Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 12:09 AM JST

PDB ID	:	5YIL
Title	:	Hoisting-loop in bacterial multidrug exporter AcrB is a highly flexible hinge that enables the large motion of the subdomains
Authors	:	Zwama, M.; Sakurai, K.; Hayashi, K.; Nakashima, R.; Kitagawa, K.; Nishino, K.; Yamaguchi, A.
Deposited on	:	2017-10-05
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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

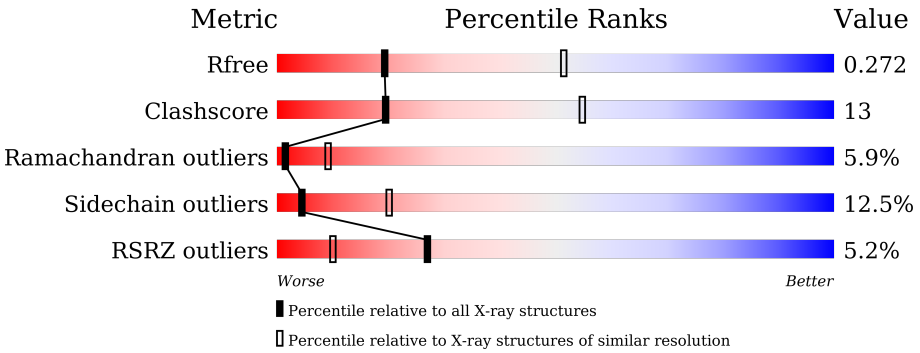
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	1050	4% 72% 24%
1	B	1050	6% 65% 28%
1	C	1050	6% 58% 33% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23566 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1041	Total	C	N	O	S	0	0	0
			7918	5091	1310	1473	44			
1	B	1030	Total	C	N	O	S	0	0	0
			7824	5037	1290	1453	44			
1	C	1030	Total	C	N	O	S	0	0	0
			7824	5037	1290	1453	44			

There are 12 discrepancies between the modelled and reference sequences:

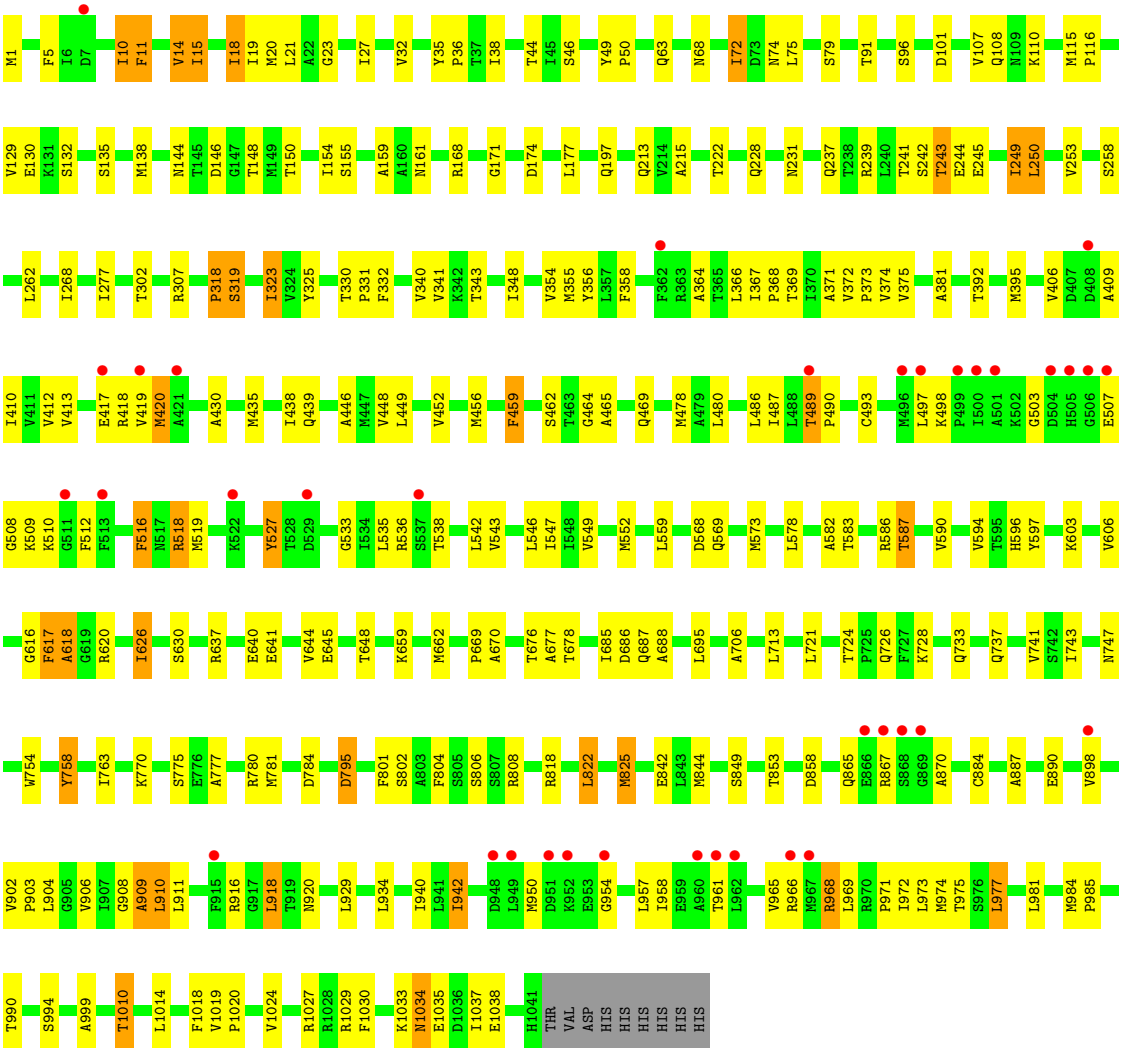
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P31224
A	1048	HIS	-	expression tag	UNP P31224
A	1049	HIS	-	expression tag	UNP P31224
A	1050	HIS	-	expression tag	UNP P31224
B	1047	HIS	-	expression tag	UNP P31224
B	1048	HIS	-	expression tag	UNP P31224
B	1049	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
C	1047	HIS	-	expression tag	UNP P31224
C	1048	HIS	-	expression tag	UNP P31224
C	1049	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224

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.

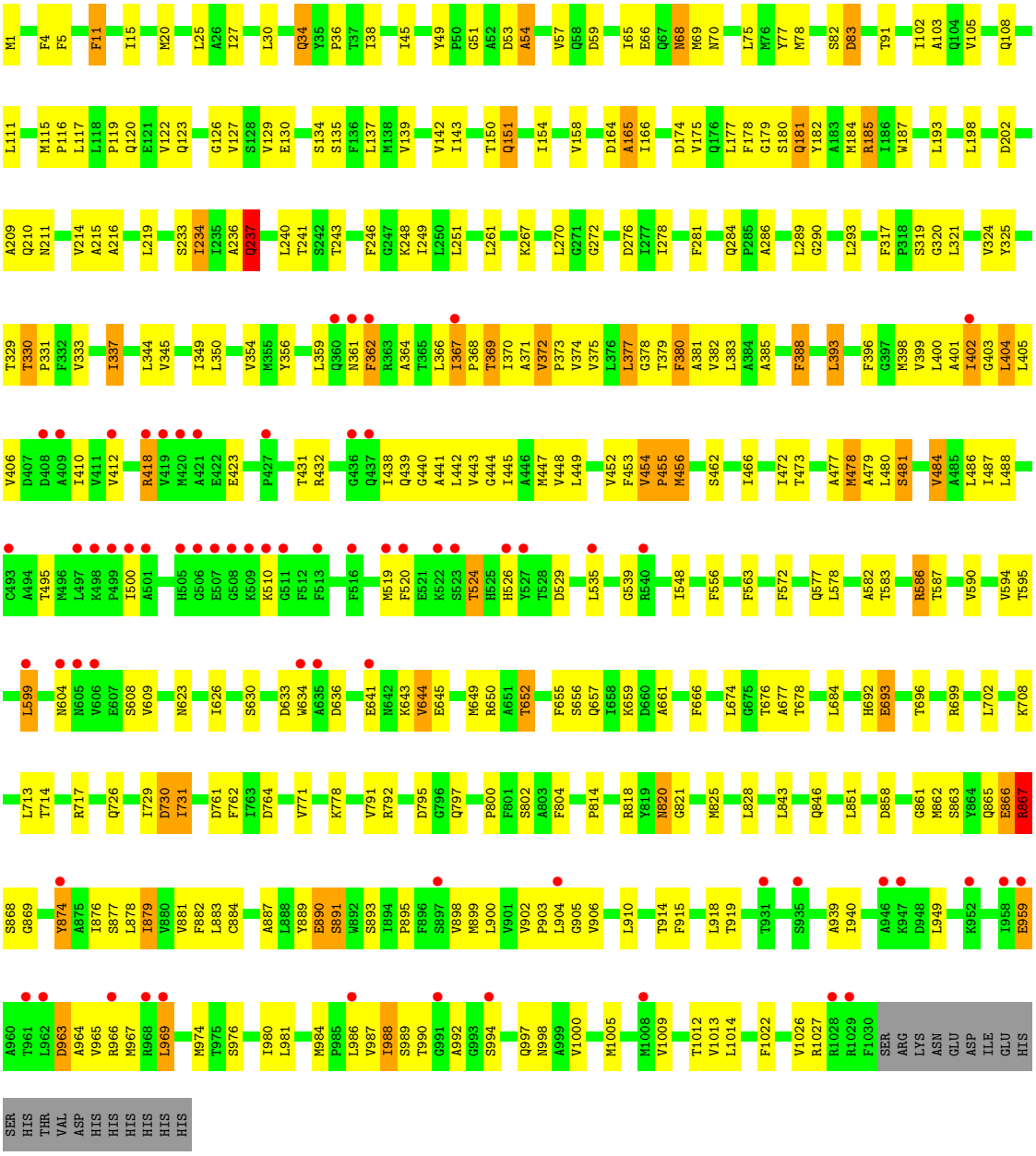
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:

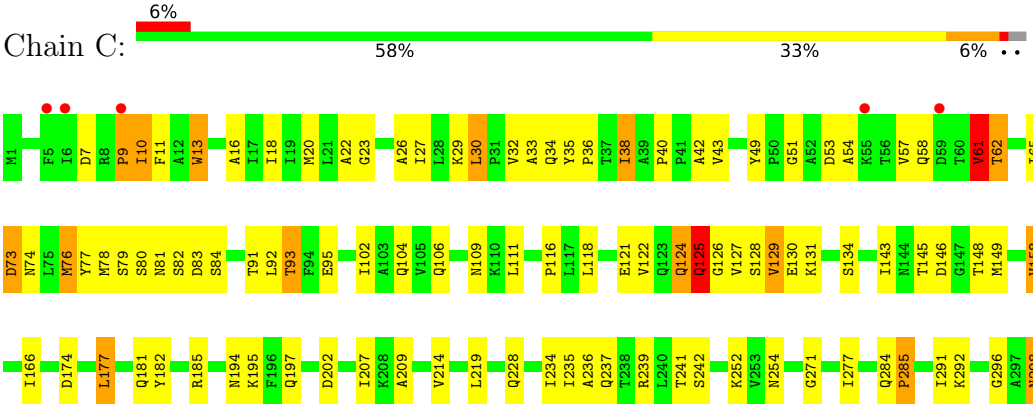


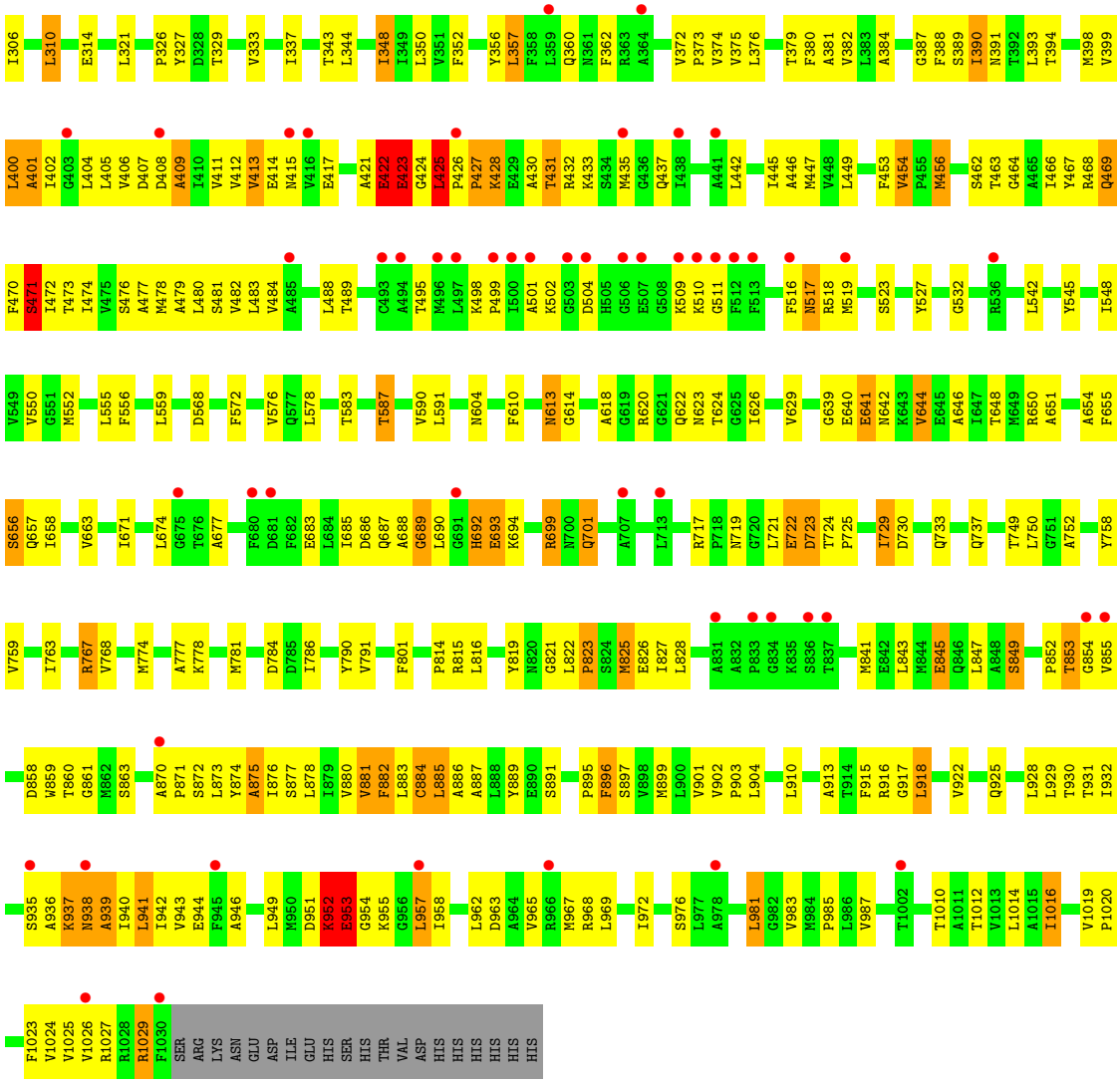
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain B:



• Molecule 1: Multidrug efflux pump subunit AcrB




I306 L310 E314 L321 P326 Y327 D328 T329 V333 I337 T343 L344 I348 I349 L350 V351 F352 Y356 L357 F358 L359 Q360 N361 F362 R363 A364 V372 P373 V374 V375 L376 T379 F380 A381 V382 L383 A384 G387 F388 S389 I390 N391 T392 L393 T394 M398 V399
L400 A401 I402 G403 L404 L405 V406 D407 D408 A409 I410 V411 V412 V413 E414 N415 V416 E417 A421 E422 E423 G424 L425 P426 P427 K428 E429 A430 T431 R432 K433 S434 M435 G436 Q437 I438 A441 L442 I445 A446 M447 V448 L449 F453 V454 P455 M456 S462 T463 G464 A465 I466 Y467 R468 Q469
F470 S471 I472 T473 I474 V475 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L488 T489 C493 A494 T495 N496 L497 K498 P499 I500 A501 K502 G503 D504 H505 G506 E507 G508 K509 K510 G511 F512 F513 F516 N517 R518 M519 S523 Y527 G532 R536 L542 Y545 I548
V549 V550 G551 M552 L555 F556 L559 D568 F572 V576 Q577 L578 T583 T587 V590 L591 N604 F610 N613 G614 A618 G619 R620 G621 Q622 N623 T624 G625 I626 V629 G639 E640 E641 N642 K643 V644 E645 A646 I647 T648 M649 R650 A651 A654 F655
S656 Q657 I658 V663 I671 L674 G675 T676 A677 F680 D681 F682 E683 L684 I685 D686 Q687 A688 G689 L690 G691 H692 E693 K694 R699 N700 Q701 A707 L713 R717 P718 N719 G720 L721 E722 D723 T724 P725 I729 D730 Q733 Q737 T749 L750 G751 A752 Y758
V759 I763 R767 V768 M774 A777 K778 M781 D784 D785 I786 Y790 V791 F801 P814 R815 L816 Y819 N820 G821 L822 P823 S824 R825 E826 I827 L828 A831 A832 P833 G834 K835 S836 T837 M841 E842 L843 M844 E845 Q846 L847 A848 S849 P852 T853 G854 V855
D858 W859 T860 G861 M862 S863 A870 P871 S872 L873 Y874 A875 I876 S877 L878 I879 V880 V881 F882 L883 C884 L885 A886 A887 L888 Y889 E890 S891 P895 F896 S897 V898 M899 L900 V901 V902 P903 L904 L910 A913 Y914 F915 R916 G917 L918 V922 Q925 L928 L929 T930 T931 I932
S935 A936 K937 N938 A939 I940 L941 I942 V943 E944 F945 A946 L949 M950 D951 K952 E953 G954 K955 G956 L957 I958 L962 D963 A964 V965 R966 M967 R968 L969 I972 S976 L977 A978 L981 G982 V983 M984 P985 L986 V987 T1002 T1010 A1011 T1012 V1013 L1014 A1015 I1016 V1019 P1020
F1023 V1024 V1025 V1026 R1027 R1028 R1029 F1030 SER ARG LYS ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.98Å 139.81Å 285.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 98.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (100.00-3.00) 94.5 (98.45-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.224 , 0.273 0.226 , 0.272	Depositor DCC
R_{free} test set	5112 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	67.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 74.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23566	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.69	0/8070	0.86	0/10957
1	B	0.64	0/7974	0.83	0/10829
1	C	0.69	0/7974	0.89	2/10829 (0.0%)
All	All	0.67	0/24018	0.86	2/32615 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	128	SER	CB-CA-C	-6.51	97.73	110.10
1	C	131	LYS	N-CA-C	-5.49	96.18	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7918	0	8059	127	0
1	B	7824	0	7976	221	0
1	C	7824	0	7976	283	0
All	All	23566	0	24011	608	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 13.

All (608) 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:344:LEU:HD23	1:B:402:ILE:CD1	1.46	1.45
1:B:449:LEU:HB3	1:B:478:MET:CE	1.52	1.37
1:B:344:LEU:CD2	1:B:402:ILE:CD1	2.18	1.20
1:B:344:LEU:CD2	1:B:402:ILE:HD11	1.79	1.12
1:B:449:LEU:HB3	1:B:478:MET:HE2	1.23	1.10
1:B:449:LEU:CB	1:B:478:MET:HE1	1.82	1.09
1:C:568:ASP:OD1	1:C:644:VAL:HG23	1.52	1.07
1:B:449:LEU:CB	1:B:478:MET:CE	2.33	1.04
1:B:404:LEU:H	1:B:404:LEU:HD12	1.22	1.02
1:B:344:LEU:HD23	1:B:402:ILE:HD13	0.98	0.97
1:B:449:LEU:HB3	1:B:478:MET:HE1	1.37	0.96
1:B:445:ILE:HG23	1:B:449:LEU:HG	1.47	0.94
1:B:731:ILE:HD13	1:B:731:ILE:H	1.30	0.93
1:B:180:SER:O	1:B:181:GLN:O	1.87	0.92
1:B:344:LEU:HD21	1:B:402:ILE:HD11	1.51	0.92
1:C:130:GLU:OE1	1:C:174:ASP:OD2	1.89	0.90
1:C:446:ALA:HB2	1:C:482:VAL:HG11	1.52	0.88
1:C:940:ILE:O	1:C:944:GLU:HB2	1.76	0.86
1:C:885:LEU:HD12	1:C:886:ALA:N	1.89	0.86
1:B:344:LEU:CD2	1:B:402:ILE:HD13	1.93	0.82
1:B:375:VAL:O	1:B:379:THR:HG23	1.80	0.80
1:B:445:ILE:O	1:B:449:LEU:HB2	1.80	0.80
1:A:410:ILE:HD11	1:A:975:THR:HG23	1.61	0.80
1:A:38:ILE:HD13	1:A:465:ALA:HB3	1.62	0.80
1:B:445:ILE:CG2	1:B:449:LEU:HG	2.13	0.78
1:B:449:LEU:CD1	1:B:478:MET:CE	2.63	0.77
1:B:449:LEU:HB2	1:B:478:MET:HE1	1.66	0.76
1:C:881:VAL:HA	1:C:884:CYS:SG	2.27	0.75
1:C:951:ASP:HB3	1:C:952:LYS:HZ2	1.52	0.75
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.22	0.75
1:C:872:SER:O	1:C:876:ILE:HG12	1.87	0.75
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.69	0.74
1:B:449:LEU:CB	1:B:478:MET:HE2	2.11	0.74
1:B:445:ILE:O	1:B:449:LEU:N	2.19	0.73
1:C:422:GLU:OE2	1:C:423:GLU:N	2.21	0.73
1:C:30:LEU:HD22	1:C:390:ILE:HG13	1.71	0.73
1:C:641:GLU:O	1:C:650:ARG:NH2	2.22	0.73
1:C:952:LYS:HE3	1:C:952:LYS:HA	1.69	0.73
1:C:104:GLN:NE2	1:C:129:VAL:O	2.22	0.72
1:C:952:LYS:O	1:C:954:GLY:N	2.23	0.72
1:B:454:VAL:O	1:B:456:MET:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:940:ILE:O	1:C:944:GLU:CB	2.37	0.71
1:B:174:ASP:C	1:B:175:VAL:HG13	2.11	0.71
1:B:401:ALA:HA	1:B:404:LEU:CD1	2.21	0.71
1:B:454:VAL:HB	1:B:455:PRO:HD3	1.71	0.71
1:C:27:ILE:HD11	1:C:380:PHE:CD2	2.26	0.71
1:B:404:LEU:HD12	1:B:404:LEU:N	2.03	0.70
1:B:889:TYR:O	1:B:891:SER:N	2.24	0.70
1:B:641:GLU:O	1:B:650:ARG:NH1	2.25	0.70
1:C:36:PRO:O	1:C:38:ILE:N	2.25	0.69
1:C:61:VAL:O	1:C:62:THR:OG1	2.08	0.69
1:C:425:LEU:HB2	1:C:426:PRO:HD2	1.74	0.69
1:C:885:LEU:HD11	1:C:895:PRO:HG3	1.73	0.69
1:B:180:SER:O	1:B:181:GLN:C	2.30	0.69
1:B:449:LEU:HD13	1:B:478:MET:HE2	1.74	0.69
1:B:449:LEU:HD13	1:B:478:MET:CE	2.23	0.68
1:C:427:PRO:O	1:C:430:ALA:N	2.27	0.67
1:A:44:THR:HG22	1:A:91:THR:HG23	1.76	0.67
1:A:348:ILE:HD11	1:A:372:VAL:HG11	1.75	0.67
1:C:36:PRO:O	1:C:38:ILE:HG23	1.93	0.67
1:C:298:ASN:O	1:C:301:ASP:N	2.28	0.67
1:C:901:VAL:HG21	1:C:939:ALA:HB2	1.76	0.67
1:A:249:ILE:O	1:A:250:LEU:HB3	1.95	0.67
1:B:174:ASP:C	1:B:175:VAL:CG1	2.64	0.66
1:A:695:LEU:HD23	1:A:825:MET:SD	2.36	0.66
1:B:174:ASP:O	1:B:175:VAL:CG1	2.43	0.66
1:B:234:ILE:HD11	1:C:729:ILE:HG21	1.78	0.66
1:C:976:SER:HB3	1:C:1012:THR:HG21	1.77	0.66
1:C:692:HIS:O	1:C:694:LYS:N	2.29	0.65
1:C:882:PHE:CE2	1:C:883:LEU:HD21	2.32	0.65
1:A:412:VAL:HG12	1:A:438:ILE:HD12	1.77	0.65
1:B:444:GLY:O	1:B:448:VAL:N	2.25	0.65
1:B:898:VAL:HG11	1:B:940:ILE:HG13	1.79	0.65
1:B:990:THR:HG23	1:B:998:ASN:HD21	1.62	0.65
1:C:940:ILE:O	1:C:944:GLU:N	2.30	0.65
1:B:379:THR:OG1	1:B:398:MET:HE3	1.97	0.64
1:B:372:VAL:HG12	1:B:373:PRO:HD3	1.80	0.64
1:C:376:LEU:HD22	1:C:398:MET:HG2	1.80	0.64
1:B:174:ASP:O	1:B:175:VAL:HG12	1.98	0.64
1:B:478:MET:O	1:B:481:SER:N	2.30	0.64
1:B:379:THR:HG21	1:B:477:ALA:HA	1.78	0.63
1:B:236:ALA:HB2	1:C:729:ILE:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:SER:O	1:C:292:LYS:HE2	1.98	0.63
1:B:401:ALA:C	1:B:403:GLY:H	2.02	0.63
1:C:36:PRO:HG2	1:C:469:GLN:NE2	2.14	0.63
1:C:129:VAL:O	1:C:129:VAL:HG12	1.97	0.63
1:B:478:MET:SD	1:B:479:ALA:N	2.72	0.62
1:C:415:ASN:OD1	1:C:968:ARG:NH2	2.32	0.62
1:C:54:ALA:CB	1:C:816:LEU:HD12	2.29	0.62
1:C:425:LEU:HB2	1:C:426:PRO:CD	2.29	0.62
1:A:228:GLN:O	1:B:583:THR:HG21	1.99	0.61
1:C:843:LEU:HD23	1:C:847:LEU:HD13	1.82	0.61
1:A:72:ILE:N	1:A:72:ILE:HD12	2.15	0.61
1:B:38:ILE:HG22	1:B:462:SER:OG	2.01	0.61
1:C:877:SER:O	1:C:881:VAL:HG22	2.00	0.61
1:B:444:GLY:O	1:B:448:VAL:HB	1.99	0.61
1:B:583:THR:HG22	1:B:586:ARG:HG3	1.81	0.61
1:C:885:LEU:HD11	1:C:895:PRO:CB	2.29	0.61
1:C:613:ASN:HD22	1:C:614:GLY:N	1.99	0.61
1:B:548:ILE:HD12	1:B:904:LEU:HD22	1.82	0.60
1:B:443:VAL:O	1:B:443:VAL:HG12	2.01	0.60
1:B:449:LEU:CD1	1:B:478:MET:SD	2.90	0.60
1:B:643:LYS:O	1:B:645:GLU:N	2.34	0.60
1:C:655:PHE:O	1:C:658:ILE:HG13	2.02	0.60
1:C:969:LEU:HA	1:C:972:ILE:HG22	1.83	0.60
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.84	0.60
1:A:277:ILE:HD11	1:A:620:ARG:HD2	1.84	0.60
1:C:143:ILE:HD12	1:C:284:GLN:HE22	1.67	0.60
1:B:77:TYR:HA	1:B:820:ASN:HD21	1.66	0.60
1:C:423:GLU:O	1:C:425:LEU:HD12	2.02	0.60
1:C:425:LEU:HD22	1:C:426:PRO:HD2	1.82	0.60
1:B:158:VAL:CG1	1:B:289:LEU:HD13	2.32	0.59
1:C:885:LEU:HD11	1:C:895:PRO:CG	2.31	0.59
1:B:139:VAL:HG13	1:B:178:PHE:HE2	1.67	0.59
1:B:599:LEU:O	1:B:599:LEU:HD12	2.03	0.59
1:C:431:THR:O	1:C:433:LYS:N	2.35	0.59
1:C:722:GLU:O	1:C:723:ASP:O	2.19	0.59
1:B:350:LEU:HD23	1:B:981:LEU:HB3	1.85	0.59
1:C:957:LEU:HD23	1:C:958:ILE:HG13	1.83	0.59
1:C:54:ALA:HB3	1:C:816:LEU:HD12	1.85	0.59
1:C:35:TYR:CE2	1:C:671:ILE:HG22	2.37	0.59
1:C:641:GLU:O	1:C:646:ALA:HB3	2.02	0.59
1:C:613:ASN:HD22	1:C:613:ASN:C	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:HA	1:B:377:LEU:HD21	1.86	0.58
1:C:724:THR:HG22	1:C:814:PRO:HD3	1.86	0.58
1:C:901:VAL:HG22	1:C:1019:VAL:HG22	1.85	0.58
1:B:452:VAL:HG13	1:B:453:PHE:N	2.19	0.58
1:B:963:ASP:HA	1:B:966:ARG:HB3	1.86	0.58
1:B:380:PHE:CE1	1:B:398:MET:HE2	2.39	0.57
1:B:403:GLY:O	1:B:406:VAL:N	2.37	0.57
1:B:379:THR:CG2	1:B:477:ALA:HA	2.34	0.57
1:C:149:MET:CE	1:C:321:LEU:HD13	2.33	0.57
1:C:699:ARG:HG3	1:C:827:ILE:HD11	1.85	0.57
1:C:121:GLU:O	1:C:125:GLN:NE2	2.38	0.57
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.37	0.57
1:B:402:ILE:HG22	1:B:402:ILE:O	2.05	0.57
1:B:403:GLY:O	1:B:406:VAL:HG12	2.04	0.57
1:B:449:LEU:HD13	1:B:478:MET:SD	2.45	0.56
1:C:425:LEU:HD13	1:C:426:PRO:O	2.05	0.56
1:C:641:GLU:HG2	1:C:642:ASN:N	2.20	0.56
1:B:730:ASP:OD1	1:B:730:ASP:N	2.38	0.56
1:C:111:LEU:HD21	1:C:127:VAL:HG21	1.86	0.56
1:C:542:LEU:HD21	1:C:1025:VAL:HG11	1.86	0.56
1:C:875:ALA:O	1:C:878:LEU:N	2.35	0.56
1:C:390:ILE:HG22	1:C:390:ILE:O	2.06	0.56
1:B:399:VAL:HA	1:B:402:ILE:HG13	1.86	0.56
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.86	0.56
1:C:641:GLU:O	1:C:646:ALA:CB	2.54	0.56
1:C:876:ILE:O	1:C:880:VAL:HG12	2.05	0.56
1:C:699:ARG:CG	1:C:827:ILE:HD11	2.36	0.56
1:B:354:VAL:HG12	1:B:974:MET:HB2	1.87	0.56
1:C:38:ILE:HD12	1:C:38:ILE:C	2.26	0.56
1:C:885:LEU:HD12	1:C:885:LEU:C	2.26	0.56
1:B:383:LEU:HD11	1:B:473:THR:HG22	1.87	0.56
1:C:76:MET:CG	1:C:95:GLU:HG3	2.36	0.56
1:A:527:TYR:CD2	1:A:969:LEU:HD22	2.41	0.56
1:C:61:VAL:HG11	1:C:122:VAL:HG21	1.88	0.56
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.88	0.55
1:A:583:THR:HG22	1:A:586:ARG:HG3	1.87	0.55
1:A:1010:THR:HG23	1:A:1014:LEU:HD13	1.86	0.55
1:C:880:VAL:O	1:C:884:CYS:HB3	2.06	0.55
1:B:5:PHE:CD2	1:B:487:ILE:HG23	2.40	0.55
1:C:424:GLY:O	1:C:425:LEU:HB3	2.06	0.55
1:B:403:GLY:O	1:B:404:LEU:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:ILE:O	1:B:990:THR:N	2.38	0.55
1:B:447:MET:HB3	1:B:884:CYS:SG	2.47	0.55
1:C:76:MET:HG2	1:C:95:GLU:HG3	1.89	0.55
1:B:178:PHE:CZ	1:B:290:GLY:N	2.75	0.55
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.88	0.55
1:B:702:LEU:HD13	1:B:851:LEU:HD11	1.89	0.55
1:B:177:LEU:O	1:B:179:GLY:N	2.38	0.55
1:C:424:GLY:C	1:C:425:LEU:HD12	2.27	0.55
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.38	0.54
1:C:9:PRO:HB2	1:C:10:ILE:HD12	1.88	0.54
1:A:159:ALA:HB2	1:A:177:LEU:HD21	1.88	0.54
1:B:818:ARG:NH1	1:B:821:GLY:O	2.38	0.54
1:C:686:ASP:HB2	1:C:823:PRO:O	2.07	0.54
1:A:904:LEU:O	1:A:1010:THR:O	2.25	0.54
1:C:38:ILE:HD13	1:C:462:SER:HB3	1.88	0.54
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.90	0.54
1:C:104:GLN:CG	1:C:129:VAL:HG12	2.36	0.54
1:C:412:VAL:HG22	1:C:442:LEU:HD11	1.88	0.54
1:B:987:VAL:HG21	1:B:1005:MET:CG	2.37	0.54
1:C:752:ALA:O	1:C:774:MET:HA	2.08	0.54
1:B:454:VAL:HB	1:B:455:PRO:CD	2.38	0.54
1:B:444:GLY:O	1:B:448:VAL:CB	2.55	0.54
1:C:146:ASP:OD1	1:C:148:THR:HG23	2.08	0.54
1:C:425:LEU:CD2	1:C:426:PRO:HD2	2.37	0.54
1:B:150:THR:OG1	1:B:151:GLN:N	2.40	0.54
1:B:449:LEU:HD12	1:B:478:MET:SD	2.48	0.54
1:A:733:GLN:HE22	1:A:743:ILE:HD13	1.73	0.54
1:C:38:ILE:HD12	1:C:38:ILE:O	2.08	0.54
1:C:38:ILE:CD1	1:C:462:SER:HB3	2.38	0.54
1:C:127:VAL:O	1:C:127:VAL:HG23	2.08	0.54
1:C:427:PRO:O	1:C:428:LYS:C	2.45	0.54
1:A:348:ILE:HD11	1:A:372:VAL:CG1	2.38	0.53
1:B:398:MET:O	1:B:402:ILE:HG13	2.08	0.53
1:C:878:LEU:HA	1:C:881:VAL:HG23	1.90	0.53
1:B:449:LEU:CD1	1:B:478:MET:HE2	2.33	0.53
1:B:980:ILE:O	1:B:984:MET:HG2	2.08	0.53
1:C:30:LEU:HD21	1:C:388:PHE:O	2.07	0.53
1:C:348:ILE:HG22	1:C:402:ILE:HG21	1.90	0.53
1:C:376:LEU:HD22	1:C:398:MET:CG	2.38	0.53
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.90	0.53
1:B:731:ILE:H	1:B:731:ILE:CD1	2.02	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1023:PHE:O	1:C:1027:ARG:HB2	2.09	0.53
1:C:124:GLN:O	1:C:125:GLN:C	2.48	0.52
1:C:57:VAL:HG13	1:C:61:VAL:HG23	1.91	0.52
1:C:692:HIS:O	1:C:693:GLU:C	2.47	0.52
1:A:20:MET:SD	1:A:374:VAL:HG12	2.50	0.52
1:A:63:GLN:HE22	1:C:767:ARG:HA	1.75	0.52
1:C:57:VAL:O	1:C:61:VAL:O	2.27	0.52
1:A:5:PHE:CD2	1:A:487:ILE:HG22	2.45	0.52
1:B:520:PHE:O	1:B:524:THR:HG22	2.10	0.52
1:C:885:LEU:CD1	1:C:895:PRO:HB3	2.40	0.52
1:A:961:THR:HG21	1:A:1024:VAL:HG13	1.91	0.52
1:B:210:GLN:HB2	1:B:249:ILE:HD12	1.92	0.52
1:C:699:ARG:CD	1:C:827:ILE:HD11	2.40	0.52
1:B:582:ALA:HB3	1:B:623:ASN:HB3	1.91	0.52
1:C:858:ASP:O	1:C:860:THR:N	2.43	0.52
1:C:877:SER:C	1:C:880:VAL:HG12	2.30	0.52
1:A:583:THR:HG22	1:A:586:ARG:CG	2.39	0.51
1:B:441:ALA:C	1:B:443:VAL:H	2.14	0.51
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.91	0.51
1:C:298:ASN:ND2	1:C:301:ASP:HB2	2.25	0.51
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.92	0.51
1:B:986:LEU:HD22	1:B:997:GLN:HE21	1.75	0.51
1:B:379:THR:OG1	1:B:398:MET:CE	2.57	0.51
1:C:946:ALA:HB1	1:C:1023:PHE:CE2	2.44	0.51
1:C:425:LEU:HD22	1:C:426:PRO:CD	2.41	0.51
1:C:470:PHE:O	1:C:471:SER:C	2.49	0.51
1:A:243:THR:HG22	1:A:268:ILE:HG22	1.91	0.51
1:A:590:VAL:O	1:A:594:VAL:HG23	2.11	0.51
1:A:743:ILE:HD12	1:C:209:ALA:HB1	1.92	0.51
1:C:641:GLU:HG2	1:C:642:ASN:H	1.75	0.51
1:C:644:VAL:O	1:C:648:THR:HG23	2.10	0.51
1:C:40:PRO:CD	1:C:674:LEU:HD11	2.41	0.51
1:A:583:THR:HG22	1:A:586:ARG:HD3	1.93	0.51
1:C:42:ALA:HB2	1:C:93:THR:HG23	1.93	0.51
1:C:453:PHE:CD2	1:C:474:ILE:HG21	2.45	0.51
1:A:942:ILE:HD11	1:A:965:VAL:HG22	1.92	0.50
1:A:72:ILE:HD13	1:A:75:LEU:HD22	1.93	0.50
1:A:687:GLN:O	1:A:688:ALA:HB2	2.12	0.50
1:B:371:ALA:HB1	1:B:488:LEU:HD23	1.93	0.50
1:B:762:PHE:CZ	1:B:764:ASP:HB2	2.47	0.50
1:C:480:LEU:O	1:C:484:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:VAL:HG23	1:B:903:PRO:HD3	1.93	0.50
1:B:180:SER:C	1:B:181:GLN:O	2.49	0.50
1:B:211:ASN:ND2	1:B:761:ASP:O	2.43	0.50
1:B:246:PHE:O	1:B:249:ILE:HG12	2.10	0.50
1:B:649:MET:O	1:B:652:THR:HG22	2.10	0.50
1:B:375:VAL:HG22	1:B:484:VAL:HG11	1.94	0.50
1:B:696:THR:O	1:B:699:ARG:HB3	2.10	0.50
1:A:413:VAL:HG12	1:A:493:CYS:SG	2.51	0.50
1:B:83:ASP:C	1:B:83:ASP:OD1	2.50	0.50
1:C:352:PHE:CG	1:C:352:PHE:O	2.65	0.50
1:C:422:GLU:O	1:C:424:GLY:N	2.44	0.50
1:A:573:MET:CE	1:A:626:ILE:HD11	2.41	0.50
1:B:406:VAL:HG22	1:B:410:ILE:HD12	1.93	0.49
1:A:818:ARG:NH1	1:A:822:LEU:HA	2.27	0.49
1:B:137:LEU:HD12	1:B:329:THR:HG22	1.94	0.49
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.41	0.49
1:C:874:TYR:O	1:C:878:LEU:N	2.46	0.49
1:A:754:TRP:CE3	1:C:234:ILE:HD11	2.47	0.49
1:B:441:ALA:O	1:B:443:VAL:N	2.44	0.49
1:A:908:GLY:O	1:A:909:ALA:HB2	2.12	0.49
1:C:937:LYS:HD3	1:C:938:ASN:HD22	1.77	0.49
1:B:120:GLN:O	1:B:123:GLN:HB3	2.11	0.49
1:B:401:ALA:O	1:B:405:LEU:HB2	2.12	0.49
1:C:411:VAL:HG21	1:C:941:LEU:HD23	1.95	0.49
1:C:519:MET:O	1:C:523:SER:OG	2.27	0.49
1:C:885:LEU:CD1	1:C:895:PRO:CB	2.91	0.49
1:A:241:THR:HG22	1:A:245:GLU:OE1	2.13	0.49
1:A:518:ARG:HE	1:A:518:ARG:HA	1.78	0.49
1:B:454:VAL:CB	1:B:455:PRO:HD3	2.38	0.49
1:B:898:VAL:HG13	1:B:939:ALA:HB3	1.93	0.49
1:C:425:LEU:HD22	1:C:426:PRO:O	2.12	0.49
1:B:111:LEU:HD21	1:B:127:VAL:CG1	2.43	0.49
1:C:688:ALA:O	1:C:689:GLY:C	2.51	0.49
1:C:882:PHE:O	1:C:885:LEU:HG	2.13	0.49
1:A:237:GLN:HG3	1:B:731:ILE:HD11	1.95	0.49
1:C:885:LEU:HD13	1:C:895:PRO:HB3	1.95	0.48
1:B:158:VAL:HG11	1:B:289:LEU:HD13	1.96	0.48
1:B:375:VAL:HG21	1:B:481:SER:HA	1.95	0.48
1:B:448:VAL:O	1:B:452:VAL:HG12	2.12	0.48
1:B:874:TYR:CE2	1:B:878:LEU:HD13	2.48	0.48
1:C:20:MET:SD	1:C:373:PRO:HB2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:943:VAL:HA	1:C:946:ALA:HB3	1.93	0.48
1:B:20:MET:HA	1:B:377:LEU:CD2	2.43	0.48
1:C:23:GLY:CA	1:C:381:ALA:HB2	2.42	0.48
1:C:578:LEU:HD13	1:C:587:THR:HB	1.94	0.48
1:A:354:VAL:O	1:A:354:VAL:HG12	2.13	0.48
1:A:685:ILE:CG2	1:A:822:LEU:HD13	2.43	0.48
1:B:143:ILE:HG22	1:B:286:ALA:HB1	1.94	0.48
1:C:424:GLY:O	1:C:425:LEU:CB	2.61	0.48
1:C:104:GLN:CG	1:C:129:VAL:CG1	2.91	0.48
1:C:16:ALA:HB1	1:C:374:VAL:HG21	1.96	0.48
1:B:142:VAL:HG12	1:B:154:ILE:CG2	2.43	0.48
1:C:13:TRP:HA	1:C:13:TRP:CE3	2.49	0.48
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.95	0.48
1:C:343:THR:HG23	1:C:985:PRO:HB2	1.96	0.48
1:A:410:ILE:HA	1:A:413:VAL:HG22	1.96	0.48
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.47	0.48
1:A:984:MET:N	1:A:985:PRO:HD2	2.29	0.48
1:C:421:ALA:O	1:C:422:GLU:O	2.30	0.48
1:A:168:ARG:HG2	1:B:69:MET:O	2.14	0.47
1:C:298:ASN:O	1:C:300:LEU:N	2.48	0.47
1:B:1022:PHE:O	1:B:1026:VAL:HG22	2.14	0.47
1:C:27:ILE:HG23	1:C:390:ILE:CD1	2.44	0.47
1:C:382:VAL:HG11	1:C:476:SER:OG	2.15	0.47
1:A:902:VAL:HB	1:A:903:PRO:HD3	1.97	0.47
1:C:388:PHE:CE2	1:C:472:ILE:HG21	2.49	0.47
1:A:11:PHE:CE1	1:B:887:ALA:HB1	2.49	0.47
1:A:957:LEU:HD23	1:A:958:ILE:HD13	1.96	0.47
1:B:53:ASP:O	1:B:54:ALA:C	2.53	0.47
1:C:214:VAL:HG23	1:C:236:ALA:HB3	1.95	0.47
1:A:596:HIS:O	1:A:597:TYR:C	2.52	0.47
1:B:396:PHE:O	1:B:400:LEU:HG	2.14	0.47
1:C:721:LEU:O	1:C:722:GLU:C	2.52	0.47
1:A:410:ILE:HD13	1:A:974:MET:CB	2.44	0.47
1:A:686:ASP:HB2	1:A:695:LEU:HD13	1.95	0.47
1:A:918:LEU:HD21	1:A:999:ALA:HB2	1.97	0.47
1:B:115:MET:N	1:B:116:PRO:CD	2.78	0.47
1:B:382:VAL:HG21	1:B:480:LEU:HD13	1.96	0.47
1:C:181:GLN:NE2	1:C:767:ARG:NH2	2.63	0.47
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.49	0.47
1:A:968:ARG:HB3	1:A:968:ARG:CZ	2.44	0.47
1:B:965:VAL:HG12	1:B:969:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:VAL:HG23	1:C:162:MET:SD	2.54	0.47
1:A:249:ILE:O	1:A:250:LEU:CB	2.59	0.47
1:B:590:VAL:O	1:B:594:VAL:HG23	2.15	0.47
1:B:1009:VAL:O	1:B:1013:VAL:HG22	2.15	0.47
1:C:360:GLN:OE1	1:C:509:LYS:NZ	2.42	0.47
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.96	0.47
1:C:1020:PRO:O	1:C:1024:VAL:HG22	2.15	0.47
1:A:758:TYR:CZ	1:A:770:LYS:HD3	2.50	0.47
1:C:639:GLY:O	1:C:642:ASN:N	2.45	0.47
1:C:375:VAL:O	1:C:379:THR:HG22	2.14	0.46
1:C:719:ASN:HD22	1:C:826:GLU:HB3	1.80	0.46
1:B:198:LEU:HD23	1:B:251:LEU:HD13	1.96	0.46
1:C:149:MET:HE1	1:C:321:LEU:HD13	1.97	0.46
1:C:578:LEU:HD11	1:C:590:VAL:HG21	1.98	0.46
1:C:655:PHE:O	1:C:657:GLN:N	2.48	0.46
1:C:965:VAL:HG21	1:C:1020:PRO:HG3	1.97	0.46
1:A:516:PHE:HA	1:A:519:MET:HB2	1.98	0.46
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.80	0.46
1:B:418:ARG:NH1	1:B:967:MET:SD	2.88	0.46
1:C:104:GLN:HG3	1:C:129:VAL:CG1	2.44	0.46
1:B:119:PRO:O	1:B:122:VAL:HG12	2.15	0.46
1:C:532:GLY:CA	1:C:962:LEU:HD21	2.45	0.46
1:C:951:ASP:HB3	1:C:952:LYS:NZ	2.28	0.46
1:B:563:PHE:HD2	1:B:677:ALA:HB2	1.80	0.46
1:C:556:PHE:HB2	1:C:910:LEU:HD11	1.97	0.46
1:A:364:ALA:HA	1:A:367:ILE:HD12	1.98	0.46
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.98	0.46
1:A:890:GLU:C	1:C:10:ILE:HD13	2.36	0.46
1:B:412:VAL:HG12	1:B:438:ILE:CD1	2.46	0.46
1:A:977:LEU:HD23	1:A:981:LEU:HD23	1.98	0.46
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.46	0.46
1:C:390:ILE:O	1:C:390:ILE:CG2	2.64	0.46
1:A:10:ILE:HG12	1:B:890:GLU:O	2.15	0.46
1:A:549:VAL:O	1:A:549:VAL:HG12	2.15	0.46
1:A:754:TRP:CE3	1:C:234:ILE:CD1	2.99	0.46
1:B:65:ILE:O	1:B:66:GLU:C	2.53	0.46
1:B:393:LEU:CD2	1:B:466:ILE:HG23	2.45	0.46
1:C:13:TRP:CZ3	1:C:488:LEU:HD11	2.50	0.46
1:B:344:LEU:CD2	1:B:402:ILE:CG1	2.91	0.46
1:C:182:TYR:HA	1:C:271:GLY:O	2.15	0.46
1:C:880:VAL:O	1:C:880:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:486:LEU:HD23	2.47	0.45
1:A:19:ILE:HG22	1:A:20:MET:N	2.31	0.45
1:A:72:ILE:HD12	1:A:72:ILE:H	1.79	0.45
1:A:695:LEU:CD2	1:A:825:MET:SD	3.03	0.45
1:C:777:ALA:O	1:C:781:MET:HG2	2.16	0.45
1:A:38:ILE:CG1	1:A:462:SER:O	2.64	0.45
1:B:379:THR:C	1:B:381:ALA:N	2.69	0.45
1:B:684:LEU:HD22	1:B:699:ARG:HA	1.97	0.45
1:C:453:PHE:CE2	1:C:474:ILE:HD13	2.52	0.45
1:C:527:TYR:OH	1:C:1016:ILE:HB	2.16	0.45
1:B:449:LEU:HD12	1:B:478:MET:CE	2.46	0.45
1:C:517:ASN:HD22	1:C:518:ARG:N	2.14	0.45
1:C:791:VAL:HG12	1:C:791:VAL:O	2.17	0.45
1:A:568:ASP:OD1	1:A:644:VAL:HG23	2.16	0.45
1:B:582:ALA:HB3	1:B:623:ASN:CB	2.46	0.45
1:C:445:ILE:HB	1:C:449:LEU:HD12	1.98	0.45
1:C:33:ALA:O	1:C:391:ASN:HA	2.17	0.45
1:C:20:MET:SD	1:C:373:PRO:CB	3.05	0.45
1:C:467:TYR:OH	1:C:925:GLN:OE1	2.30	0.45
1:A:578:LEU:HD13	1:A:587:THR:HB	1.98	0.45
1:A:446:ALA:HA	1:A:478:MET:HE2	1.99	0.45
1:A:972:ILE:HG22	1:A:973:LEU:HD12	1.98	0.45
1:A:171:GLY:O	1:A:302:THR:HG21	2.17	0.45
1:A:222:THR:HG21	1:B:276:ASP:CG	2.37	0.45
1:C:400:LEU:O	1:C:401:ALA:CB	2.63	0.45
1:A:318:PRO:O	1:A:319:SER:O	2.35	0.45
1:B:137:LEU:HD12	1:B:329:THR:CG2	2.46	0.45
1:C:207:ILE:HG22	1:C:759:VAL:HG11	1.99	0.45
1:C:453:PHE:HA	1:C:456:MET:HG2	1.99	0.45
1:C:875:ALA:O	1:C:878:LEU:HB2	2.17	0.45
1:A:559:LEU:HD23	1:A:920:ASN:HB2	2.00	0.44
1:A:706:ALA:HB1	1:A:713:LEU:HD13	1.98	0.44
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.99	0.44
1:B:634:TRP:CE3	1:B:992:ALA:HB2	2.52	0.44
1:B:1013:VAL:HG23	1:B:1014:LEU:HD12	1.99	0.44
1:C:207:ILE:CG2	1:C:759:VAL:HG11	2.47	0.44
1:A:777:ALA:O	1:A:781:MET:HG2	2.17	0.44
1:B:375:VAL:HG22	1:B:484:VAL:CG1	2.47	0.44
1:B:401:ALA:C	1:B:403:GLY:N	2.68	0.44
1:C:688:ALA:HB3	1:C:854:GLY:HA3	1.99	0.44
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:VAL:HA	1:B:402:ILE:CD1	2.48	0.44
1:C:545:TYR:O	1:C:548:ILE:HG13	2.17	0.44
1:C:651:ALA:O	1:C:654:ALA:N	2.50	0.44
1:A:11:PHE:HA	1:A:14:VAL:HG22	1.99	0.44
1:A:146:ASP:OD1	1:A:148:THR:HG23	2.18	0.44
1:A:409:ALA:HA	1:A:489:THR:HG21	2.00	0.44
1:C:181:GLN:NE2	1:C:767:ARG:HH22	2.15	0.44
1:C:343:THR:O	1:C:344:LEU:C	2.56	0.44
1:B:30:LEU:HD11	1:B:380:PHE:O	2.18	0.44
1:C:124:GLN:O	1:C:126:GLY:N	2.51	0.44
1:C:372:VAL:CG2	1:C:373:PRO:HD3	2.46	0.44
1:C:478:MET:O	1:C:479:ALA:C	2.56	0.44
1:C:498:LYS:HB2	1:C:499:PRO:CD	2.48	0.44
1:A:323:ILE:HG23	1:A:325:TYR:CE2	2.52	0.44
1:A:330:THR:O	1:A:331:PRO:C	2.55	0.44
1:A:1019:VAL:N	1:A:1020:PRO:CD	2.81	0.44
1:B:185:ARG:HG3	1:B:187:TRP:CE2	2.53	0.44
1:C:472:ILE:O	1:C:476:SER:OG	2.30	0.44
1:A:542:LEU:CD2	1:A:546:LEU:HD21	2.48	0.44
1:B:184:MET:HB3	1:B:771:VAL:HG22	2.00	0.44
1:C:26:ALA:O	1:C:30:LEU:HB2	2.18	0.44
1:C:65:ILE:HG13	1:C:118:LEU:HD21	1.99	0.44
1:C:181:GLN:HE21	1:C:767:ARG:NH2	2.16	0.44
1:C:885:LEU:HD21	1:C:895:PRO:HB2	1.99	0.44
1:A:318:PRO:O	1:A:319:SER:C	2.56	0.44
1:A:763:ILE:HD11	1:B:59:ASP:HB3	2.00	0.44
1:B:330:THR:HB	1:B:331:PRO:HD3	1.99	0.44
1:A:72:ILE:HD13	1:A:75:LEU:CD2	2.47	0.44
1:A:115:MET:N	1:A:116:PRO:CD	2.80	0.44
1:A:332:PHE:CD2	1:A:332:PHE:C	2.90	0.44
1:A:449:LEU:HD12	1:A:478:MET:HE1	1.99	0.44
1:B:151:GLN:NE2	1:B:278:ILE:HA	2.33	0.44
1:B:366:LEU:HD13	1:B:369:THR:HG22	1.99	0.44
1:B:478:MET:SD	1:B:478:MET:C	2.96	0.44
1:B:655:PHE:O	1:B:656:SER:C	2.56	0.44
1:C:34:GLN:O	1:C:35:TYR:HD1	2.01	0.44
1:B:444:GLY:O	1:B:448:VAL:HG23	2.18	0.43
1:B:876:ILE:HA	1:B:879:ILE:HG22	2.00	0.43
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.98	0.43
1:C:587:THR:HG21	1:C:623:ASN:HA	2.00	0.43
1:C:845:GLU:O	1:C:849:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:LYS:C	1:C:954:GLY:H	2.19	0.43
1:B:182:TYR:CD2	1:B:270:LEU:HD23	2.54	0.43
1:B:344:LEU:HD23	1:B:402:ILE:CG1	2.36	0.43
1:B:5:PHE:CE2	1:B:487:ILE:HG23	2.53	0.43
1:C:26:ALA:HB1	1:C:384:ALA:HB3	2.00	0.43
1:B:997:GLN:O	1:B:1000:VAL:HG22	2.19	0.43
1:B:1013:VAL:HG23	1:B:1014:LEU:CD1	2.48	0.43
1:C:399:VAL:O	1:C:401:ALA:N	2.52	0.43
1:C:639:GLY:O	1:C:641:GLU:N	2.51	0.43
1:C:873:LEU:O	1:C:877:SER:N	2.33	0.43
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.52	0.43
1:B:166:ILE:HD13	1:B:289:LEU:CD2	2.49	0.43
1:C:166:ILE:HD11	1:C:310:LEU:CD1	2.48	0.43
1:C:194:ASN:ND2	1:C:790:TYR:CG	2.86	0.43
1:C:277:ILE:N	1:C:277:ILE:CD1	2.82	0.43
1:A:23:GLY:CA	1:A:381:ALA:HB2	2.44	0.43
1:A:420:MET:SD	1:A:430:ALA:HB3	2.59	0.43
1:B:994:SER:O	1:B:998:ASN:ND2	2.52	0.43
1:C:425:LEU:HD13	1:C:425:LEU:C	2.39	0.43
1:A:906:VAL:HG12	1:A:910:LEU:CD2	2.49	0.43
1:B:399:VAL:CA	1:B:402:ILE:HG13	2.49	0.43
1:B:866:GLU:O	1:B:867:ARG:HB2	2.18	0.43
1:C:30:LEU:HD22	1:C:390:ILE:CG1	2.46	0.43
1:B:108:GLN:HE21	1:C:109:ASN:HD22	1.67	0.43
1:B:403:GLY:HA2	1:B:406:VAL:HG12	2.01	0.43
1:B:449:LEU:O	1:B:453:PHE:HB2	2.19	0.43
1:C:952:LYS:HA	1:C:952:LYS:CE	2.42	0.43
1:B:731:ILE:HA	1:B:804:PHE:O	2.19	0.43
1:B:878:LEU:HA	1:B:881:VAL:HG22	2.00	0.43
1:C:30:LEU:HD12	1:C:384:ALA:HB2	1.99	0.43
1:A:1:MET:HE2	1:A:486:LEU:HD23	2.01	0.42
1:A:448:VAL:HG12	1:A:884:CYS:CB	2.49	0.42
1:A:676:THR:O	1:A:678:THR:N	2.52	0.42
1:A:961:THR:HG21	1:A:1024:VAL:CG1	2.48	0.42
1:B:102:ILE:O	1:B:105:VAL:HG12	2.19	0.42
1:C:399:VAL:HA	1:C:402:ILE:HD11	2.01	0.42
1:C:916:ARG:O	1:C:918:LEU:N	2.52	0.42
1:A:107:VAL:HG12	1:A:108:GLN:N	2.34	0.42
1:A:332:PHE:CD1	1:A:569:GLN:HA	2.54	0.42
1:A:583:THR:HG21	1:C:228:GLN:O	2.19	0.42
1:A:743:ILE:HG22	1:A:747:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:CG1	1:B:453:PHE:N	2.81	0.42
1:C:350:LEU:HD13	1:C:981:LEU:HD22	2.00	0.42
1:C:478:MET:O	1:C:481:SER:N	2.52	0.42
1:B:374:VAL:O	1:B:378:GLY:N	2.51	0.42
1:B:382:VAL:O	1:B:385:ALA:HB3	2.19	0.42
1:C:327:TYR:CD2	1:C:327:TYR:O	2.72	0.42
1:A:215:ALA:HB1	1:B:51:GLY:C	2.40	0.42
1:B:11:PHE:CD1	1:B:15:ILE:HD11	2.54	0.42
1:B:185:ARG:NH1	1:B:272:GLY:O	2.43	0.42
1:B:333:VAL:O	1:B:337:ILE:HD12	2.19	0.42
1:B:692:HIS:O	1:B:693:GLU:C	2.57	0.42
1:C:895:PRO:C	1:C:897:SER:N	2.73	0.42
1:A:887:ALA:HB1	1:C:11:PHE:HD2	1.84	0.42
1:B:578:LEU:HD13	1:B:587:THR:HG23	2.01	0.42
1:B:731:ILE:HG12	1:B:731:ILE:O	2.18	0.42
1:C:36:PRO:HD3	1:C:391:ASN:ND2	2.34	0.42
1:C:904:LEU:O	1:C:1010:THR:O	2.36	0.42
1:B:903:PRO:HA	1:B:906:VAL:HG22	2.01	0.42
1:C:326:PRO:CB	1:C:610:PHE:HB2	2.50	0.42
1:C:357:LEU:HD21	1:C:516:PHE:CZ	2.55	0.42
1:C:572:PHE:CZ	1:C:629:VAL:HG11	2.54	0.42
1:C:878:LEU:HA	1:C:881:VAL:CG2	2.49	0.42
1:A:68:ASN:O	1:A:110:LYS:HB3	2.20	0.42
1:A:583:THR:HG22	1:A:586:ARG:CD	2.49	0.42
1:B:454:VAL:CB	1:B:455:PRO:CD	2.97	0.42
1:C:160:ALA:HA	1:C:767:ARG:NH2	2.35	0.42
1:C:422:GLU:O	1:C:502:LYS:O	2.38	0.42
1:C:885:LEU:C	1:C:885:LEU:CD1	2.88	0.42
1:A:130:GLU:OE2	1:A:174:ASP:OD2	2.37	0.42
1:C:453:PHE:O	1:C:454:VAL:HG23	2.20	0.42
1:B:903:PRO:O	1:B:905:GLY:N	2.53	0.42
1:B:906:VAL:O	1:B:910:LEU:HD13	2.20	0.42
1:C:194:ASN:O	1:C:195:LYS:C	2.58	0.42
1:A:213:GLN:HB2	1:A:239:ARG:HG2	2.01	0.42
1:A:410:ILE:HD13	1:A:974:MET:HB2	2.01	0.42
1:B:27:ILE:CG2	1:B:380:PHE:HD2	2.33	0.42
1:B:45:ILE:HG12	1:B:129:VAL:HG22	2.02	0.42
1:B:216:ALA:HB1	1:B:234:ILE:O	2.19	0.42
1:C:409:ALA:HA	1:C:489:THR:HG21	2.02	0.42
1:C:928:LEU:O	1:C:931:THR:N	2.53	0.42
1:A:641:GLU:N	1:A:641:GLU:OE1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:CD1	1:C:333:VAL:HG11	2.50	0.41
1:C:655:PHE:C	1:C:657:GLN:N	2.73	0.41
1:A:372:VAL:HB	1:A:373:PRO:CD	2.49	0.41
1:B:367:ILE:HB	1:B:368:PRO:CD	2.50	0.41
1:B:445:ILE:CG2	1:B:449:LEU:CG	2.91	0.41
1:C:36:PRO:HG2	1:C:469:GLN:HE22	1.84	0.41
1:C:474:ILE:O	1:C:477:ALA:N	2.53	0.41
1:C:882:PHE:CD1	1:C:882:PHE:C	2.92	0.41
1:C:940:ILE:O	1:C:944:GLU:CA	2.68	0.41
1:B:595:THR:HG22	1:B:609:VAL:CG2	2.50	0.41
1:B:882:PHE:HB2	1:B:899:MET:HE1	2.01	0.41
1:C:34:GLN:OE1	1:C:35:TYR:CE1	2.73	0.41
1:C:425:LEU:CB	1:C:426:PRO:CD	2.97	0.41
1:A:144:ASN:HB2	1:A:154:ILE:HD11	2.03	0.41
1:B:976:SER:OG	1:B:1012:THR:HG21	2.21	0.41
1:A:410:ILE:HD13	1:A:974:MET:HB3	2.03	0.41
1:A:578:LEU:HD11	1:A:590:VAL:HG21	2.03	0.41
1:B:236:ALA:O	1:B:237:GLN:C	2.58	0.41
1:C:425:LEU:CD1	1:C:426:PRO:O	2.67	0.41
1:C:877:SER:O	1:C:880:VAL:HG12	2.21	0.41
1:B:572:PHE:CD2	1:B:644:VAL:HG23	2.56	0.41
1:C:576:VAL:HG22	1:C:663:VAL:HG22	2.02	0.41
1:A:918:LEU:HD21	1:A:999:ALA:CB	2.51	0.41
1:B:102:ILE:O	1:B:103:ALA:C	2.59	0.41
1:C:74:ASN:O	1:C:95:GLU:N	2.52	0.41
1:C:819:TYR:N	1:C:821:GLY:O	2.53	0.41
1:C:902:VAL:HB	1:C:903:PRO:HD3	2.02	0.41
1:C:949:LEU:HD23	1:C:953:GLU:HB3	2.02	0.41
1:A:371:ALA:O	1:A:374:VAL:HG22	2.21	0.41
1:B:20:MET:CA	1:B:377:LEU:HD21	2.51	0.41
1:B:27:ILE:HG22	1:B:380:PHE:CD2	2.55	0.41
1:C:129:VAL:O	1:C:129:VAL:CG1	2.68	0.41
1:C:298:ASN:C	1:C:300:LEU:N	2.73	0.41
1:A:15:ILE:HA	1:A:18:ILE:HG22	2.03	0.41
1:A:916:ARG:HG3	1:A:916:ARG:O	2.19	0.41
1:B:317:PHE:CG	1:B:321:LEU:HD23	2.56	0.41
1:B:987:VAL:HG11	1:B:1005:MET:HG3	2.02	0.41
1:C:13:TRP:HA	1:C:13:TRP:HE3	1.83	0.41
1:C:406:VAL:O	1:C:407:ASP:C	2.58	0.41
1:C:409:ALA:O	1:C:413:VAL:HB	2.20	0.41
1:C:412:VAL:O	1:C:412:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:THR:OG1	1:C:725:PRO:N	2.53	0.41
1:C:749:THR:O	1:C:750:LEU:C	2.59	0.41
1:C:937:LYS:CD	1:C:938:ASN:HD22	2.33	0.41
1:A:726:GLN:NE2	1:C:235:ILE:CD1	2.84	0.41
1:B:5:PHE:CE2	1:B:487:ILE:HD12	2.55	0.41
1:B:164:ASP:O	1:B:165:ALA:HB2	2.21	0.41
1:B:609:VAL:HG13	1:B:609:VAL:O	2.21	0.41
1:B:868:SER:HA	1:B:869:GLY:HA3	1.88	0.41
1:B:964:ALA:HA	1:B:967:MET:HE3	2.02	0.41
1:C:464:GLY:O	1:C:468:ARG:HG3	2.20	0.41
1:B:445:ILE:O	1:B:449:LEU:CB	2.61	0.40
1:C:40:PRO:HD2	1:C:674:LEU:HD11	2.03	0.40
1:C:882:PHE:O	1:C:885:LEU:CD1	2.69	0.40
1:B:240:LEU:CD2	1:B:249:ILE:HD11	2.52	0.40
1:C:284:GLN:HE21	1:C:284:GLN:HB3	1.61	0.40
1:C:952:LYS:HE3	1:C:952:LYS:CA	2.47	0.40
1:A:456:MET:HA	1:A:459:PHE:CD2	2.57	0.40
1:A:617:PHE:O	1:A:618:ALA:HB2	2.21	0.40
1:A:968:ARG:HG2	1:A:971:PRO:HG3	2.04	0.40
1:B:324:VAL:HG12	1:B:325:TYR:H	1.87	0.40
1:C:72:ILE:O	1:C:73:ASP:C	2.60	0.40
1:C:76:MET:SD	1:C:95:GLU:HA	2.61	0.40
1:C:878:LEU:O	1:C:881:VAL:N	2.46	0.40
1:C:882:PHE:HA	1:C:899:MET:HE1	2.02	0.40
1:A:728:LYS:HA	1:C:235:ILE:O	2.22	0.40
1:A:898:VAL:HG11	1:A:940:ILE:HA	2.04	0.40
1:B:388:PHE:CE2	1:B:472:ILE:HG21	2.55	0.40
1:C:555:LEU:O	1:C:559:LEU:N	2.55	0.40
1:C:677:ALA:HB1	1:C:717:ARG:HH21	1.87	0.40
1:C:69:MET:HE2	1:C:92:LEU:HD21	2.04	0.40
1:C:382:VAL:HG12	1:C:472:ILE:HD11	2.03	0.40
1:C:470:PHE:HA	1:C:473:THR:HG22	2.02	0.40
1:C:901:VAL:HG12	1:C:935:SER:HB3	2.03	0.40
1:C:983:VAL:HG12	1:C:983:VAL:O	2.22	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	1039/1050 (99%)	877 (84%)	116 (11%)	46 (4%)	2 15
1	B	1028/1050 (98%)	825 (80%)	148 (14%)	55 (5%)	2 11
1	C	1028/1050 (98%)	791 (77%)	155 (15%)	82 (8%)	1 4
All	All	3095/3150 (98%)	2493 (80%)	419 (14%)	183 (6%)	1 9

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	SER
1	A	366	LEU
1	A	464	GLY
1	A	543	VAL
1	A	582	ALA
1	A	677	ALA
1	A	865	GLN
1	A	909	ALA
1	A	1033	LYS
1	B	68	ASN
1	B	165	ALA
1	B	181	GLN
1	B	215	ALA
1	B	337	ILE
1	B	362	PHE
1	B	633	ASP
1	B	636	ASP
1	B	644	VAL
1	B	659	LYS
1	B	861	GLY
1	B	863	SER
1	B	890	GLU
1	B	988	ILE
1	B	989	SER

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Mol	Chain	Res	Type
1	C	7	ASP
1	C	9	PRO
1	C	10	ILE
1	C	62	THR
1	C	82	SER
1	C	83	ASP
1	C	124	GLN
1	C	125	GLN
1	C	401	ALA
1	C	422	GLU
1	C	425	LEU
1	C	431	THR
1	C	432	ARG
1	C	644	VAL
1	C	689	GLY
1	C	693	GLU
1	C	723	ASP
1	C	853	THR
1	C	859	TRP
1	C	870	ALA
1	C	917	GLY
1	C	922	VAL
1	C	936	ALA
1	C	953	GLU
1	A	161	ASN
1	A	318	PRO
1	A	420	MET
1	A	435	MET
1	A	439	GLN
1	A	503	GLY
1	A	508	GLY
1	A	616	GLY
1	A	618	ALA
1	A	670	ALA
1	A	994	SER
1	A	1018	PHE
1	A	1034	ASN
1	A	1035	GLU
1	B	34	GLN
1	B	209	ALA
1	B	237	GLN
1	B	319	SER

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Mol	Chain	Res	Type
1	B	359	LEU
1	B	364	ALA
1	B	388	PHE
1	B	432	ARG
1	B	440	GLY
1	B	455	PRO
1	B	456	MET
1	B	778	LYS
1	B	802	SER
1	B	867	ARG
1	C	51	GLY
1	C	61	VAL
1	C	296	GLY
1	C	298	ASN
1	C	299	ALA
1	C	356	TYR
1	C	362	PHE
1	C	400	LEU
1	C	409	ALA
1	C	428	LYS
1	C	437	GLN
1	C	471	SER
1	C	510	LYS
1	C	511	GLY
1	C	640	GLU
1	C	656	SER
1	C	687	GLN
1	C	701	GLN
1	C	722	GLU
1	C	778	LYS
1	C	855	VAL
1	C	861	GLY
1	C	887	ALA
1	C	952	LYS
1	C	957	LEU
1	C	1029	ARG
1	A	21	LEU
1	A	250	LEU
1	A	490	PRO
1	A	533	GLY
1	A	645	GLU
1	A	669	PRO

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Mol	Chain	Res	Type
1	A	795	ASP
1	A	867	ARG
1	A	950	MET
1	B	135	SER
1	B	243	THR
1	B	320	GLY
1	B	367	ILE
1	B	657	GLN
1	B	661	ALA
1	B	678	THR
1	B	795	ASP
1	B	814	PRO
1	B	866	GLU
1	B	959	GLU
1	C	53	ASP
1	C	81	ASN
1	C	106	GLN
1	C	423	GLU
1	C	427	PRO
1	C	454	VAL
1	C	618	ALA
1	C	896	PHE
1	A	35	TYR
1	A	459	PHE
1	A	507	GLU
1	A	538	THR
1	B	36	PRO
1	B	380	PHE
1	B	439	GLN
1	B	800	PRO
1	B	820	ASN
1	C	73	ASP
1	C	390	ILE
1	C	501	ALA
1	C	871	PRO
1	C	875	ALA
1	C	913	ALA
1	C	915	PHE
1	C	955	LYS
1	A	358	PHE
1	A	418	ARG
1	A	509	LYS

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Mol	Chain	Res	Type
1	B	54	ALA
1	B	431	THR
1	B	510	LYS
1	B	895	PRO
1	C	22	ALA
1	C	683	GLU
1	C	692	HIS
1	C	852	PRO
1	C	939	ALA
1	A	929	LEU
1	A	1037	ILE
1	B	402	ILE
1	B	442	LEU
1	B	454	VAL
1	B	539	GLY
1	B	676	THR
1	B	949	LEU
1	C	76	MET
1	C	285	PRO
1	C	387	GLY
1	C	825	MET
1	C	929	LEU
1	C	942	ILE
1	A	368	PRO
1	A	954	GLY
1	C	685	ILE
1	C	823	PRO
1	A	419	VAL
1	C	129	VAL
1	C	822	LEU
1	A	870	ALA
1	C	932	ILE
1	A	14	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	847/856 (99%)	748 (88%)	99 (12%)	5 22
1	B	836/856 (98%)	737 (88%)	99 (12%)	5 22
1	C	836/856 (98%)	719 (86%)	117 (14%)	3 16
All	All	2519/2568 (98%)	2204 (88%)	315 (12%)	4 20

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	PHE
1	A	15	ILE
1	A	18	ILE
1	A	27	ILE
1	A	32	VAL
1	A	46	SER
1	A	49	TYR
1	A	50	PRO
1	A	72	ILE
1	A	74	ASN
1	A	79	SER
1	A	96	SER
1	A	101	ASP
1	A	129	VAL
1	A	132	SER
1	A	135	SER
1	A	138	MET
1	A	150	THR
1	A	155	SER
1	A	197	GLN
1	A	231	ASN
1	A	242	SER
1	A	243	THR
1	A	244	GLU
1	A	249	ILE
1	A	253	VAL
1	A	258	SER
1	A	262	LEU
1	A	307	ARG
1	A	323	ILE
1	A	341	VAL
1	A	343	THR
1	A	355	MET

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Mol	Chain	Res	Type
1	A	356	TYR
1	A	369	THR
1	A	375	VAL
1	A	392	THR
1	A	406	VAL
1	A	417	GLU
1	A	452	VAL
1	A	480	LEU
1	A	489	THR
1	A	497	LEU
1	A	498	LYS
1	A	510	LYS
1	A	512	PHE
1	A	516	PHE
1	A	518	ARG
1	A	527	TYR
1	A	535	LEU
1	A	536	ARG
1	A	547	ILE
1	A	552	MET
1	A	587	THR
1	A	603	LYS
1	A	606	VAL
1	A	617	PHE
1	A	626	ILE
1	A	630	SER
1	A	637	ARG
1	A	640	GLU
1	A	648	THR
1	A	659	LYS
1	A	662	MET
1	A	721	LEU
1	A	724	THR
1	A	737	GLN
1	A	741	VAL
1	A	758	TYR
1	A	784	ASP
1	A	795	ASP
1	A	801	PHE
1	A	802	SER
1	A	804	PHE
1	A	806	SER

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Mol	Chain	Res	Type
1	A	808	ARG
1	A	822	LEU
1	A	825	MET
1	A	842	GLU
1	A	844	MET
1	A	849	SER
1	A	853	THR
1	A	858	ASP
1	A	910	LEU
1	A	911	LEU
1	A	918	LEU
1	A	934	LEU
1	A	942	ILE
1	A	966	ARG
1	A	968	ARG
1	A	977	LEU
1	A	990	THR
1	A	1010	THR
1	A	1027	ARG
1	A	1029	ARG
1	A	1030	PHE
1	A	1034	ASN
1	A	1038	GLU
1	B	1	MET
1	B	4	PHE
1	B	11	PHE
1	B	25	LEU
1	B	34	GLN
1	B	49	TYR
1	B	57	VAL
1	B	68	ASN
1	B	70	ASN
1	B	75	LEU
1	B	78	MET
1	B	82	SER
1	B	83	ASP
1	B	91	THR
1	B	117	LEU
1	B	130	GLU
1	B	134	SER
1	B	151	GLN
1	B	185	ARG

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Mol	Chain	Res	Type
1	B	193	LEU
1	B	214	VAL
1	B	219	LEU
1	B	233	SER
1	B	234	ILE
1	B	237	GLN
1	B	241	THR
1	B	267	LYS
1	B	284	GLN
1	B	293	LEU
1	B	330	THR
1	B	345	VAL
1	B	349	ILE
1	B	356	TYR
1	B	361	ASN
1	B	362	PHE
1	B	369	THR
1	B	370	ILE
1	B	372	VAL
1	B	377	LEU
1	B	393	LEU
1	B	404	LEU
1	B	418	ARG
1	B	423	GLU
1	B	478	MET
1	B	481	SER
1	B	484	VAL
1	B	486	LEU
1	B	495	THR
1	B	500	ILE
1	B	519	MET
1	B	524	THR
1	B	526	HIS
1	B	529	ASP
1	B	535	LEU
1	B	556	PHE
1	B	577	GLN
1	B	586	ARG
1	B	599	LEU
1	B	604	ASN
1	B	608	SER
1	B	626	ILE

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Mol	Chain	Res	Type
1	B	630	SER
1	B	652	THR
1	B	666	PHE
1	B	674	LEU
1	B	693	GLU
1	B	708	LYS
1	B	713	LEU
1	B	714	THR
1	B	717	ARG
1	B	726	GLN
1	B	729	ILE
1	B	730	ASP
1	B	731	ILE
1	B	791	VAL
1	B	797	GLN
1	B	825	MET
1	B	828	LEU
1	B	843	LEU
1	B	846	GLN
1	B	858	ASP
1	B	862	MET
1	B	865	GLN
1	B	867	ARG
1	B	874	TYR
1	B	877	SER
1	B	879	ILE
1	B	883	LEU
1	B	891	SER
1	B	893	SER
1	B	900	LEU
1	B	914	THR
1	B	915	PHE
1	B	918	LEU
1	B	919	THR
1	B	959	GLU
1	B	963	ASP
1	B	969	LEU
1	B	1027	ARG
1	C	13	TRP
1	C	18	ILE
1	C	29	LYS
1	C	30	LEU

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Mol	Chain	Res	Type
1	C	32	VAL
1	C	38	ILE
1	C	43	VAL
1	C	49	TYR
1	C	58	GLN
1	C	61	VAL
1	C	77	TYR
1	C	78	MET
1	C	79	SER
1	C	80	SER
1	C	84	SER
1	C	91	THR
1	C	93	THR
1	C	102	ILE
1	C	125	GLN
1	C	145	THR
1	C	158	VAL
1	C	177	LEU
1	C	185	ARG
1	C	197	GLN
1	C	202	ASP
1	C	237	GLN
1	C	239	ARG
1	C	241	THR
1	C	242	SER
1	C	252	LYS
1	C	254	ASN
1	C	285	PRO
1	C	300	LEU
1	C	301	ASP
1	C	310	LEU
1	C	314	GLU
1	C	329	THR
1	C	337	ILE
1	C	348	ILE
1	C	357	LEU
1	C	389	SER
1	C	394	THR
1	C	404	LEU
1	C	408	ASP
1	C	413	VAL
1	C	414	GLU

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Mol	Chain	Res	Type
1	C	417	GLU
1	C	422	GLU
1	C	423	GLU
1	C	425	LEU
1	C	435	MET
1	C	447	MET
1	C	456	MET
1	C	463	THR
1	C	469	GLN
1	C	471	SER
1	C	483	LEU
1	C	495	THR
1	C	504	ASP
1	C	517	ASN
1	C	550	VAL
1	C	552	MET
1	C	583	THR
1	C	587	THR
1	C	591	LEU
1	C	604	ASN
1	C	613	ASN
1	C	620	ARG
1	C	622	GLN
1	C	624	THR
1	C	626	ILE
1	C	641	GLU
1	C	656	SER
1	C	690	LEU
1	C	699	ARG
1	C	701	GLN
1	C	729	ILE
1	C	730	ASP
1	C	733	GLN
1	C	737	GLN
1	C	758	TYR
1	C	763	ILE
1	C	767	ARG
1	C	768	VAL
1	C	784	ASP
1	C	786	ILE
1	C	801	PHE
1	C	815	ARG

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Mol	Chain	Res	Type
1	C	825	MET
1	C	828	LEU
1	C	841	MET
1	C	845	GLU
1	C	849	SER
1	C	853	THR
1	C	863	SER
1	C	881	VAL
1	C	882	PHE
1	C	884	CYS
1	C	885	LEU
1	C	889	TYR
1	C	891	SER
1	C	896	PHE
1	C	918	LEU
1	C	930	THR
1	C	937	LYS
1	C	938	ASN
1	C	941	LEU
1	C	952	LYS
1	C	953	GLU
1	C	963	ASP
1	C	967	MET
1	C	981	LEU
1	C	987	VAL
1	C	1014	LEU
1	C	1016	ILE
1	C	1026	VAL
1	C	1029	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	GLN
1	A	68	ASN
1	A	231	ASN
1	A	596	HIS
1	A	726	GLN
1	A	737	GLN
1	A	925	GLN
1	A	998	ASN

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Mol	Chain	Res	Type
1	B	34	GLN
1	B	108	GLN
1	B	151	GLN
1	B	191	ASN
1	B	197	GLN
1	B	237	GLN
1	B	284	GLN
1	B	469	GLN
1	B	569	GLN
1	B	604	ASN
1	B	605	ASN
1	B	642	ASN
1	B	797	GLN
1	B	820	ASN
1	B	865	GLN
1	B	997	GLN
1	B	998	ASN
1	C	70	ASN
1	C	104	GLN
1	C	109	ASN
1	C	181	GLN
1	C	228	GLN
1	C	284	GLN
1	C	298	ASN
1	C	469	GLN
1	C	525	HIS
1	C	613	ASN
1	C	657	GLN
1	C	719	ASN
1	C	733	GLN
1	C	744	ASN
1	C	820	ASN
1	C	938	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1041/1050 (99%)	0.07	37 (3%)	42	17	21, 70, 147, 190	0
1	B	1030/1050 (98%)	0.26	66 (6%)	19	6	27, 98, 147, 173	0
1	C	1030/1050 (98%)	0.24	58 (5%)	24	8	24, 87, 142, 207	0
All	All	3101/3150 (98%)	0.19	161 (5%)	27	10	21, 86, 147, 207	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	ILE	9.7
1	C	6	ILE	5.8
1	C	497	LEU	5.5
1	C	707	ALA	5.4
1	B	497	LEU	5.2
1	B	986	LEU	5.0
1	B	527	TYR	4.8
1	C	511	GLY	4.6
1	C	1030	PHE	4.5
1	C	512	PHE	4.5
1	C	426	PRO	4.4
1	A	501	ALA	4.2
1	B	408	ASP	4.2
1	B	421	ALA	4.1
1	A	954	GLY	4.0
1	C	516	PHE	3.9
1	C	5	PHE	3.9
1	B	606	VAL	3.9
1	B	604	ASN	3.9
1	B	1028	ARG	3.8
1	B	526	HIS	3.8
1	B	507	GLU	3.7
1	A	419	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	501	ALA	3.7
1	B	419	VAL	3.6
1	B	634	TRP	3.6
1	C	496	MET	3.6
1	A	868	SER	3.6
1	B	516	PHE	3.5
1	A	506	GLY	3.4
1	A	511	GLY	3.4
1	C	513	PHE	3.3
1	B	509	LYS	3.3
1	C	408	ASP	3.3
1	C	507	GLU	3.3
1	C	55	LYS	3.3
1	A	505	HIS	3.2
1	C	935	SER	3.2
1	C	504	ASP	3.2
1	B	501	ALA	3.2
1	A	961	THR	3.1
1	A	869	GLY	3.1
1	C	500	ILE	3.1
1	C	503	GLY	3.1
1	B	511	GLY	3.1
1	C	494	ALA	3.1
1	C	438	ILE	3.1
1	C	938	ASN	3.1
1	B	412	VAL	3.1
1	B	522	LYS	3.1
1	C	509	LYS	3.0
1	B	510	LYS	3.0
1	A	513	PHE	3.0
1	C	833	PRO	3.0
1	B	1029	ARG	3.0
1	B	520	PHE	3.0
1	C	681	ASP	3.0
1	A	417	GLU	2.9
1	B	535	LEU	2.9
1	A	866	GLU	2.9
1	C	441	ALA	2.9
1	B	523	SER	2.9
1	B	505	HIS	2.9
1	C	836	SER	2.9
1	A	967	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	499	PRO	2.8
1	B	605	ASN	2.8
1	B	500	ILE	2.8
1	B	361	ASN	2.7
1	C	966	ARG	2.7
1	B	931	THR	2.7
1	C	506	GLY	2.7
1	A	867	ARG	2.7
1	A	898	VAL	2.6
1	B	962	LEU	2.6
1	B	513	PHE	2.6
1	B	968	ARG	2.6
1	B	498	LYS	2.6
1	B	506	GLY	2.6
1	B	437	GLN	2.5
1	A	504	ASP	2.5
1	A	421	ALA	2.5
1	B	961	THR	2.5
1	B	959	GLU	2.5
1	C	364	ALA	2.5
1	C	675	GLY	2.5
1	B	360	GLN	2.5
1	C	1002	THR	2.5
1	A	949	LEU	2.5
1	C	691	GLY	2.5
1	C	834	GLY	2.5
1	B	874	TYR	2.4
1	A	537	SER	2.4
1	B	635	ALA	2.4
1	C	536	ARG	2.4
1	B	935	SER	2.4
1	C	493	CYS	2.4
1	B	599	LEU	2.4
1	B	362	PHE	2.4
1	B	994	SER	2.4
1	C	435	MET	2.4
1	C	510	LYS	2.4
1	A	496	MET	2.4
1	C	945	PHE	2.4
1	B	946	ALA	2.4
1	B	966	ARG	2.4
1	B	991	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	952	LYS	2.4
1	B	427	PRO	2.3
1	C	519	MET	2.3
1	B	402	ILE	2.3
1	B	947	LYS	2.3
1	A	962	LEU	2.3
1	B	904	LEU	2.3
1	C	855	VAL	2.3
1	C	837	THR	2.3
1	C	403	GLY	2.3
1	B	897	SER	2.3
1	B	499	PRO	2.3
1	B	409	ALA	2.3
1	A	489	THR	2.2
1	C	680	PHE	2.2
1	C	415	ASN	2.2
1	A	408	ASP	2.2
1	B	367	ILE	2.2
1	C	831	ALA	2.2
1	A	522	LYS	2.2
1	B	958	ILE	2.2
1	C	359	LEU	2.2
1	B	1008	MET	2.2
1	A	7	ASP	2.2
1	B	420	MET	2.2
1	B	519	MET	2.2
1	A	948	ASP	2.2
1	C	499	PRO	2.2
1	A	507	GLU	2.2
1	C	9	PRO	2.1
1	A	966	ARG	2.1
1	C	978	ALA	2.1
1	A	362	PHE	2.1
1	B	508	GLY	2.1
1	A	915	PHE	2.1
1	C	870	ALA	2.1
1	C	957	LEU	2.1
1	A	960	ALA	2.1
1	B	493	CYS	2.1
1	A	529	ASP	2.1
1	B	540	ARG	2.1
1	B	436	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	418	ARG	2.1
1	C	1026	VAL	2.1
1	C	713	LEU	2.0
1	A	951	ASP	2.0
1	A	497	LEU	2.0
1	B	969	LEU	2.0
1	C	854	GLY	2.0
1	B	641	GLU	2.0
1	C	59	ASP	2.0
1	B	952	LYS	2.0
1	C	416	VAL	2.0
1	C	485	ALA	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.