:HG22	1:A:854:LEU:CD2	2.42	0.50
1:B:119:VAL:CG1	1:B:175:PHE:HA	2.42	0.50
1:B:156:PHE:HB3	1:B:157:PRO:HD2	1.94	0.50
1:B:346:LYS:HB2	1:B:347:GLU:OE2	2.11	0.50
1:B:510:LYS:HB3	1:B:512:LEU:CD2	2.42	0.50
1:B:577:HIS:O	1:B:580:SER:HB3	2.12	0.50
1:A:25:TYR:CE2	1:A:313:MET:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ILE:HG22	1:A:582:ILE:CD1	2.41	0.50
1:B:313:MET:CE	1:B:318:LEU:CD1	2.88	0.50
1:A:180:VAL:O	1:A:183:ALA:HB3	2.11	0.50
1:B:320:PHE:CE2	1:B:361:VAL:CG2	2.95	0.50
1:B:495:MET:HE1	1:B:841:VAL:HG22	1.93	0.50
1:A:174:ARG:O	1:A:286:LEU:CD1	2.59	0.50
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.12	0.50
1:A:154:PHE:HA	1:A:155:SER:HB3	1.93	0.50
1:A:652:VAL:HB	1:A:905:THR:HG23	1.92	0.50
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.47	0.50
1:A:760:ASP:OD2	1:A:764:LYS:CE	2.53	0.50
1:B:290:LYS:O	1:B:295:LYS:HE3	2.10	0.50
1:B:574:LEU:O	1:B:577:HIS:HB3	2.11	0.50
1:B:844:LYS:HZ3	1:B:848:ASN:ND2	2.05	0.50
1:A:66:THR:CG2	1:A:256:CYS:HB3	2.39	0.50
1:B:229:ILE:O	1:B:234:THR:HA	2.12	0.50
1:A:512:LEU:N	1:A:512:LEU:HD13	2.27	0.50
1:A:638:ARG:O	1:A:641:ILE:HB	2.12	0.50
1:A:786:PHE:CE1	1:A:790:ILE:HG13	2.47	0.50
1:B:426:ARG:HH21	5:B:1007:CIT:C4	2.18	0.50
1:B:513:PRO:HB2	1:B:703:MET:HE3	1.93	0.50
1:B:666:ALA:CA	1:B:672:CYS:HB3	2.41	0.50
1:B:759:ILE:O	1:B:762:THR:HB	2.12	0.50
1:B:768:PHE:CE1	1:B:811:SER:HB3	2.47	0.50
1:A:799:GLN:O	1:A:802:ALA:HB3	2.11	0.49
1:B:84:ASP:HA	1:B:153:THR:HB	1.93	0.49
1:B:118:ILE:CD1	1:B:129:HIS:HD2	2.25	0.49
1:B:553:VAL:HG11	1:B:899:LYS:HG3	1.94	0.49
1:A:430:THR:HG23	1:A:433:ARG:NH2	2.28	0.49
1:B:98:ASN:C	1:B:103:GLN:O	2.50	0.49
1:B:141:ARG:HD2	1:B:141:ARG:N	2.27	0.49
1:B:325:THR:HG21	1:B:360:GLY:HA3	1.93	0.49
1:B:467:HIS:O	1:B:468:ARG:C	2.50	0.49
1:A:528:PHE:CZ	1:A:906:ALA:HA	2.47	0.49
1:A:408:THR:OG1	1:A:409:THR:N	2.45	0.49
1:B:786:PHE:CD1	1:B:787:LEU:N	2.80	0.49
1:B:307:ARG:HG2	1:B:307:ARG:NH1	2.27	0.49
1:B:529:LEU:O	1:B:598:LEU:HA	2.13	0.49
1:A:221:ASP:OD1	1:A:222:GLN:N	2.46	0.49
1:A:796:ALA:O	1:A:799:GLN:HB3	2.13	0.49
1:B:791:GLU:O	1:B:792:SER:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:THR:O	1:A:392:ALA:N	2.46	0.49
1:A:422:GLN:HG3	1:A:425:ARG:NH2	2.22	0.49
1:A:611:LEU:HG	1:A:653:ALA:HB2	1.94	0.49
1:B:350:HIS:O	1:B:353:LYS:HB3	2.13	0.49
1:B:764:LYS:HE2	6:B:1124:HOH:O	2.12	0.49
1:A:510:LYS:HB3	1:A:512:LEU:HD13	1.89	0.48
1:A:711:ALA:O	1:A:714:ASP:HB2	2.12	0.48
1:A:786:PHE:CZ	1:A:790:ILE:CG1	2.96	0.48
1:B:390:LEU:CD2	1:B:427:PHE:HZ	2.22	0.48
1:B:538:PHE:CG	1:B:562:ILE:HD11	2.48	0.48
1:B:598:LEU:HD22	1:B:651:VAL:HG22	1.95	0.48
1:A:22:ILE:HD11	1:A:370:SER:HB3	1.94	0.48
1:A:579:VAL:HA	1:A:582:ILE:HD12	1.95	0.48
1:B:275:THR:O	1:B:278:ASP:N	2.47	0.48
1:B:320:PHE:CE2	1:B:361:VAL:CB	2.96	0.48
1:B:347:GLU:O	1:B:348:GLY:C	2.52	0.48
1:A:361:VAL:O	1:A:361:VAL:HG23	2.13	0.48
1:A:602:PHE:CE2	1:A:633:VAL:HG11	2.48	0.48
1:A:786:PHE:CE2	1:A:790:ILE:CD1	2.83	0.48
1:A:786:PHE:CD2	1:A:807:LEU:HD11	2.48	0.48
1:A:854:LEU:HD12	1:A:854:LEU:C	2.33	0.48
1:B:173:LYS:CE	2:B:1001:BGC:O5	2.53	0.48
1:B:471:GLU:HG2	6:B:1129:HOH:O	2.09	0.48
1:B:818:LEU:O	1:B:822:VAL:HG23	2.13	0.48
1:A:162:LYS:C	1:A:164:ASP:H	2.16	0.48
1:A:520:PRO:CG	1:A:663:MET:HE3	2.43	0.48
1:A:786:PHE:CZ	1:A:790:ILE:CD1	2.96	0.48
1:B:204:VAL:HG12	1:B:460:ALA:CB	2.41	0.48
1:B:320:PHE:CE2	1:B:361:VAL:HG11	2.48	0.48
1:A:637:LEU:O	1:A:641:ILE:HG12	2.14	0.48
1:B:398:ARG:HB2	1:B:406:LEU:HD22	1.96	0.48
1:A:156:PHE:HB3	1:A:157:PRO:CD	2.44	0.48
1:A:496:GLU:O	1:A:500:ARG:HG3	2.14	0.48
1:B:189:LEU:CD2	1:B:203:ILE:HD11	2.35	0.48
1:B:320:PHE:HE2	1:B:361:VAL:CG2	2.21	0.48
1:A:264:PHE:HB3	1:A:293:PHE:CB	2.44	0.48
1:A:623:PHE:N	1:A:623:PHE:CD2	2.80	0.48
1:A:767:LEU:HD22	1:A:768:PHE:CE2	2.48	0.48
1:B:531:LEU:HD22	1:B:598:LEU:HD11	1.95	0.48
1:A:412:VAL:CG1	1:A:413:ASP:N	2.76	0.47
1:B:159:GLN:HA	1:B:159:GLN:OE1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASN:O	1:B:204:VAL:HG23	2.14	0.47
1:A:56:ASN:N	1:A:57:PRO:CD	2.76	0.47
1:A:406:LEU:HG	1:A:408:THR:HG22	1.96	0.47
1:A:781:ILE:HG22	1:A:782:PHE:N	2.28	0.47
1:B:291:GLN:O	1:B:295:LYS:HG3	2.15	0.47
1:B:612:ASP:HB3	1:B:652:VAL:O	2.14	0.47
1:A:66:THR:HG21	1:A:256:CYS:CB	2.40	0.47
1:A:67:PHE:CZ	1:A:161:SER:O	2.67	0.47
1:B:159:GLN:HB3	1:B:167:ILE:HB	1.96	0.47
1:A:261:TRP:O	1:A:264:PHE:HB2	2.15	0.47
1:A:721:ILE:HD12	1:A:722:ARG:N	2.28	0.47
1:A:854:LEU:HD12	1:A:855:ASN:O	2.15	0.47
1:B:235:ASN:HB2	6:B:1136:HOH:O	2.15	0.47
1:A:199:TYR:CE2	1:A:201:ALA:HB2	2.49	0.47
1:A:520:PRO:HG3	1:A:663:MET:HE3	1.96	0.47
1:A:838:MET:O	1:A:841:VAL:N	2.47	0.47
1:B:718:LEU:C	1:B:720:ASP:N	2.68	0.47
1:A:43:PHE:O	1:A:47:MET:HG3	2.15	0.47
1:A:154:PHE:CA	1:A:155:SER:HB2	2.45	0.47
1:B:841:VAL:HG12	1:B:842:VAL:N	2.29	0.47
1:A:101:LYS:N	1:A:101:LYS:CD	2.77	0.47
1:A:287:ASN:O	1:A:295:LYS:NZ	2.45	0.47
1:A:564:ILE:CG1	1:A:565:GLU:H	2.16	0.47
1:B:69:ARG:O	1:B:70:SER:HB3	2.15	0.47
1:B:330:THR:HG21	1:B:333:LYS:HE2	1.96	0.47
1:B:491:MET:O	1:B:495:MET:HG3	2.15	0.47
1:A:693:VAL:O	1:A:693:VAL:HG12	2.15	0.47
1:B:395:ASN:OD1	1:B:398:ARG:NH2	2.48	0.47
1:B:724:HIS:CE1	1:B:728:LEU:HD11	2.49	0.47
1:A:71:ILE:HA	1:A:215:MET:SD	2.54	0.47
1:A:238:TYR:O	1:A:256:CYS:HA	2.15	0.47
1:A:241:GLU:O	1:A:244:HIS:HB2	2.14	0.47
1:B:163:ILE:HG13	1:B:205:ALA:CB	2.44	0.47
1:B:306:VAL:O	1:B:307:ARG:C	2.54	0.47
1:B:628:CYS:HB2	6:B:1123:HOH:O	2.14	0.47
1:B:781:ILE:HG22	1:B:782:PHE:N	2.31	0.46
1:B:505:ASN:HB2	6:B:1111:HOH:O	2.15	0.46
1:B:579:VAL:HG21	1:B:640:ALA:HB3	1.96	0.46
1:B:488:LYS:HE3	1:B:840:ALA:HA	1.97	0.46
1:B:755:ARG:HD2	1:B:778:THR:O	2.16	0.46
1:B:797:LEU:HD21	1:B:817:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:CG2	1:A:219:TYR:OH	2.63	0.46
1:A:511:MET:O	1:A:705:ILE:HD12	2.16	0.46
1:A:718:LEU:C	1:A:720:ASP:N	2.68	0.46
1:B:596:MET:HB3	1:B:597:PRO:HD2	1.97	0.46
1:A:44:ARG:HA	1:A:47:MET:CE	2.45	0.46
1:A:76:GLU:HG2	1:A:455:MET:SD	2.56	0.46
1:A:320:PHE:CE2	1:A:361:VAL:HG11	2.51	0.46
1:A:380:PHE:CE2	1:A:426:ARG:CD	2.99	0.46
1:A:652:VAL:HG21	1:A:909:VAL:CG2	2.46	0.46
1:A:398:ARG:HB3	1:A:398:ARG:HH11	1.80	0.46
1:A:647:PHE:CD1	1:A:647:PHE:N	2.83	0.46
1:B:119:VAL:HG12	1:B:120:HIS:HD2	1.80	0.46
1:B:844:LYS:HZ2	1:B:848:ASN:HD21	1.61	0.46
1:B:83:LEU:HB2	1:B:152:PHE:HD1	1.81	0.46
1:B:616:LEU:HD12	1:B:618:THR:H	1.81	0.46
1:A:52:SER:HA	1:A:246:ASP:OD2	2.16	0.45
1:A:619:TRP:CD1	1:A:624:LYS:HA	2.51	0.45
1:B:42:ARG:HH11	1:B:270:LEU:HD23	1.80	0.45
1:B:105:VAL:HG21	1:B:219:TYR:HE2	1.81	0.45
1:B:147:LYS:HD3	1:B:147:LYS:H	1.81	0.45
1:B:346:LYS:C	1:B:347:GLU:CD	2.74	0.45
1:B:492:ARG:NE	1:B:844:LYS:HG3	2.32	0.45
1:B:735:ASN:OD1	1:B:735:ASN:N	2.48	0.45
1:A:311:VAL:O	1:A:315:LYS:HG3	2.15	0.45
1:A:666:ALA:HA	1:A:669:GLU:O	2.15	0.45
1:B:683:ASN:HA	1:B:709:TRP:CD1	2.51	0.45
1:B:797:LEU:HD13	1:B:813:CYS:HB3	1.98	0.45
1:A:687:MET:SD	1:A:704:CYS:HB2	2.56	0.45
1:B:30:ARG:HG2	1:B:377:ILE:HG23	1.98	0.45
1:B:126:LEU:O	1:B:130:VAL:HG23	2.17	0.45
1:B:666:ALA:HA	1:B:672:CYS:CB	2.45	0.45
1:B:716:GLY:C	1:B:718:LEU:H	2.19	0.45
1:B:718:LEU:C	1:B:720:ASP:H	2.20	0.45
1:B:725:TYR:O	1:B:729:VAL:HG23	2.16	0.45
1:B:772:ILE:HG22	1:B:777:LYS:HD2	1.96	0.45
1:B:513:PRO:CB	1:B:703:MET:HE2	2.46	0.45
1:B:862:GLY:HA2	3:B:1004:0WK:O6	2.16	0.45
1:B:899:LYS:O	1:B:903:LEU:HG	2.17	0.45
1:A:58:THR:O	1:A:58:THR:HG22	2.17	0.45
1:A:154:PHE:C	1:A:156:PHE:H	2.17	0.45
1:A:727:ARG:O	1:A:731:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:VAL:HG23	1:B:509:VAL:N	2.32	0.45
1:B:650:ASP:OD2	1:B:912:ARG:NH1	2.41	0.45
1:A:317:GLY:HA2	1:A:322:GLY:HA2	1.99	0.45
1:A:539:ARG:HH11	1:A:557:ASN:ND2	2.15	0.45
1:A:846:ARG:HA	1:A:854:LEU:HD22	1.98	0.45
1:A:156:PHE:CZ	1:A:175:PHE:CD2	2.94	0.45
1:A:357:THR:OG1	1:A:363:PRO:HG2	2.17	0.45
1:A:564:ILE:CA	6:A:1164:HOH:O	2.63	0.45
1:A:569:GLY:O	1:A:626:THR:HG23	2.17	0.45
1:A:652:VAL:HG12	1:A:652:VAL:O	2.16	0.45
1:B:431:LEU:HD22	1:B:442:PHE:HZ	1.82	0.45
1:B:843:ASP:HB3	6:B:1113:HOH:O	2.17	0.45
1:A:88:SER:OG	3:A:1002:0WK:O3P	2.34	0.45
1:A:110:GLU:HG2	1:A:112:TYR:CE1	2.52	0.45
1:A:897:SER:O	1:A:898:GLY:C	2.55	0.45
1:B:509:VAL:HB	6:B:1110:HOH:O	2.16	0.45
1:B:515:PHE:O	1:B:611:LEU:HD13	2.16	0.45
1:A:763:LYS:HG3	1:A:772:ILE:HD11	1.99	0.45
1:A:781:ILE:HD13	1:A:781:ILE:HA	1.75	0.45
1:B:481:LYS:O	1:B:485:LEU:HG	2.16	0.45
1:A:26:LEU:HD21	1:A:309:ILE:HG23	1.99	0.45
1:A:107:MET:O	1:A:107:MET:HG3	2.17	0.45
1:A:166:ALA:O	1:A:184:ASP:HA	2.17	0.45
1:A:579:VAL:HG13	1:A:641:ILE:HD13	1.99	0.45
1:A:913:THR:HG22	1:A:913:THR:O	2.17	0.45
1:A:364:SER:C	1:A:366:ASP:H	2.20	0.44
1:A:390:LEU:HD23	1:A:427:PHE:HZ	1.82	0.44
1:A:691:LYS:HA	1:A:699:ASP:CB	2.44	0.44
1:B:400:ASN:N	1:B:400:ASN:HD22	2.15	0.44
1:A:162:LYS:HD2	1:A:164:ASP:HB3	1.99	0.44
1:A:202:ASN:OD1	1:A:202:ASN:O	2.35	0.44
1:A:801:ARG:HG3	1:A:811:SER:O	2.17	0.44
1:B:608:GLN:HG2	1:B:614:GLY:HA2	2.00	0.44
1:B:642:LYS:C	1:B:644:ARG:H	2.19	0.44
1:A:124:SER:O	1:A:128:ASP:HB2	2.17	0.44
1:A:306:VAL:O	1:A:308:LEU:N	2.51	0.44
1:B:71:ILE:HB	1:B:72:PRO:HD2	1.99	0.44
1:B:325:THR:OG1	1:B:359:LEU:O	2.34	0.44
1:B:568:GLN:HA	1:B:624:LYS:O	2.16	0.44
1:B:797:LEU:HD21	1:B:817:ILE:HD11	1.99	0.44
1:B:828:ARG:NH2	1:B:874:ILE:CD1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:VAL:HB	1:A:858:VAL:HG22	1.99	0.44
1:A:754:VAL:HA	1:A:757:ILE:HD12	2.00	0.44
1:B:342:ILE:CG2	1:B:372:GLN:HA	2.47	0.44
1:A:657:ASP:OD1	1:A:657:ASP:N	2.50	0.44
1:B:374:VAL:O	1:B:375:CYS:C	2.56	0.44
1:B:870:HIS:C	6:B:1146:HOH:O	2.55	0.44
1:A:128:ASP:HA	1:A:192:ALA:HB1	1.98	0.44
1:A:521:ASP:OD2	1:A:523:THR:HG23	2.17	0.44
1:A:853:ARG:HD3	1:A:885:LYS:O	2.18	0.44
1:B:373:HIS:O	1:B:377:ILE:HG13	2.18	0.44
1:B:542:LEU:HD13	1:B:542:LEU:C	2.38	0.44
1:A:149:PRO:HG3	1:A:461:TYR:CE1	2.51	0.44
1:A:425:ARG:NH2	1:A:426:ARG:NE	2.65	0.44
1:A:709:TRP:CD1	1:A:709:TRP:C	2.90	0.44
1:B:545:ILE:O	1:B:546:ARG:CD	2.57	0.44
1:B:31:LEU:HD11	1:B:381:ARG:HG3	1.99	0.44
1:A:26:LEU:HD21	1:A:309:ILE:CG2	2.48	0.44
1:A:67:PHE:CB	1:A:163:ILE:HB	2.47	0.44
1:A:110:GLU:CG	1:A:111:VAL:N	2.80	0.44
1:A:385:LEU:O	1:A:386:VAL:C	2.54	0.44
1:A:510:LYS:CB	1:A:512:LEU:CD1	2.86	0.44
1:A:541:LEU:N	1:A:541:LEU:HD12	2.32	0.44
1:A:718:LEU:HB2	6:A:1102:HOH:O	2.18	0.44
1:B:285:SER:OG	1:B:295:LYS:NZ	2.51	0.44
1:B:306:VAL:HG11	1:B:334:PHE:CE2	2.53	0.44
1:A:156:PHE:HB3	1:A:157:PRO:HD2	1.99	0.43
1:A:173:LYS:NZ	2:A:1001:BGC:O6	2.50	0.43
1:A:304:GLU:CD	1:A:307:ARG:HE	2.21	0.43
1:B:640:ALA:HA	1:B:643:ARG:NE	2.32	0.43
1:B:661:THR:O	1:B:662:MET:C	2.55	0.43
1:B:762:THR:HG22	1:B:772:ILE:CD1	2.46	0.43
1:A:763:LYS:CG	1:A:772:ILE:HD11	2.48	0.43
1:A:853:ARG:HH11	1:A:853:ARG:HG2	1.82	0.43
1:A:551:ARG:HB2	6:A:1155:HOH:O	2.18	0.43
1:A:652:VAL:HG21	1:A:909:VAL:HG22	2.00	0.43
1:B:508:VAL:HG23	1:B:509:VAL:H	1.82	0.43
1:A:211:VAL:HG22	1:A:256:CYS:SG	2.59	0.43
1:B:851:LEU:HD23	1:B:851:LEU:N	2.34	0.43
1:A:235:ASN:OD1	1:A:236:ALA:N	2.50	0.43
1:B:98:ASN:HD21	1:B:101:LYS:HD2	1.83	0.43
1:B:539:ARG:NH2	1:B:559:ILE:HD11	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:LYS:HB3	1:B:592:LYS:HE2	1.67	0.43
1:B:680:THR:O	1:B:746:SER:CB	2.62	0.43
1:A:245:ILE:HD11	1:A:257:ILE:HG12	1.99	0.43
1:A:320:PHE:CD2	1:A:361:VAL:HG11	2.54	0.43
1:A:491:MET:O	1:A:495:MET:HG3	2.18	0.43
1:A:721:ILE:HD13	1:A:744:MET:HE1	2.00	0.43
1:B:124:SER:N	6:B:1172:HOH:O	2.51	0.43
1:B:186:VAL:HG22	1:B:206:VAL:HG21	2.00	0.43
1:B:510:LYS:HB3	1:B:512:LEU:HD21	2.01	0.43
1:B:598:LEU:HD23	1:B:598:LEU:C	2.39	0.43
1:B:745:ILE:O	1:B:750:LEU:HG	2.19	0.43
1:B:784:THR:CG2	1:B:864:LEU:HA	2.48	0.43
1:A:26:LEU:HD11	1:A:309:ILE:HG21	2.01	0.43
1:A:422:GLN:CG	1:A:425:ARG:HH21	2.23	0.43
1:A:519:THR:O	1:A:520:PRO:C	2.56	0.43
1:A:755:ARG:HH11	1:A:755:ARG:HG2	1.84	0.43
1:A:632:ASP:C	1:A:632:ASP:OD1	2.56	0.43
1:B:21:LYS:HB3	1:B:21:LYS:HZ2	1.83	0.43
1:B:142:LYS:HA	1:B:142:LYS:HE2	2.00	0.43
1:B:172:THR:HG21	1:B:291:GLN:HE21	1.83	0.43
1:B:492:ARG:CZ	1:B:844:LYS:HG3	2.49	0.43
1:B:563:PRO:CD	1:B:566:ILE:HD12	2.40	0.43
1:A:60:THR:HB	1:A:263:ALA:O	2.18	0.43
1:A:228:LEU:HB3	1:A:412:VAL:HG22	2.01	0.43
1:A:242:LEU:C	1:A:244:HIS:H	2.21	0.43
1:B:389:THR:O	1:B:392:ALA:N	2.51	0.43
1:A:18:GLN:OE1	1:A:366:ASP:O	2.37	0.43
1:A:413:ASP:OD1	1:A:414:GLY:N	2.50	0.43
1:A:614:GLY:O	1:A:632:ASP:HA	2.19	0.43
1:A:845:ILE:CG2	1:A:854:LEU:HD21	2.49	0.43
1:B:107:MET:HE1	1:B:451:LYS:HB2	2.01	0.43
1:B:118:ILE:CD1	1:B:129:HIS:CD2	2.94	0.43
1:B:713:GLY:HA2	1:B:717:CYS:SG	2.59	0.43
1:A:371:VAL:O	1:A:374:VAL:N	2.52	0.42
1:A:619:TRP:HZ2	1:A:625:ALA:HB3	1.83	0.42
1:A:860:VAL:HG12	1:A:861:ASP:N	2.34	0.42
1:B:168:LEU:HD23	1:B:180:VAL:HG12	2.01	0.42
1:B:238:TYR:CE2	1:B:240:GLU:HB2	2.53	0.42
1:B:603:SER:HB2	1:B:621:LYS:HZ1	1.84	0.42
1:B:147:LYS:HD3	1:B:147:LYS:N	2.34	0.42
1:B:426:ARG:NH2	5:B:1007:CIT:H41	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:MET:HB3	1:B:591:ILE:HG12	2.00	0.42
1:A:632:ASP:OD1	1:A:634:VAL:N	2.52	0.42
1:B:66:THR:CG2	1:B:256:CYS:O	2.62	0.42
1:B:167:ILE:HA	1:B:183:ALA:O	2.18	0.42
1:B:217:CYS:SG	1:B:411:GLY:CA	3.07	0.42
1:B:412:VAL:CG1	1:B:413:ASP:N	2.82	0.42
1:B:665:CYS:O	1:B:669:GLU:HB3	2.19	0.42
1:B:796:ALA:O	1:B:799:GLN:HB3	2.19	0.42
1:A:77:LYS:HA	1:A:97:VAL:O	2.20	0.42
1:A:168:LEU:HD22	1:A:180:VAL:HG12	1.98	0.42
1:A:355:ILE:O	1:A:358:ARG:HB2	2.20	0.42
1:A:853:ARG:HG2	1:A:853:ARG:NH1	2.34	0.42
1:B:342:ILE:O	1:B:342:ILE:HG22	2.19	0.42
1:A:97:VAL:HG21	1:A:105:VAL:HG22	2.01	0.42
1:A:730:ASP:OD1	1:A:737:GLY:N	2.45	0.42
1:B:405:ARG:NH1	1:B:438:SER:HA	2.34	0.42
1:B:570:THR:OG1	1:B:573:GLU:HG3	2.20	0.42
1:B:763:LYS:HG3	1:B:772:ILE:HD11	2.02	0.42
1:B:782:PHE:CD1	1:B:786:PHE:CE1	2.93	0.42
1:A:199:TYR:HE2	1:A:201:ALA:HB2	1.83	0.42
1:A:216:THR:HG23	1:A:451:LYS:HB3	2.01	0.42
1:A:484:LEU:HB3	1:A:882:LEU:HD11	2.01	0.42
1:A:598:LEU:HD13	1:A:649:LEU:HD13	2.01	0.42
1:A:639:ASP:O	1:A:643:ARG:HG3	2.20	0.42
1:A:684:ALA:O	1:A:707:MET:HB2	2.18	0.42
1:B:266:ASP:HA	1:B:292:LEU:HD12	2.01	0.42
1:B:693:VAL:HG12	1:B:693:VAL:O	2.20	0.42
1:A:61:VAL:HG12	1:A:63:MET:HG2	2.01	0.42
5:A:1007:CIT:O3	5:A:1007:CIT:O7	2.37	0.42
1:B:211:VAL:HA	1:B:237:CYS:SG	2.59	0.42
1:B:275:THR:O	1:B:277:PHE:N	2.53	0.42
1:B:492:ARG:NH2	1:B:844:LYS:HG3	2.34	0.42
1:B:579:VAL:HA	1:B:582:ILE:CG1	2.49	0.42
1:B:639:ASP:O	1:B:643:ARG:HG3	2.19	0.42
1:B:728:LEU:HD23	1:B:728:LEU:HA	1.83	0.42
1:A:168:LEU:CD2	1:A:180:VAL:CG1	2.95	0.42
1:B:758:LEU:O	1:B:759:ILE:C	2.57	0.42
1:A:67:PHE:CE2	1:A:161:SER:C	2.93	0.42
1:A:168:LEU:HD22	1:A:180:VAL:CG1	2.50	0.42
1:A:347:GLU:OE2	1:A:347:GLU:CA	2.65	0.42
1:A:398:ARG:HG3	1:A:406:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:MET:HE2	1:B:451:LYS:HG3	2.00	0.42
1:B:225:GLU:C	1:B:226:VAL:HG23	2.40	0.42
1:B:545:ILE:HG23	1:B:553:VAL:HG22	2.00	0.42
1:B:669:GLU:HA	1:B:670:PRO:HD2	1.79	0.42
1:A:171:TRP:NE1	1:A:177:ALA:N	2.56	0.42
1:A:486:GLU:O	1:A:490:ARG:HG3	2.20	0.42
1:B:22:ILE:HD11	1:B:370:SER:HB3	2.02	0.42
1:B:46:GLU:HG3	1:B:264:PHE:CE1	2.55	0.42
1:B:489:LYS:O	1:B:492:ARG:HB3	2.20	0.42
1:B:583:SER:HB2	1:B:647:PHE:CE2	2.51	0.42
1:B:683:ASN:HB3	2:B:1003:BGC:H5	2.02	0.42
1:B:795:LEU:HD11	1:B:799:GLN:HG2	2.01	0.42
1:A:245:ILE:HD11	1:A:257:ILE:CG1	2.50	0.41
1:A:378:VAL:O	1:A:381:ARG:HB3	2.20	0.41
1:A:510:LYS:HA	1:A:510:LYS:HD3	1.61	0.41
1:A:652:VAL:O	1:A:653:ALA:HB2	2.20	0.41
1:A:795:LEU:CD1	1:A:799:GLN:HG2	2.39	0.41
1:B:249:GLU:HB3	1:B:797:LEU:HD12	2.01	0.41
1:B:853:ARG:HA	1:B:885:LYS:O	2.20	0.41
1:A:147:LYS:H	1:A:147:LYS:HG2	1.47	0.41
1:A:615:ILE:HA	1:A:631:HIS:O	2.20	0.41
1:B:119:VAL:CG1	1:B:174:ARG:O	2.68	0.41
1:B:649:LEU:C	1:B:649:LEU:CD1	2.87	0.41
1:B:712:PHE:HE1	1:B:717:CYS:HG	1.63	0.41
1:B:797:LEU:HD11	1:B:817:ILE:HD11	2.01	0.41
1:B:856:VAL:O	1:B:856:VAL:HG13	2.21	0.41
1:B:897:SER:O	1:B:898:GLY:C	2.57	0.41
1:A:81:ILE:HG13	1:A:148:LEU:HD13	2.03	0.41
1:A:230:ILE:HB	1:A:417:TYR:HB2	2.01	0.41
1:A:515:PHE:HA	1:A:703:MET:SD	2.60	0.41
1:A:607:GLN:HB2	1:A:617:ILE:HD11	2.02	0.41
1:A:755:ARG:HG2	1:A:755:ARG:NH1	2.35	0.41
1:A:907:VAL:O	1:A:911:LEU:HG	2.19	0.41
1:B:91:ARG:HB2	1:B:91:ARG:HH11	1.84	0.41
1:B:174:ARG:HG2	1:B:300:MET:CE	2.50	0.41
1:B:263:ALA:O	1:B:266:ASP:CG	2.58	0.41
1:B:315:LYS:HG2	1:B:324:ILE:HD13	1.98	0.41
1:B:539:ARG:HB2	1:B:558:LYS:O	2.20	0.41
1:A:407:ARG:HG2	1:A:439:ASP:HB2	2.02	0.41
1:A:425:ARG:NH2	1:A:426:ARG:HE	2.18	0.41
1:A:693:VAL:C	1:A:695:MET:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:MET:O	1:A:708:GLU:HB2	2.21	0.41
1:A:331:ARG:HD2	1:B:588:TYR:CE2	2.55	0.41
1:B:306:VAL:O	1:B:309:ILE:N	2.53	0.41
1:B:384:ASN:HD22	1:B:384:ASN:HA	1.57	0.41
1:B:539:ARG:HH11	1:B:557:ASN:HD21	1.65	0.41
1:B:584:ASP:O	1:B:587:ASP:HB2	2.20	0.41
1:B:813:CYS:O	1:B:814:ASP:C	2.57	0.41
1:B:907:VAL:HG21	6:B:1158:HOH:O	2.20	0.41
1:A:85:LEU:O	1:A:155:SER:OG	2.38	0.41
1:A:107:MET:HE3	1:A:451:LYS:HE2	2.03	0.41
1:A:258:ASN:OD1	1:A:258:ASN:C	2.59	0.41
1:A:700:GLN:HE21	1:A:700:GLN:HA	1.85	0.41
1:A:790:ILE:H	1:A:790:ILE:HG12	1.74	0.41
1:B:700:GLN:HG3	6:B:1161:HOH:O	2.20	0.41
1:A:315:LYS:CA	1:A:324:ILE:HD11	2.42	0.41
1:A:724:HIS:HA	1:A:727:ARG:NH1	2.36	0.41
1:A:786:PHE:HD1	1:A:787:LEU:N	2.18	0.41
1:B:343:GLU:HG3	1:B:420:HIS:HE1	1.86	0.41
1:A:48:LYS:HB2	1:A:48:LYS:HE3	1.77	0.41
1:A:81:ILE:HB	1:A:150:VAL:HG22	2.01	0.41
1:A:912:ARG:HG3	1:A:912:ARG:HH11	1.84	0.41
1:B:217:CYS:SG	1:B:411:GLY:HA3	2.61	0.41
1:B:347:GLU:CB	1:B:351:ASN:HD21	2.22	0.41
1:B:418:LYS:HD2	6:B:1151:HOH:O	2.20	0.41
1:B:595:ARG:CD	1:B:648:ASP:OD2	2.69	0.41
1:B:664:THR:OG1	1:B:900:GLY:N	2.50	0.41
1:A:151:GLY:HA3	1:A:457:THR:OG1	2.21	0.41
1:A:560:TYR:OH	1:A:585:PHE:HB2	2.21	0.41
1:A:619:TRP:CZ2	1:A:625:ALA:HB3	2.55	0.41
1:B:266:ASP:HA	1:B:292:LEU:CD1	2.50	0.41
1:B:342:ILE:HG22	1:B:372:GLN:HG3	2.03	0.41
1:B:501:LYS:HB3	1:B:695:MET:SD	2.60	0.41
1:B:539:ARG:HB3	1:B:559:ILE:HD13	2.03	0.41
1:B:578:ILE:C	1:B:582:ILE:HG12	2.41	0.41
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.81	0.41
1:A:255:MET:HG3	1:A:256:CYS:N	2.36	0.41
1:A:259:THR:O	1:A:260:GLU:HB2	2.20	0.41
1:B:213:THR:HG22	1:B:214:MET:N	2.36	0.41
1:B:376:THR:O	1:B:380:PHE:HB2	2.21	0.41
1:B:383:ALA:HA	1:B:423:TYR:CZ	2.56	0.41
1:A:93:LEU:HD11	1:A:450:GLY:CA	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASN:O	1:A:211:VAL:N	2.54	0.40
1:A:265:GLY:C	1:A:267:ASP:H	2.25	0.40
1:B:168:LEU:CD2	1:B:180:VAL:HG12	2.51	0.40
1:B:640:ALA:HB2	1:B:643:ARG:HH21	1.85	0.40
1:B:786:PHE:CE2	1:B:807:LEU:CD1	3.04	0.40
1:A:185:VAL:HG23	1:A:186:VAL:N	2.36	0.40
1:A:203:ILE:HD13	1:A:203:ILE:H	1.87	0.40
1:A:226:VAL:HB	1:A:410:VAL:HG22	2.04	0.40
1:A:480:THR:CG2	1:A:483:MET:CE	2.92	0.40
1:B:579:VAL:HA	1:B:582:ILE:HG12	2.03	0.40
1:B:637:LEU:HD23	1:B:651:VAL:HG21	2.04	0.40
1:A:80:PHE:HE2	1:A:458:ALA:HA	1.84	0.40
1:A:361:VAL:CG2	1:A:361:VAL:O	2.70	0.40
1:A:531:LEU:HD13	1:A:598:LEU:HD11	2.03	0.40
1:B:541:LEU:HD13	1:B:898:GLY:HA2	2.04	0.40
1:B:751:GLY:HA3	1:B:782:PHE:O	2.22	0.40
1:A:683:ASN:OD1	1:A:684:ALA:N	2.51	0.40
1:A:809:LEU:HD23	1:A:809:LEU:HA	1.94	0.40
1:A:912:ARG:C	1:A:914:GLU:N	2.74	0.40
1:B:62:LYS:O	1:B:63:MET:HB2	2.21	0.40
1:B:467:HIS:O	1:B:470:ILE:N	2.55	0.40
1:B:772:ILE:O	1:B:773:SER:C	2.59	0.40
1:B:831:ALA:HA	1:B:871:PHE:CZ	2.55	0.40
1:A:142:LYS:HB3	1:A:142:LYS:HE2	1.90	0.40
1:A:234:THR:H	1:A:294:GLU:HG3	1.86	0.40
1:A:467:HIS:O	1:A:468:ARG:C	2.60	0.40
1:A:488:LYS:O	1:A:491:MET:HB3	2.22	0.40
1:A:691:LYS:CA	1:A:699:ASP:HB2	2.47	0.40
1:B:230:ILE:CD1	1:B:386:VAL:HG11	2.43	0.40
1:B:339:VAL:O	1:B:339:VAL:HG12	2.22	0.40
1:B:422:GLN:HB3	1:B:426:ARG:NE	2.37	0.40
1:B:579:VAL:CG2	1:B:640:ALA:HB3	2.51	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	897/917 (98%)	794 (88%)	97 (11%)	6 (1%)	22	60
1	B	897/917 (98%)	777 (87%)	114 (13%)	6 (1%)	22	60
All	All	1794/1834 (98%)	1571 (88%)	211 (12%)	12 (1%)	22	60

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ILE
1	A	251	ASP
1	A	694	GLU
1	A	307	ARG
1	B	276	GLU
1	B	307	ARG
1	B	781	ILE
1	B	694	GLU
1	B	717	CYS
1	A	155	SER
1	A	594	PRO
1	B	693	VAL

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	774/788 (98%)	726 (94%)	48 (6%)	18	52
1	B	774/788 (98%)	732 (95%)	42 (5%)	22	57
All	All	1548/1576 (98%)	1458 (94%)	90 (6%)	20	55

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	27	TYR
1	A	80	PHE
1	A	93	LEU
1	A	96	GLN
1	A	102	ASN
1	A	147	LYS
1	A	159	GLN
1	A	163	ILE
1	A	165	GLU
1	A	174	ARG
1	A	202	ASN
1	A	203	ILE
1	A	208	ASN
1	A	213	THR
1	A	222	GLN
1	A	232	THR
1	A	249	GLU
1	A	261	TRP
1	A	269	SER
1	A	281	ILE
1	A	305	LEU
1	A	321	GLU
1	A	358	ARG
1	A	399	ASP
1	A	408	THR
1	A	422	GLN
1	A	481	LYS
1	A	508	VAL
1	A	512	LEU
1	A	550	LYS
1	A	565	GLU
1	A	566	ILE
1	A	570	THR
1	A	596	MET
1	A	609	THR
1	A	665	CYS
1	A	703	MET
1	A	709	TRP
1	A	714	ASP
1	A	767	LEU
1	A	769	ARG
1	A	781	ILE

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Mol	Chain	Res	Type
1	A	786	PHE
1	A	792	SER
1	A	810	ASN
1	A	854	LEU
1	A	887	ASN
1	B	41	THR
1	B	93	LEU
1	B	99	HIS
1	B	102	ASN
1	B	114	THR
1	B	116	GLU
1	B	147	LYS
1	B	170	THR
1	B	213	THR
1	B	249	GLU
1	B	261	TRP
1	B	281	ILE
1	B	318	LEU
1	B	320	PHE
1	B	321	GLU
1	B	345	ASN
1	B	346	LYS
1	B	347	GLU
1	B	379	SER
1	B	380	PHE
1	B	382	SER
1	B	405	ARG
1	B	424	SER
1	B	432	ARG
1	B	437	ASP
1	B	481	LYS
1	B	531	LEU
1	B	562	ILE
1	B	591	ILE
1	B	669	GLU
1	B	703	MET
1	B	709	TRP
1	B	721	ILE
1	B	769	ARG
1	B	771	GLN
1	B	775	THR
1	B	777	LYS

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Mol	Chain	Res	Type
1	B	786	PHE
1	B	798	LEU
1	B	805	GLN
1	B	854	LEU
1	B	872	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	102	ASN
1	A	104	ASN
1	A	125	GLN
1	A	159	GLN
1	A	190	ASN
1	A	208	ASN
1	A	258	ASN
1	A	373	HIS
1	A	384	ASN
1	A	400	ASN
1	A	466	GLN
1	A	506	ASN
1	A	557	ASN
1	A	700	GLN
1	A	771	GLN
1	A	799	GLN
1	A	805	GLN
1	A	806	GLN
1	A	810	ASN
1	A	887	ASN
1	B	18	GLN
1	B	98	ASN
1	B	99	HIS
1	B	120	HIS
1	B	125	GLN
1	B	129	HIS
1	B	202	ASN
1	B	351	ASN
1	B	384	ASN
1	B	400	ASN
1	B	420	HIS
1	B	466	GLN

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Mol	Chain	Res	Type
1	B	469	GLN
1	B	502	GLN
1	B	506	ASN
1	B	557	ASN
1	B	607	GLN
1	B	771	GLN
1	B	799	GLN
1	B	805	GLN
1	B	806	GLN
1	B	832	GLN
1	B	848	ASN
1	B	870	HIS
1	B	887	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BGC	A	1001	-	12,12,12	0.38	0	17,17,17	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BGC	B	1003	-	12,12,12	0.46	0	17,17,17	1.34	2 (11%)
3	0WK	B	1002	-	15,15,15	0.45	0	22,22,22	0.78	0
5	CIT	B	1007	-	12,12,12	1.00	0	17,17,17	1.46	1 (5%)
2	BGC	A	1003	-	12,12,12	0.31	0	17,17,17	1.40	2 (11%)
5	CIT	A	1007	-	12,12,12	1.00	0	17,17,17	1.64	1 (5%)
3	0WK	A	1004	-	15,15,15	0.48	0	22,22,22	0.79	0
3	0WK	B	1004	-	15,15,15	0.43	0	22,22,22	0.85	0
3	0WK	A	1002	-	15,15,15	0.46	0	22,22,22	0.94	0
2	BGC	B	1001	-	12,12,12	0.34	0	17,17,17	0.94	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
2	BGC	B	1003	-	-	0/2/22/22	0/1/1/1
3	0WK	B	1002	-	-	2/6/23/23	0/1/1/1
5	CIT	B	1007	-	-	9/16/16/16	-
2	BGC	A	1003	-	-	2/2/22/22	0/1/1/1
5	CIT	A	1007	-	-	9/16/16/16	-
3	0WK	A	1004	-	-	4/6/23/23	0/1/1/1
3	0WK	B	1004	-	-	4/6/23/23	0/1/1/1
3	0WK	A	1002	-	-	2/6/23/23	0/1/1/1
2	BGC	B	1001	-	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1007	CIT	O6-C6-C3	4.61	121.06	113.05
5	B	1007	CIT	O6-C6-C3	3.98	119.97	113.05
2	A	1003	BGC	O5-C1-C2	-3.69	103.70	110.28
2	B	1003	BGC	O5-C1-C2	-3.54	103.96	110.28
2	A	1001	BGC	C6-C5-C4	-3.06	105.83	113.00
2	B	1003	BGC	C1-O5-C5	-2.83	108.32	113.66
2	A	1003	BGC	C6-C5-C4	-2.66	106.78	113.00
2	B	1001	BGC	C1-O5-C5	-2.23	109.46	113.66

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	0WK	C6-O6-P-O2P
3	A	1004	0WK	C6-O6-P-O2P
3	A	1004	0WK	C6-O6-P-O3P
3	B	1004	0WK	C6-O6-P-O3P
5	A	1007	CIT	C2-C3-C4-C5
5	A	1007	CIT	O7-C3-C4-C5
5	A	1007	CIT	C6-C3-C4-C5
5	A	1007	CIT	O7-C3-C6-O5
5	A	1007	CIT	O7-C3-C6-O6
5	B	1007	CIT	O7-C3-C6-O5
5	B	1007	CIT	O7-C3-C6-O6
5	B	1007	CIT	C4-C3-C6-O5
5	B	1007	CIT	C4-C3-C6-O6
2	B	1001	BGC	O5-C5-C6-O6
3	A	1002	0WK	C5-C6-O6-P
2	B	1001	BGC	C4-C5-C6-O6
2	A	1003	BGC	O5-C5-C6-O6
3	B	1002	0WK	C5-C6-O6-P
2	A	1003	BGC	C4-C5-C6-O6
5	A	1007	CIT	C2-C3-C6-O6
5	A	1007	CIT	C4-C3-C6-O5
5	B	1007	CIT	C1-C2-C3-C6
3	A	1004	0WK	C6-O6-P-O1P
5	B	1007	CIT	C1-C2-C3-O7
5	A	1007	CIT	C4-C3-C6-O6
3	B	1004	0WK	C6-O6-P-O2P
5	B	1007	CIT	C1-C2-C3-C4
3	B	1004	0WK	C5-C6-O6-P
3	A	1004	0WK	C5-C6-O6-P
3	B	1004	0WK	C6-O6-P-O1P
5	A	1007	CIT	C2-C3-C6-O5
3	B	1002	0WK	C6-O6-P-O2P
5	B	1007	CIT	C6-C3-C4-C5
5	B	1007	CIT	O7-C3-C4-C5

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	BGC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1003	BGC	1	0
5	B	1007	CIT	4	0
2	A	1003	BGC	3	0
5	A	1007	CIT	1	0
3	B	1004	0WK	1	0
3	A	1002	0WK	2	0
2	B	1001	BGC	3	0

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	899/917 (98%)	-0.30	4 (0%)	92	79	45, 76, 106, 143	0
1	B	899/917 (98%)	-0.35	2 (0%)	95	87	44, 76, 106, 143	0
All	All	1798/1834 (98%)	-0.32	6 (0%)	94	84	44, 76, 106, 143	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	ASP	3.6
1	A	29	MET	3.6
1	A	310	LEU	3.3
1	A	26	LEU	2.9
1	A	16	ASP	2.8
1	B	548	GLY	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CIT	B	1007	13/13	0.68	0.27	124,126,127,127	0
5	CIT	A	1007	13/13	0.74	0.41	127,127,129,129	0
4	NA	A	1005	1/1	0.89	0.09	74,74,74,74	0
4	NA	B	1005	1/1	0.90	0.12	77,77,77,77	0
2	BGC	B	1001	12/12	0.91	0.31	78,79,79,80	0
4	NA	B	1006	1/1	0.92	0.08	54,54,54,54	0
2	BGC	A	1001	12/12	0.92	0.50	80,81,81,82	0
2	BGC	B	1003	12/12	0.92	0.26	53,55,56,56	0
3	0WK	A	1002	15/15	0.94	0.32	79,80,80,80	0
2	BGC	A	1003	12/12	0.95	0.21	51,54,55,56	0
4	NA	A	1006	1/1	0.95	0.05	55,55,55,55	0
3	0WK	B	1002	15/15	0.95	0.21	77,78,78,78	0
3	0WK	A	1004	15/15	0.96	0.22	59,60,61,61	0
3	0WK	B	1004	15/15	0.96	0.29	60,60,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.