Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:52 AM EDT

PDB ID	:	1NO7
Title	:	Structure of the Large Protease Resistant Upper Domain of VP5, the Major Capsid Protein of Herpes Simplex Virus-1
Authors	:	Bowman, B.R.; Baker, M.L.; Rixon, F.J.; Chiu, W.; Quiocho, F.A.
Deposited on	:	2003-01-15
Resolution	:	2.90 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 (1)) were used in the production of this report:

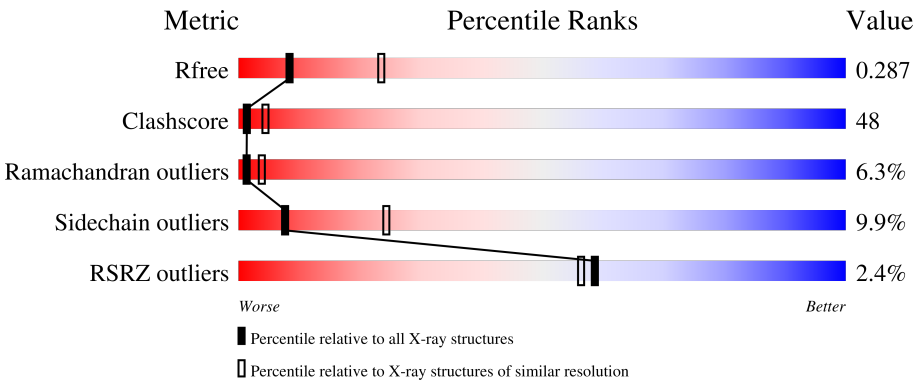
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	604	3%; 31%; 47%; 10%; • ; 10%
1	B	604	2%; 33%; 46%; 9%; 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8179 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 Major capsid protein.

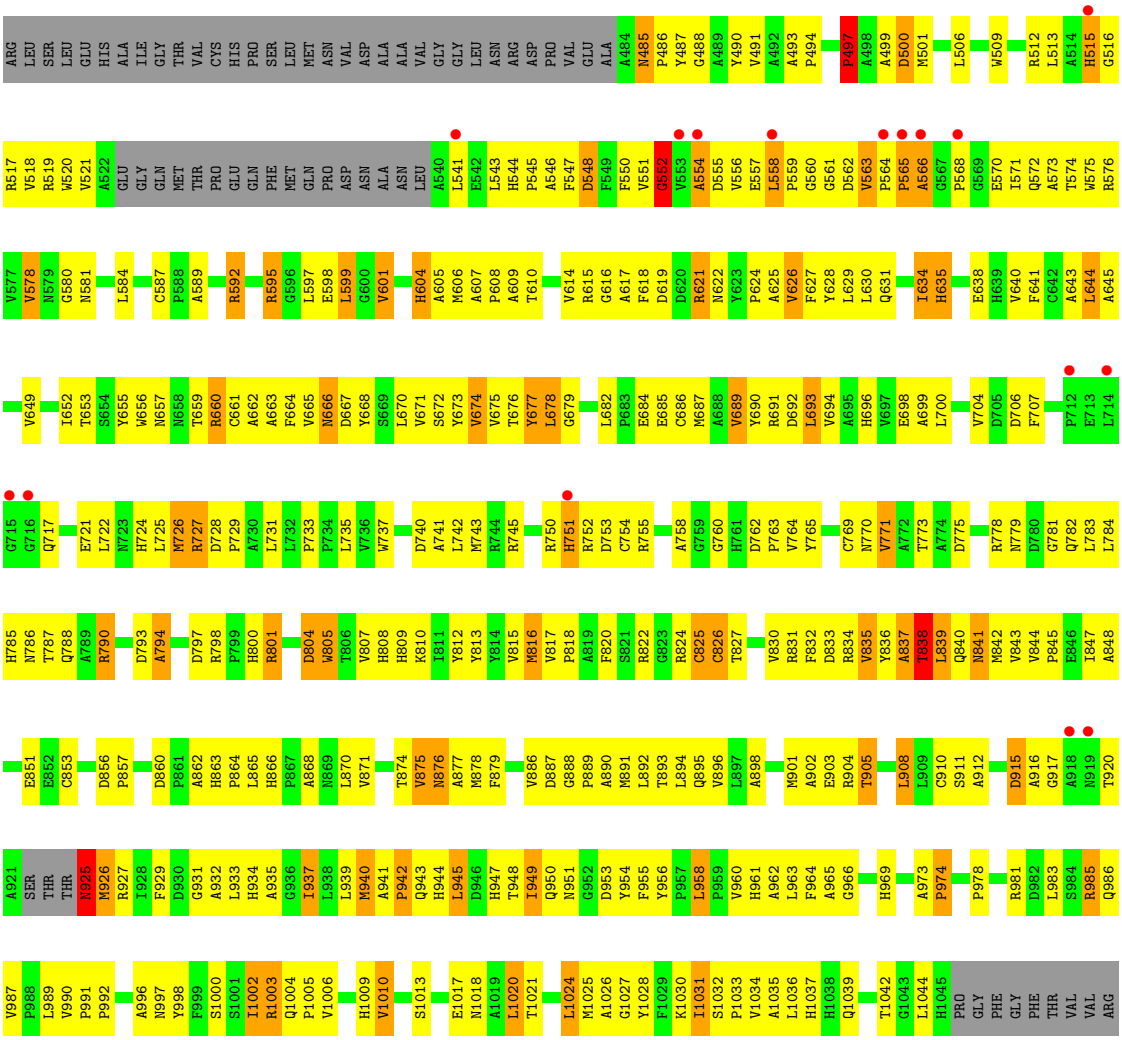
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	542	4121	2609	747	740	25	0	0	0
			Total	C	N	O	S			
1	B	534	4058	2573	734	726	25	0	0	0

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.

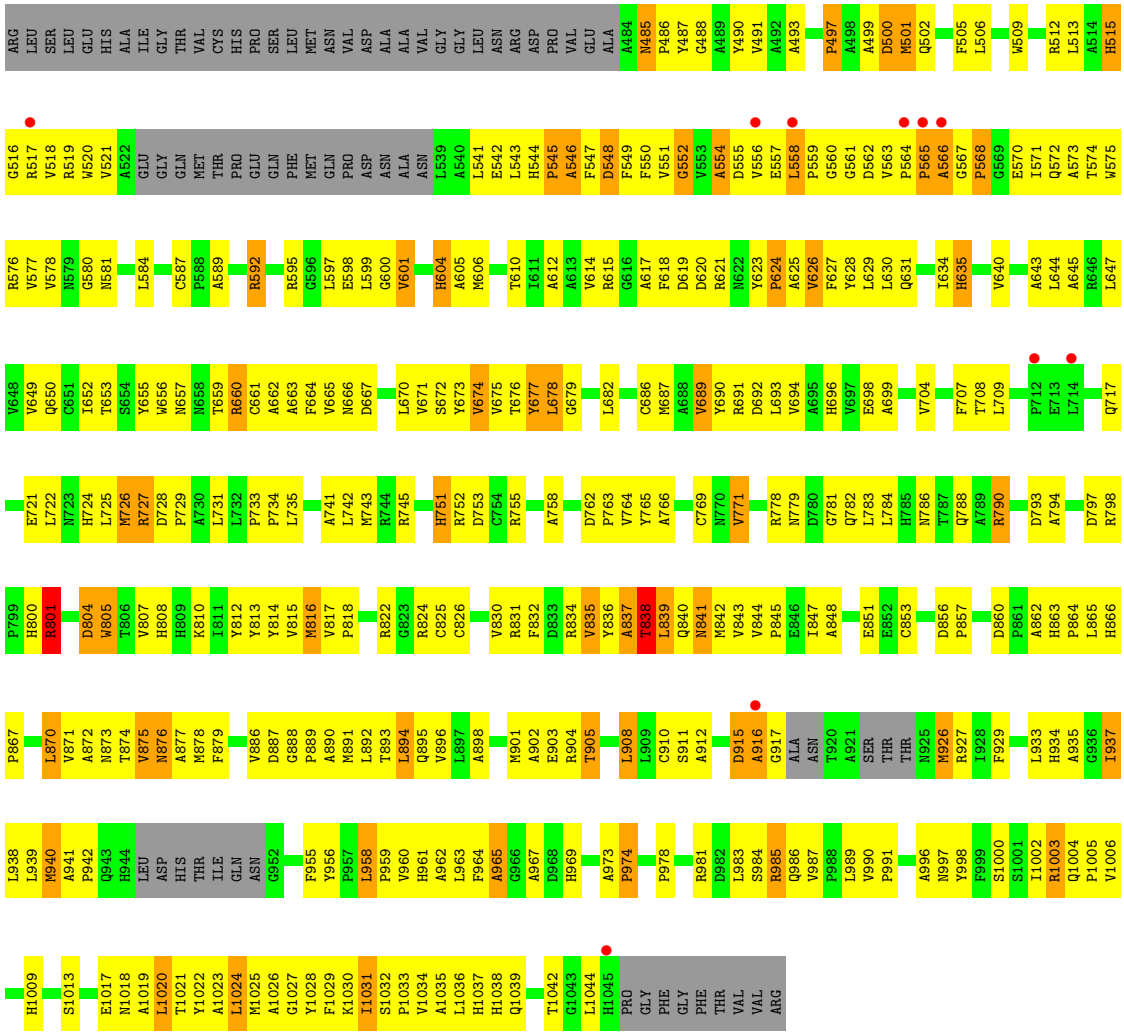
• Molecule 1: Major capsid protein

Chain A: 3% 31% 47% 10% • 10%



• Molecule 1: Major capsid protein

Chain B: 2% 33% 46% 9% 12%


ARG LEU SER LEU GLU HIS ALA ILE GLY THR VAL CYS HIS PRO SER LEU MET ASN VAL ASP ALA ALA VAL GLY GLY LEU ASN ARG ASP PRO VAL GLU ALA A484 M485 P486 Y487 G488 A489 Y490 V491 A492 A493 P497 A498 A499 D500 M501 Q502 F505 L506 W509 R512 L513 A514 H515
G516 R517 V518 R519 W520 V521 A522 GLU GLY GLN MET THR PRO GLU GLN PHE MET GLN PRO ASP ASN ALA ASN L539 A540 L541 E542 L543 H544 P545 A546 F547 D548 F549 F550 V551 G552 V553 A554 D555 V556 E557 L558 P559 G560 G561 D562 V563 P564 P565 A566 G567 P568 G569 E570 I571 Q572 A573 T574 W575
R576 V577 V578 N579 G580 N581 L584 C587 P588 A589 R592 R595 G596 L597 E598 L599 G600 V601 H604 A605 M606 T610 I611 A612 A613 V614 R615 G616 A617 F618 D619 D620 R621 N622 Y623 P624 A625 V626 F627 Y628 L629 L630 Q631 I634 H635 V640 A643 L644 A645 R646 L647
V648 V649 Q650 C651 I652 T653 S654 Y655 W656 N657 N658 T659 R660 C661 A662 A663 F664 V665 N666 D667 L670 V671 S672 Y673 V674 V675 T676 Y677 L678 G679 L682 C686 M687 A688 V689 Y690 R691 D692 L693 V694 A695 H696 V697 E698 A699 V704 F707 T708 L709 P712 E713 L714 Q717
E721 L722 N723 H724 L725 M726 R727 D728 P729 A730 L731 L732 P733 P734 L735 A741 L742 M743 R744 R745 H751 R752 D753 G754 R755 A758 D762 P763 V764 Y765 A766 C769 N770 V771 R778 N779 D780 G781 Q782 L783 L784 H785 N786 T787 Q788 A789 R790 D793 A794 D797 R798
P799 H800 R801 D804 W805 T806 V807 H808 H809 K810 I811 Y812 Y813 Y814 V815 M816 V817 P818 R822 G823 R824 C825 C826 V830 R831 F832 D833 R834 V835 Y836 A837 T838 L839 Q840 N841 M842 V843 V844 P845 E846 I847 A848 E851 E852 C853 D856 P857 D860 P861 A862 H863 P864 L865 H866
P867 L870 V871 A872 N873 T874 V875 N876 A877 M878 F879 V886 D887 G888 P889 A890 M891 L892 T893 L894 Q895 V896 L897 A898 M901 A902 E903 R904 T905 L908 L909 C910 S911 A912 D915 A916 G917 ALA ASN T920 A921 SER THR THR N925 M926 R927 I928 F929 L933 H934 A935 G936 I937
L938 L939 M940 A941 P942 Q943 H944 LEU ASP HIS THR ILE GLN ASN G952 F955 Y956 P957 L958 P959 V960 H961 A962 L963 F964 A965 G966 A967 D968 H969 A973 P974 P978 R981 D982 L983 S984 R985 Q986 V987 P988 L989 V990 P991 A996 N997 Y998 F999 S1000 S1001 I1002 R1003 Q1004 P1005 V1006
H1009 S1013 E1017 N1018 A1019 L1020 T1021 Y1022 A1023 L1024 M1025 A1026 G1027 Y1028 F1029 K1030 I1031 S1032 P1033 V1034 A1035 L1036 H1037 H1038 Q1039 T1042 G1043 L1044 H1045 PRO GLY PHE GLY PHE THR VAL VAL ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	99.07Å 99.07Å 454.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.90 48.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.3 (47.09-2.90) 91.4 (48.40-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.255 , 0.289 0.253 , 0.287	Depositor DCC
R_{free} test set	4747 reflections (9.29%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8179	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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)

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	0.65	4/4235 (0.1%)	1.00	16/5798 (0.3%)
1	B	0.59	2/4169 (0.0%)	0.98	12/5704 (0.2%)
All	All	0.62	6/8404 (0.1%)	0.99	28/11502 (0.2%)

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	1	2
1	B	1	1
All	All	2	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	GLY	C-N	-16.74	0.95	1.34
1	A	800	HIS	CB-CG	-15.89	1.21	1.50
1	B	800	HIS	CB-CG	-15.58	1.22	1.50
1	B	801	ARG	CB-CG	-11.61	1.21	1.52
1	A	555	ASP	C-N	-9.62	1.11	1.34
1	A	794	ALA	N-CA	-5.28	1.35	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	677	TYR	CB-CG-CD2	-29.83	103.10	121.00
1	B	677	TYR	CB-CG-CD1	29.36	138.61	121.00
1	A	677	TYR	CB-CG-CD2	-29.19	103.49	121.00
1	A	677	TYR	CB-CG-CD1	28.97	138.38	121.00
1	A	800	HIS	CA-CB-CG	14.48	138.21	113.60
1	B	800	HIS	CA-CB-CG	14.10	137.57	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	554	ALA	N-CA-C	13.45	147.30	111.00
1	A	554	ALA	N-CA-C	13.44	147.29	111.00
1	A	677	TYR	N-CA-C	12.70	145.28	111.00
1	A	677	TYR	CB-CA-C	-11.27	87.86	110.40
1	B	677	TYR	N-CA-C	10.82	140.22	111.00
1	B	677	TYR	CB-CA-C	-10.31	89.78	110.40
1	A	677	TYR	CA-CB-CG	9.47	131.40	113.40
1	B	677	TYR	CA-CB-CG	9.08	130.65	113.40
1	A	925	ASN	N-CA-C	8.63	134.31	111.00
1	A	678	LEU	N-CA-CB	-7.90	94.59	110.40
1	B	801	ARG	CA-CB-CG	7.52	129.94	113.40
1	A	555	ASP	C-N-CA	7.36	140.09	121.70
1	A	920	THR	C-N-CA	-7.01	104.18	121.70
1	A	552	GLY	C-N-CA	6.94	139.06	121.70
1	A	555	ASP	CA-C-N	6.83	132.22	117.20
1	B	678	LEU	N-CA-CB	-6.50	97.40	110.40
1	B	800	HIS	CB-CG-ND1	-5.91	108.42	123.20
1	A	800	HIS	CB-CG-ND1	-5.40	109.71	123.20
1	A	555	ASP	CA-C-O	-5.27	109.03	120.10
1	B	555	ASP	CA-C-O	-5.25	109.07	120.10
1	B	552	GLY	CA-C-N	-5.04	106.11	117.20
1	A	554	ALA	CB-CA-C	-5.01	102.59	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	554	ALA	CA
1	B	554	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	552	GLY	Mainchain
1	A	801	ARG	Mainchain
1	B	801	ARG	Mainchain

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4121	0	3986	400	0
1	B	4058	0	3932	381	0
All	All	8179	0	7918	774	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 48.

All (774) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:PHE:HA	1:A:940:MET:HE3	1.13	1.10
1:B:926:MET:HE2	1:B:926:MET:HA	1.24	1.08
1:A:610:THR:HG22	1:A:689:VAL:HA	1.37	1.07
1:B:618:PHE:HA	1:B:940:MET:HE3	1.09	1.05
1:A:949:ILE:HD12	1:A:949:ILE:H	1.20	1.03
1:B:610:THR:HG22	1:B:689:VAL:HA	1.42	1.00
1:A:945:LEU:HD22	1:B:612:ALA:HB2	1.39	0.99
1:B:618:PHE:CA	1:B:940:MET:HE3	1.96	0.96
1:B:788:GLN:HE21	1:B:794:ALA:HA	1.28	0.95
1:A:696:HIS:HE2	1:A:1021:THR:HG21	1.33	0.94
1:A:943:GLN:HG3	1:A:949:ILE:HG12	1.49	0.93
1:A:629:LEU:HD12	1:A:629:LEU:H	1.32	0.91
1:A:621:ARG:HG3	1:B:619:ASP:HB3	1.51	0.91
1:A:925:ASN:OD1	1:A:925:ASN:N	1.97	0.90
1:A:727:ARG:NH1	1:A:727:ARG:HB3	1.87	0.89
1:A:727:ARG:HB3	1:A:727:ARG:HH11	1.37	0.89
1:B:926:MET:HA	1:B:926:MET:CE	2.02	0.89
1:A:610:THR:CG2	1:A:689:VAL:HA	2.04	0.88
1:A:618:PHE:HA	1:A:940:MET:CE	2.03	0.88
1:A:874:THR:HG22	1:A:876:ASN:H	1.38	0.87
1:A:626:VAL:HG22	1:A:878:MET:HB3	1.56	0.87
1:B:556:VAL:HG21	1:B:565:PRO:HD2	1.57	0.86
1:B:626:VAL:HG22	1:B:878:MET:HB3	1.57	0.86
1:A:787:THR:HB	1:A:801:ARG:HH21	1.40	0.86
1:A:787:THR:O	1:A:801:ARG:NH2	2.08	0.86
1:B:618:PHE:HA	1:B:940:MET:CE	2.03	0.85
1:B:629:LEU:HD12	1:B:629:LEU:H	1.40	0.85
1:A:949:ILE:HD12	1:A:949:ILE:N	1.90	0.85
1:A:822:ARG:HB2	1:A:824:ARG:HH12	1.42	0.84
1:A:618:PHE:CA	1:A:940:MET:HE3	2.03	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:THR:HG22	1:B:876:ASN:H	1.41	0.84
1:B:631:GLN:HE21	1:B:667:ASP:HB2	1.42	0.84
1:A:631:GLN:HE21	1:A:667:ASP:HB2	1.42	0.83
1:B:696:HIS:HE2	1:B:1021:THR:HG21	1.44	0.82
1:A:660:ARG:HH11	1:A:660:ARG:HG2	1.45	0.82
1:A:552:GLY:HA3	1:A:572:GLN:HG3	1.60	0.81
1:B:782:GLN:H	1:B:904:ARG:HH22	1.29	0.81
1:A:782:GLN:H	1:A:904:ARG:HH22	1.27	0.81
1:B:822:ARG:HB2	1:B:824:ARG:HH12	1.47	0.80
1:A:898:ALA:HA	1:A:901:MET:HE3	1.63	0.80
1:A:622:ASN:HD21	1:B:620:ASP:HA	1.47	0.79
1:B:997:ASN:HD21	1:B:1004:GLN:H	1.28	0.79
1:B:610:THR:CG2	1:B:689:VAL:HA	2.12	0.79
1:A:610:THR:HG21	1:A:692:ASP:HB3	1.65	0.78
1:A:817:VAL:HB	1:A:818:PRO:HD3	1.65	0.78
1:A:644:LEU:HD12	1:A:644:LEU:H	1.48	0.78
1:A:973:ALA:HB1	1:A:974:PRO:HD2	1.65	0.78
1:A:933:LEU:HG	1:A:960:VAL:CG1	2.13	0.78
1:B:817:VAL:HB	1:B:818:PRO:HD3	1.64	0.78
1:A:704:VAL:HG11	1:A:727:ARG:HG3	1.66	0.77
1:A:816:MET:HE2	1:A:816:MET:HA	1.66	0.77
1:A:554:ALA:HB3	1:A:568:PRO:O	1.85	0.77
1:B:610:THR:HG21	1:B:692:ASP:CB	2.15	0.77
1:B:704:VAL:HG11	1:B:727:ARG:HG3	1.65	0.77
1:A:1020:LEU:O	1:A:1024:LEU:HD12	1.84	0.77
1:B:973:ALA:HB1	1:B:974:PRO:HD2	1.67	0.77
1:B:1020:LEU:O	1:B:1024:LEU:HD12	1.83	0.76
1:B:727:ARG:HB3	1:B:727:ARG:NH1	2.02	0.75
1:B:905:THR:HA	1:B:935:ALA:HB3	1.67	0.75
1:A:610:THR:HG21	1:A:692:ASP:CB	2.17	0.75
1:A:653:THR:HG22	1:A:657:ASN:HD21	1.52	0.75
1:B:1002:ILE:HD11	1:B:1006:VAL:HG11	1.68	0.74
1:B:816:MET:HA	1:B:816:MET:HE2	1.69	0.74
1:A:1035:ALA:HB1	1:A:1039:GLN:NE2	2.02	0.74
1:A:987:VAL:O	1:A:989:LEU:HD22	1.87	0.74
1:A:631:GLN:NE2	1:A:667:ASP:HB2	2.02	0.74
1:A:905:THR:HB	1:A:935:ALA:O	1.88	0.74
1:B:610:THR:HG21	1:B:692:ASP:HB3	1.70	0.74
1:B:635:HIS:HD1	1:B:635:HIS:H	1.35	0.73
1:B:598:GLU:O	1:B:601:VAL:HG22	1.88	0.73
1:B:905:THR:HB	1:B:935:ALA:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:LEU:O	1:B:634:ILE:HG13	1.89	0.72
1:B:836:TYR:O	1:B:840:GLN:HG2	1.88	0.72
1:A:790:ARG:HG3	1:A:790:ARG:HH11	1.54	0.72
1:B:604:HIS:HD2	1:B:696:HIS:ND1	1.86	0.72
1:A:606:MET:H	1:A:1018:ASN:HD21	1.37	0.72
1:B:660:ARG:HG2	1:B:660:ARG:HH11	1.53	0.72
1:A:836:TYR:O	1:A:840:GLN:HG2	1.89	0.72
1:A:933:LEU:HG	1:A:960:VAL:HG11	1.71	0.72
1:A:696:HIS:NE2	1:A:1021:THR:HG21	2.05	0.71
1:B:631:GLN:NE2	1:B:667:ASP:HB2	2.03	0.71
1:A:645:ALA:O	1:A:649:VAL:HG23	1.91	0.71
1:A:844:VAL:HG21	1:A:892:LEU:CD2	2.21	0.71
1:B:830:VAL:HB	1:B:832:PHE:CE1	2.25	0.71
1:A:844:VAL:HG21	1:A:892:LEU:HD21	1.73	0.71
1:A:1002:ILE:HD11	1:A:1006:VAL:HG11	1.73	0.70
1:B:790:ARG:HG3	1:B:790:ARG:HH11	1.56	0.70
1:A:491:VAL:HG11	1:A:929:PHE:CD2	2.26	0.70
1:B:1035:ALA:HB1	1:B:1039:GLN:NE2	2.06	0.70
1:B:727:ARG:HB3	1:B:727:ARG:HH11	1.55	0.70
1:B:615:ARG:HG2	1:B:619:ASP:OD2	1.92	0.69
1:A:554:ALA:CB	1:A:568:PRO:O	2.40	0.69
1:B:490:TYR:O	1:B:996:ALA:HB2	1.92	0.69
1:A:556:VAL:HG21	1:A:565:PRO:HD2	1.73	0.69
1:A:764:VAL:HG13	1:A:782:GLN:HG3	1.74	0.69
1:A:778:ARG:HD2	1:A:903:GLU:OE1	1.92	0.69
1:A:1006:VAL:O	1:A:1009:HIS:HB3	1.92	0.69
1:B:521:VAL:HG21	1:B:987:VAL:HG13	1.73	0.69
1:B:1002:ILE:HD12	1:B:1028:TYR:CE1	2.27	0.69
1:B:574:THR:HG21	1:B:998:TYR:O	1.92	0.69
1:A:905:THR:HA	1:A:935:ALA:HB3	1.75	0.69
1:A:949:ILE:H	1:A:949:ILE:CD1	1.85	0.69
1:B:521:VAL:HG11	1:B:987:VAL:HG22	1.74	0.69
1:B:653:THR:HG22	1:B:657:ASN:HD21	1.56	0.68
1:A:487:TYR:HB3	1:A:520:TRP:HH2	1.58	0.68
1:A:892:LEU:O	1:A:895:GLN:HG3	1.92	0.68
1:A:997:ASN:HD21	1:A:1004:GLN:H	1.40	0.68
1:B:487:TYR:HB3	1:B:520:TRP:HH2	1.58	0.68
1:B:645:ALA:O	1:B:649:VAL:HG23	1.93	0.68
1:B:911:SER:HB3	1:B:929:PHE:HD1	1.58	0.68
1:A:519:ARG:NH2	1:A:551:VAL:HG23	2.09	0.68
1:A:1002:ILE:HD12	1:A:1028:TYR:CE1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:ALA:HA	1:B:901:MET:HE3	1.76	0.68
1:A:521:VAL:HG11	1:A:987:VAL:HG22	1.76	0.68
1:B:606:MET:H	1:B:1018:ASN:HD21	1.40	0.68
1:A:615:ARG:HG2	1:A:619:ASP:OD2	1.93	0.68
1:A:589:ALA:O	1:A:592:ARG:HG2	1.94	0.68
1:A:905:THR:HG23	1:A:956:TYR:OH	1.93	0.67
1:B:576:ARG:HA	1:B:1003:ARG:HH21	1.59	0.67
1:A:652:ILE:HG12	1:A:663:ALA:CB	2.24	0.67
1:B:933:LEU:HG	1:B:960:VAL:CG1	2.24	0.67
1:A:604:HIS:HD2	1:A:696:HIS:ND1	1.92	0.66
1:A:490:TYR:O	1:A:996:ALA:HB2	1.96	0.66
1:B:519:ARG:HH12	1:B:550:PHE:HA	1.60	0.66
1:A:893:THR:O	1:A:896:VAL:HG23	1.95	0.66
1:B:942:PRO:HB3	1:B:969:HIS:CD2	2.31	0.66
1:B:987:VAL:O	1:B:989:LEU:HD22	1.96	0.66
1:A:519:ARG:HH22	1:A:551:VAL:H	1.42	0.66
1:A:911:SER:HB3	1:A:929:PHE:HD1	1.61	0.66
1:B:933:LEU:HG	1:B:960:VAL:HG11	1.78	0.66
1:B:893:THR:O	1:B:896:VAL:HG23	1.95	0.66
1:A:822:ARG:HB2	1:A:824:ARG:NH1	2.10	0.66
1:B:788:GLN:HG2	1:B:793:ASP:O	1.96	0.65
1:A:614:VAL:HG21	1:A:693:LEU:CD1	2.26	0.65
1:A:499:ALA:HB2	1:A:956:TYR:CE2	2.32	0.64
1:A:597:LEU:C	1:A:597:LEU:HD13	2.16	0.64
1:B:652:ILE:HG21	1:B:682:LEU:HD23	1.79	0.64
1:B:778:ARG:HD2	1:B:903:GLU:OE1	1.97	0.64
1:B:844:VAL:HG21	1:B:892:LEU:CD2	2.27	0.64
1:B:490:TYR:OH	1:B:561:GLY:HA3	1.97	0.64
1:B:745:ARG:HH22	1:B:911:SER:N	1.96	0.64
1:B:764:VAL:HG13	1:B:782:GLN:HG3	1.79	0.64
1:B:1006:VAL:O	1:B:1009:HIS:HB3	1.98	0.64
1:A:745:ARG:NH2	1:A:910:CYS:HB2	2.13	0.64
1:B:519:ARG:HH22	1:B:551:VAL:H	1.43	0.64
1:B:822:ARG:HB2	1:B:824:ARG:NH1	2.13	0.64
1:B:825:CYS:SG	1:B:938:LEU:HD11	2.38	0.64
1:A:815:VAL:O	1:A:818:PRO:HD2	1.98	0.64
1:B:887:ASP:OD1	1:B:889:PRO:HD2	1.98	0.64
1:A:606:MET:N	1:A:1018:ASN:HD21	1.96	0.64
1:B:892:LEU:O	1:B:895:GLN:HG3	1.98	0.63
1:B:644:LEU:HD12	1:B:644:LEU:H	1.63	0.63
1:A:652:ILE:HG12	1:A:663:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:LEU:O	1:A:969:HIS:HE1	1.81	0.63
1:B:606:MET:N	1:B:1018:ASN:HD21	1.97	0.63
1:A:490:TYR:OH	1:A:561:GLY:HA3	1.97	0.63
1:A:621:ARG:HG3	1:B:619:ASP:CB	2.27	0.63
1:A:726:MET:HE2	1:A:726:MET:HA	1.80	0.63
1:A:742:LEU:O	1:A:742:LEU:HD23	1.99	0.63
1:B:844:VAL:HG21	1:B:892:LEU:HD21	1.81	0.63
1:A:663:ALA:N	1:A:690:TYR:OH	2.31	0.62
1:A:726:MET:HA	1:A:726:MET:CE	2.29	0.62
1:A:1024:LEU:O	1:A:1028:TYR:HD2	1.82	0.62
1:B:491:VAL:HG11	1:B:929:PHE:CD2	2.35	0.62
1:B:788:GLN:NE2	1:B:794:ALA:HA	2.09	0.62
1:A:644:LEU:HD12	1:A:644:LEU:N	2.13	0.62
1:A:790:ARG:HG3	1:A:790:ARG:NH1	2.14	0.62
1:B:490:TYR:HE1	1:B:556:VAL:HG11	1.65	0.62
1:B:626:VAL:HA	1:B:629:LEU:HD13	1.82	0.62
1:B:726:MET:HA	1:B:726:MET:CE	2.30	0.61
1:A:830:VAL:HB	1:A:832:PHE:CE1	2.35	0.61
1:B:597:LEU:HD13	1:B:597:LEU:C	2.19	0.61
1:B:1034:VAL:O	1:B:1037:HIS:HB3	1.99	0.61
1:A:841:ASN:O	1:A:841:ASN:CG	2.39	0.61
1:B:986:GLN:HG3	1:B:987:VAL:HG23	1.83	0.61
1:B:659:THR:O	1:B:661:CYS:N	2.34	0.61
1:B:815:VAL:O	1:B:818:PRO:HD2	2.00	0.61
1:B:544:HIS:ND1	1:B:545:PRO:HD2	2.16	0.61
1:B:834:ARG:O	1:B:838:THR:HG23	2.01	0.61
1:A:519:ARG:HH12	1:A:550:PHE:HA	1.64	0.60
1:A:717:GLN:HE22	1:A:752:ARG:HH11	1.48	0.60
1:A:948:THR:HA	1:A:953:ASP:OD2	2.01	0.60
1:B:816:MET:HE2	1:B:816:MET:CA	2.28	0.60
1:B:1009:HIS:CD2	1:B:1013:SER:HB2	2.37	0.60
1:A:575:TRP:CZ2	1:A:1031:ILE:HG22	2.37	0.60
1:B:696:HIS:NE2	1:B:1021:THR:HG21	2.16	0.60
1:A:614:VAL:HG21	1:A:693:LEU:HD11	1.84	0.60
1:A:887:ASP:OD1	1:A:889:PRO:HD2	2.00	0.60
1:B:663:ALA:N	1:B:690:TYR:OH	2.35	0.60
1:B:581:ASN:HD21	1:B:1003:ARG:H	1.49	0.59
1:A:499:ALA:HA	1:A:956:TYR:CE1	2.37	0.59
1:A:653:THR:O	1:A:657:ASN:ND2	2.35	0.59
1:B:581:ASN:ND2	1:B:1003:ARG:H	2.00	0.59
1:B:790:ARG:HG3	1:B:790:ARG:NH1	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:842:MET:SD	1:B:891:MET:HG2	2.43	0.59
1:A:517:ARG:HH22	1:A:986:GLN:HE21	1.51	0.59
1:A:788:GLN:HG2	1:A:793:ASP:O	2.03	0.59
1:B:788:GLN:HE21	1:B:794:ALA:CA	2.08	0.59
1:B:804:ASP:HB3	1:B:808:HIS:HE1	1.68	0.59
1:A:764:VAL:HG12	1:A:781:GLY:O	2.03	0.59
1:B:519:ARG:NH2	1:B:551:VAL:HG23	2.17	0.59
1:A:488:GLY:O	1:A:996:ALA:HB1	2.03	0.59
1:B:614:VAL:HG21	1:B:693:LEU:CD1	2.32	0.59
1:A:659:THR:O	1:A:661:CYS:N	2.35	0.59
1:A:694:VAL:O	1:A:698:GLU:HG3	2.03	0.59
1:A:911:SER:HB3	1:A:929:PHE:CD1	2.38	0.59
1:A:610:THR:HG22	1:A:689:VAL:CA	2.25	0.59
1:B:911:SER:HB3	1:B:929:PHE:CD1	2.36	0.59
1:A:576:ARG:HA	1:A:1003:ARG:HH21	1.67	0.58
1:A:986:GLN:HG3	1:A:987:VAL:HG23	1.86	0.58
1:A:997:ASN:HD21	1:A:1004:GLN:HB2	1.67	0.58
1:B:652:ILE:HG12	1:B:663:ALA:CB	2.33	0.58
1:B:653:THR:O	1:B:657:ASN:ND2	2.36	0.58
1:B:771:VAL:HG13	1:B:898:ALA:O	2.04	0.58
1:A:629:LEU:H	1:A:629:LEU:CD1	2.13	0.58
1:A:933:LEU:HD11	1:A:958:LEU:HD23	1.84	0.58
1:A:947:HIS:O	1:A:951:ASN:HB2	2.03	0.58
1:B:758:ALA:HB2	1:B:763:PRO:HB3	1.85	0.58
1:A:598:GLU:O	1:A:601:VAL:HG22	2.04	0.58
1:A:666:ASN:HB3	1:A:940:MET:SD	2.44	0.58
1:A:1035:ALA:HB1	1:A:1039:GLN:HE21	1.69	0.58
1:B:722:LEU:O	1:B:1030:LYS:HG3	2.03	0.58
1:A:575:TRP:HZ2	1:A:1031:ILE:HG22	1.69	0.58
1:A:668:TYR:OH	1:A:694:VAL:HG13	2.04	0.58
1:B:556:VAL:HG21	1:B:565:PRO:CD	2.29	0.58
1:A:678:LEU:HB3	1:A:682:LEU:HD11	1.86	0.58
1:B:488:GLY:N	1:B:520:TRP:CH2	2.72	0.58
1:A:521:VAL:HG21	1:A:987:VAL:HG13	1.86	0.57
1:A:834:ARG:O	1:A:838:THR:HG23	2.04	0.57
1:B:564:PRO:O	1:B:566:ALA:N	2.37	0.57
1:A:745:ARG:HH22	1:A:911:SER:N	2.01	0.57
1:A:804:ASP:HB3	1:A:808:HIS:HE1	1.69	0.57
1:A:660:ARG:HG2	1:A:660:ARG:NH1	2.12	0.57
1:A:630:LEU:O	1:A:634:ILE:HG13	2.04	0.57
1:A:784:LEU:HB3	1:A:786:ASN:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LEU:HD13	1:A:597:LEU:O	2.03	0.57
1:B:554:ALA:HB3	1:B:568:PRO:HG2	1.86	0.57
1:A:945:LEU:HD12	1:A:945:LEU:H	1.68	0.57
1:A:745:ARG:CZ	1:A:910:CYS:HB2	2.34	0.57
1:A:764:VAL:HG13	1:A:782:GLN:HA	1.87	0.57
1:B:983:LEU:C	1:B:983:LEU:HD13	2.26	0.57
1:A:816:MET:HE2	1:A:816:MET:CA	2.27	0.56
1:B:804:ASP:HB3	1:B:808:HIS:CE1	2.40	0.56
1:A:983:LEU:HD13	1:A:983:LEU:C	2.26	0.56
1:B:644:LEU:HD12	1:B:644:LEU:N	2.20	0.56
1:A:488:GLY:N	1:A:520:TRP:CH2	2.73	0.56
1:A:722:LEU:O	1:A:1030:LYS:HG3	2.05	0.56
1:B:589:ALA:O	1:B:592:ARG:HG2	2.05	0.56
1:B:652:ILE:HG21	1:B:682:LEU:CD2	2.35	0.56
1:B:784:LEU:HB3	1:B:786:ASN:OD1	2.05	0.56
1:B:905:THR:HG23	1:B:956:TYR:OH	2.04	0.56
1:B:905:THR:CG2	1:B:956:TYR:OH	2.53	0.56
1:A:905:THR:CG2	1:A:956:TYR:OH	2.52	0.56
1:A:499:ALA:HB2	1:A:956:TYR:CZ	2.40	0.56
1:A:771:VAL:HG13	1:A:898:ALA:O	2.05	0.56
1:A:815:VAL:C	1:A:818:PRO:HD2	2.26	0.56
1:A:1034:VAL:O	1:A:1037:HIS:HB3	2.05	0.56
1:B:816:MET:HA	1:B:816:MET:CE	2.34	0.56
1:B:604:HIS:CD2	1:B:696:HIS:HA	2.39	0.56
1:B:605:ALA:HA	1:B:1018:ASN:ND2	2.20	0.56
1:A:788:GLN:HE21	1:A:794:ALA:HA	1.69	0.56
1:A:837:ALA:O	1:A:839:LEU:N	2.39	0.56
1:B:997:ASN:ND2	1:B:1004:GLN:H	2.02	0.56
1:A:1009:HIS:CD2	1:A:1013:SER:HB2	2.40	0.56
1:B:1035:ALA:HB1	1:B:1039:GLN:HE21	1.70	0.56
1:A:491:VAL:HG21	1:A:929:PHE:HD2	1.71	0.55
1:A:758:ALA:HB2	1:A:763:PRO:HB3	1.86	0.55
1:B:745:ARG:CZ	1:B:910:CYS:HB2	2.36	0.55
1:B:491:VAL:HG21	1:B:929:PHE:HD2	1.71	0.55
1:B:628:TYR:HB3	1:B:955:PHE:CZ	2.40	0.55
1:B:656:TRP:CD2	1:B:686:CYS:HB2	2.41	0.55
1:B:662:ALA:HB3	1:B:665:VAL:CG1	2.36	0.55
1:B:815:VAL:C	1:B:818:PRO:HD2	2.27	0.55
1:B:580:GLY:O	1:B:592:ARG:NH2	2.37	0.55
1:A:707:PHE:CD1	1:A:1044:LEU:HD13	2.40	0.55
1:A:1000:SER:C	1:A:1002:ILE:H	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ARG:HG2	1:B:660:ARG:NH1	2.21	0.55
1:A:581:ASN:HD21	1:A:1003:ARG:H	1.54	0.55
1:B:678:LEU:HB3	1:B:682:LEU:HD11	1.89	0.55
1:B:845:PRO:HG2	1:B:862:ALA:O	2.05	0.55
1:A:662:ALA:HB3	1:A:665:VAL:CG1	2.37	0.55
1:A:678:LEU:HB3	1:A:682:LEU:CD1	2.37	0.55
1:A:843:VAL:HG12	1:A:843:VAL:O	2.07	0.55
1:A:945:LEU:H	1:A:945:LEU:CD1	2.20	0.55
1:A:997:ASN:ND2	1:A:1004:GLN:HB2	2.21	0.55
1:B:652:ILE:HG12	1:B:663:ALA:HB3	1.88	0.55
1:A:1024:LEU:O	1:A:1028:TYR:CD2	2.60	0.55
1:B:745:ARG:NH2	1:B:910:CYS:HB2	2.22	0.55
1:B:764:VAL:HG13	1:B:782:GLN:HA	1.88	0.55
1:A:512:ARG:NH2	1:A:563:VAL:HG12	2.21	0.54
1:A:735:LEU:HD23	1:A:933:LEU:HB2	1.88	0.54
1:A:948:THR:O	1:A:953:ASP:HB2	2.07	0.54
1:B:554:ALA:HB2	1:B:568:PRO:O	2.08	0.54
1:B:961:HIS:HE2	1:B:1002:ILE:HG23	1.71	0.54
1:B:549:PHE:CD2	1:B:573:ALA:HB2	2.43	0.54
1:B:841:ASN:CG	1:B:841:ASN:O	2.43	0.54
1:A:724:HIS:HD2	1:A:726:MET:H	1.55	0.54
1:A:890:ALA:O	1:A:893:THR:OG1	2.20	0.54
1:A:581:ASN:ND2	1:A:1003:ARG:H	2.06	0.54
1:A:564:PRO:O	1:A:566:ALA:N	2.40	0.54
1:A:574:THR:HG21	1:A:998:TYR:O	2.07	0.54
1:B:499:ALA:HA	1:B:956:TYR:CE1	2.42	0.54
1:B:876:ASN:N	1:B:876:ASN:HD22	2.05	0.54
1:A:839:LEU:HD22	1:A:894:LEU:HD13	1.89	0.54
1:B:1000:SER:C	1:B:1002:ILE:H	2.09	0.54
1:B:742:LEU:CD1	1:B:908:LEU:HD21	2.38	0.54
1:A:804:ASP:O	1:A:807:VAL:HB	2.08	0.54
1:B:742:LEU:HD23	1:B:742:LEU:O	2.08	0.54
1:A:961:HIS:HE2	1:A:1002:ILE:HG23	1.73	0.53
1:B:888:GLY:O	1:B:892:LEU:HD23	2.08	0.53
1:A:742:LEU:CD1	1:A:908:LEU:HD21	2.39	0.53
1:B:764:VAL:HG12	1:B:781:GLY:O	2.08	0.53
1:B:499:ALA:HB2	1:B:956:TYR:CE2	2.43	0.53
1:A:717:GLN:HE22	1:A:752:ARG:NH1	2.06	0.53
1:A:804:ASP:HB3	1:A:808:HIS:CE1	2.44	0.53
1:B:666:ASN:HB3	1:B:940:MET:SD	2.48	0.53
1:A:905:THR:CB	1:A:935:ALA:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:879:PHE:HE2	1:B:886:VAL:HG21	1.73	0.53
1:A:652:ILE:HG21	1:A:682:LEU:HD23	1.91	0.53
1:B:678:LEU:CD1	1:B:682:LEU:HD11	2.39	0.53
1:A:643:ALA:HB1	1:A:896:VAL:HG21	1.90	0.53
1:A:644:LEU:H	1:A:644:LEU:CD1	2.20	0.53
1:A:943:GLN:CG	1:A:949:ILE:HG12	2.30	0.53
1:B:672:SER:HG	1:B:805:TRP:HZ3	1.57	0.53
1:B:879:PHE:CE2	1:B:886:VAL:HG21	2.44	0.53
1:A:655:TYR:CE2	1:A:661:CYS:HB2	2.44	0.53
1:A:672:SER:HG	1:A:805:TRP:HZ3	1.57	0.53
1:A:942:PRO:HB3	1:A:969:HIS:CD2	2.44	0.53
1:B:743:MET:HG3	1:B:765:TYR:CE2	2.44	0.53
1:B:610:THR:HA	1:B:689:VAL:HG22	1.90	0.52
1:A:497:PRO:HB2	1:A:500:ASP:HB2	1.91	0.52
1:A:629:LEU:HD12	1:A:629:LEU:N	2.11	0.52
1:B:890:ALA:O	1:B:893:THR:OG1	2.26	0.52
1:A:978:PRO:HA	1:A:981:ARG:HG3	1.91	0.52
1:B:678:LEU:HB3	1:B:682:LEU:CD1	2.39	0.52
1:B:724:HIS:HD2	1:B:726:MET:H	1.58	0.52
1:A:638:GLU:OE1	1:A:801:ARG:NH1	2.43	0.52
1:A:735:LEU:CD2	1:A:933:LEU:HB2	2.39	0.52
1:B:801:ARG:HG3	1:B:805:TRP:CD1	2.44	0.52
1:B:837:ALA:O	1:B:839:LEU:N	2.43	0.52
1:A:628:TYR:HB3	1:A:955:PHE:CZ	2.45	0.52
1:A:841:ASN:ND2	1:A:874:THR:HA	2.24	0.52
1:B:643:ALA:HB1	1:B:896:VAL:HG21	1.90	0.52
1:B:905:THR:CB	1:B:935:ALA:O	2.55	0.52
1:A:604:HIS:CD2	1:A:696:HIS:HA	2.45	0.52
1:A:876:ASN:N	1:A:876:ASN:HD22	2.08	0.52
1:A:1004:GLN:O	1:A:1005:PRO:C	2.49	0.52
1:B:843:VAL:O	1:B:843:VAL:HG12	2.10	0.52
1:A:601:VAL:HG23	1:A:601:VAL:O	2.10	0.52
1:B:726:MET:HA	1:B:726:MET:HE2	1.90	0.52
1:A:610:THR:HA	1:A:689:VAL:HG22	1.93	0.51
1:B:545:PRO:O	1:B:576:ARG:HD2	2.09	0.51
1:B:751:HIS:O	1:B:751:HIS:ND1	2.43	0.51
1:B:554:ALA:CB	1:B:568:PRO:O	2.58	0.51
1:B:635:HIS:CD2	1:B:902:ALA:HB2	2.45	0.51
1:B:694:VAL:O	1:B:698:GLU:HG3	2.10	0.51
1:A:618:PHE:O	1:A:941:ALA:HB2	2.10	0.51
1:B:497:PRO:HB2	1:B:500:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:TRP:HZ2	1:B:660:ARG:NH2	2.08	0.51
1:B:662:ALA:HB3	1:B:665:VAL:HG13	1.92	0.51
1:B:618:PHE:O	1:B:941:ALA:HB2	2.10	0.51
1:B:1029:PHE:CD1	1:B:1044:LEU:HD21	2.45	0.51
1:A:656:TRP:CD2	1:A:686:CYS:HB2	2.46	0.51
1:B:635:HIS:ND1	1:B:635:HIS:N	2.59	0.51
1:B:617:ALA:C	1:B:940:MET:HE1	2.31	0.51
1:B:836:TYR:CE1	1:B:901:MET:HB2	2.46	0.51
1:B:1000:SER:C	1:B:1002:ILE:N	2.64	0.51
1:B:717:GLN:HE22	1:B:752:ARG:HH11	1.57	0.51
1:B:874:THR:O	1:B:877:ALA:N	2.44	0.51
1:B:517:ARG:HD2	1:B:518:VAL:H	1.76	0.51
1:B:652:ILE:CG2	1:B:682:LEU:HD23	2.41	0.51
1:B:629:LEU:HD12	1:B:629:LEU:N	2.18	0.50
1:B:875:VAL:HG23	1:B:879:PHE:CE1	2.45	0.50
1:B:959:PRO:HB3	1:B:965:ALA:HB2	1.93	0.50
1:A:605:ALA:HA	1:A:1018:ASN:ND2	2.26	0.50
1:B:575:TRP:CZ2	1:B:1031:ILE:HG22	2.46	0.50
1:B:801:ARG:HD3	1:B:805:TRP:CE2	2.46	0.50
1:B:848:ALA:HB3	1:B:851:GLU:HG3	1.93	0.50
1:A:615:ARG:O	1:A:618:PHE:N	2.44	0.50
1:B:505:PHE:CE2	1:B:991:PRO:HA	2.46	0.50
1:B:563:VAL:HG12	1:B:564:PRO:HD2	1.93	0.50
1:B:978:PRO:HA	1:B:981:ARG:HG3	1.94	0.50
1:B:997:ASN:HD21	1:B:1004:GLN:HB2	1.75	0.50
1:A:696:HIS:O	1:A:699:ALA:N	2.45	0.50
1:A:784:LEU:CD1	1:A:902:ALA:HA	2.42	0.50
1:B:673:TYR:O	1:B:675:VAL:N	2.44	0.50
1:B:546:ALA:C	1:B:547:PHE:CD1	2.85	0.50
1:B:552:GLY:HA3	1:B:572:GLN:HG3	1.93	0.50
1:A:656:TRP:CE2	1:A:686:CYS:HB2	2.46	0.50
1:B:517:ARG:HH22	1:B:986:GLN:HE21	1.59	0.50
1:B:1017:GLU:N	1:B:1017:GLU:OE2	2.45	0.50
1:A:517:ARG:HD2	1:A:518:VAL:H	1.77	0.50
1:A:545:PRO:O	1:A:576:ARG:HD2	2.12	0.50
1:A:673:TYR:O	1:A:675:VAL:N	2.44	0.50
1:B:673:TYR:O	1:B:676:THR:N	2.45	0.50
1:B:845:PRO:CG	1:B:862:ALA:O	2.60	0.50
1:A:769:CYS:HB3	1:A:901:MET:O	2.11	0.50
1:A:830:VAL:HG22	1:A:955:PHE:CD2	2.47	0.50
1:B:576:ARG:CA	1:B:1003:ARG:HH21	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:THR:HG21	1:A:954:TYR:OH	2.12	0.49
1:A:848:ALA:O	1:A:851:GLU:HB2	2.12	0.49
1:A:947:HIS:O	1:A:951:ASN:CB	2.60	0.49
1:B:962:ALA:N	1:B:990:VAL:HG21	2.27	0.49
1:A:544:HIS:ND1	1:A:545:PRO:HD2	2.27	0.49
1:A:845:PRO:HG2	1:A:862:ALA:O	2.12	0.49
1:A:997:ASN:ND2	1:A:1004:GLN:H	2.09	0.49
1:A:842:MET:SD	1:A:891:MET:HG2	2.52	0.49
1:B:1031:ILE:O	1:B:1036:LEU:HD23	2.12	0.49
1:A:626:VAL:HA	1:A:629:LEU:HD13	1.93	0.49
1:B:997:ASN:ND2	1:B:1004:GLN:HB2	2.28	0.49
1:B:743:MET:HE2	1:B:765:TYR:CE2	2.48	0.49
1:B:493:ALA:HB2	1:B:560:GLY:HA2	1.95	0.49
1:B:961:HIS:NE2	1:B:1002:ILE:HG23	2.27	0.49
1:A:824:ARG:O	1:A:825:CYS:HB3	2.11	0.49
1:B:735:LEU:CD2	1:B:933:LEU:HB2	2.43	0.49
1:B:872:ALA:O	1:B:873:ASN:HB2	2.13	0.49
1:B:1039:GLN:HG2	1:B:1044:LEU:HD23	1.95	0.49
1:A:546:ALA:C	1:A:547:PHE:CD1	2.86	0.49
1:A:580:GLY:O	1:A:592:ARG:NH2	2.44	0.49
1:B:707:PHE:HA	1:B:1042:THR:HG21	1.95	0.49
1:A:758:ALA:C	1:A:760:GLY:H	2.16	0.49
1:A:826:CYS:HB3	1:A:969:HIS:ND1	2.28	0.49
1:A:841:ASN:O	1:A:874:THR:HG23	2.12	0.49
1:A:1000:SER:C	1:A:1002:ILE:N	2.65	0.48
1:B:655:TYR:CE2	1:B:661:CYS:HB2	2.48	0.48
1:B:707:PHE:CD1	1:B:1044:LEU:HD13	2.48	0.48
1:A:816:MET:HA	1:A:816:MET:CE	2.39	0.48
1:A:847:ILE:HD13	1:A:853:CYS:HA	1.95	0.48
1:A:875:VAL:HG23	1:A:879:PHE:CE1	2.49	0.48
1:B:597:LEU:HD13	1:B:597:LEU:O	2.13	0.48
1:A:724:HIS:HD2	1:A:726:MET:N	2.11	0.48
1:B:614:VAL:HG13	1:B:665:VAL:HG11	1.94	0.48
1:A:485:ASN:C	1:A:485:ASN:HD22	2.16	0.48
1:A:682:LEU:HD12	1:A:682:LEU:N	2.28	0.48
1:A:751:HIS:O	1:A:751:HIS:ND1	2.46	0.48
1:B:733:PRO:HB3	1:B:810:LYS:CG	2.44	0.48
1:A:635:HIS:CD2	1:A:902:ALA:HB2	2.48	0.48
1:B:575:TRP:O	1:B:576:ARG:C	2.51	0.48
1:B:581:ASN:HD21	1:B:1003:ARG:N	2.11	0.48
1:B:584:LEU:HD23	1:B:592:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:CYS:HB3	1:B:901:MET:O	2.14	0.48
1:A:643:ALA:HB3	1:A:644:LEU:HD12	1.96	0.48
1:B:664:PHE:HB3	1:B:670:LEU:HD12	1.96	0.48
1:B:687:MET:HG3	1:B:691:ARG:NE	2.29	0.48
1:A:548:ASP:O	1:A:573:ALA:HA	2.14	0.48
1:A:597:LEU:C	1:A:597:LEU:CD1	2.83	0.48
1:A:860:ASP:OD1	1:A:862:ALA:HB3	2.13	0.48
1:A:1020:LEU:O	1:A:1020:LEU:HD12	2.14	0.48
1:B:485:ASN:C	1:B:485:ASN:HD22	2.16	0.48
1:B:512:ARG:NH2	1:B:563:VAL:HG12	2.29	0.48
1:B:707:PHE:C	1:B:1042:THR:HG21	2.35	0.48
1:B:863:HIS:ND1	1:B:864:PRO:HD2	2.28	0.48
1:A:515:HIS:ND1	1:A:516:GLY:N	2.62	0.48
1:A:621:ARG:CG	1:B:619:ASP:HB3	2.35	0.48
1:A:626:VAL:CG2	1:A:878:MET:HB3	2.36	0.48
1:A:743:MET:HG3	1:A:765:TYR:CE2	2.49	0.47
1:B:505:PHE:CD2	1:B:991:PRO:HA	2.49	0.47
1:B:601:VAL:HG23	1:B:601:VAL:O	2.14	0.47
1:B:841:ASN:ND2	1:B:874:THR:HA	2.29	0.47
1:A:961:HIS:NE2	1:A:1002:ILE:HG23	2.28	0.47
1:B:544:HIS:CE1	1:B:545:PRO:HD2	2.48	0.47
1:B:682:LEU:N	1:B:682:LEU:HD12	2.29	0.47
1:B:1032:SER:HB2	1:B:1033:PRO:HD2	1.94	0.47
1:A:820:PHE:CD2	1:A:1017:GLU:HG2	2.49	0.47
1:B:662:ALA:CB	1:B:665:VAL:HG13	2.44	0.47
1:A:727:ARG:HH11	1:A:727:ARG:CB	2.19	0.47
1:A:741:ALA:O	1:A:745:ARG:HB2	2.14	0.47
1:B:565:PRO:O	1:B:566:ALA:C	2.52	0.47
1:B:893:THR:C	1:B:895:GLN:H	2.18	0.47
1:A:617:ALA:C	1:A:940:MET:HE1	2.35	0.47
1:B:515:HIS:ND1	1:B:516:GLY:N	2.63	0.47
1:B:627:PHE:CD1	1:B:627:PHE:N	2.82	0.47
1:B:804:ASP:O	1:B:807:VAL:HB	2.15	0.47
1:B:985:ARG:HG2	1:B:985:ARG:HH11	1.79	0.47
1:B:985:ARG:HG2	1:B:985:ARG:NH1	2.29	0.47
1:A:485:ASN:HD22	1:A:486:PRO:HD2	1.79	0.47
1:A:911:SER:CB	1:A:929:PHE:CD1	2.97	0.47
1:B:488:GLY:O	1:B:996:ALA:HB1	2.15	0.47
1:A:1039:GLN:HG2	1:A:1044:LEU:HD23	1.97	0.47
1:A:563:VAL:HG12	1:A:564:PRO:HD2	1.96	0.47
1:A:985:ARG:HH11	1:A:985:ARG:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:782:GLN:O	1:B:904:ARG:NH2	2.47	0.47
1:A:558:LEU:N	1:A:559:PRO:HD2	2.30	0.47
1:A:945:LEU:CD2	1:B:612:ALA:HB2	2.29	0.47
1:B:735:LEU:HD23	1:B:933:LEU:HB2	1.96	0.47
1:B:546:ALA:O	1:B:575:TRP:HD1	1.97	0.47
1:A:961:HIS:ND1	1:A:963:LEU:HB2	2.29	0.46
1:B:721:GLU:OE1	1:B:729:PRO:HG3	2.15	0.46
1:B:753:ASP:OD1	1:B:755:ARG:NH1	2.48	0.46
1:B:558:LEU:N	1:B:559:PRO:HD2	2.30	0.46
1:A:557:GLU:C	1:A:559:PRO:HD2	2.35	0.46
1:A:584:LEU:HD23	1:A:592:ARG:HH11	1.80	0.46
1:A:848:ALA:HB3	1:A:851:GLU:HG3	1.97	0.46
1:A:911:SER:CB	1:A:929:PHE:HD1	2.27	0.46
1:A:985:ARG:HG2	1:A:985:ARG:NH1	2.30	0.46
1:B:841:ASN:O	1:B:874:THR:HG23	2.14	0.46
1:A:578:VAL:HB	1:A:1027:GLY:O	2.14	0.46
1:B:724:HIS:CD2	1:B:725:LEU:N	2.83	0.46
1:A:487:TYR:C	1:A:487:TYR:CD2	2.88	0.46
1:B:871:VAL:O	1:B:874:THR:HB	2.15	0.46
1:A:758:ALA:HA	1:A:908:LEU:HD12	1.98	0.46
1:A:863:HIS:ND1	1:A:864:PRO:HD2	2.30	0.46
1:B:724:HIS:HD2	1:B:726:MET:N	2.13	0.46
1:B:784:LEU:CD1	1:B:902:ALA:HA	2.46	0.46
1:A:565:PRO:O	1:A:566:ALA:C	2.54	0.46
1:A:606:MET:HE2	1:A:696:HIS:CD2	2.50	0.46
1:A:673:TYR:O	1:A:676:THR:N	2.48	0.46
1:A:944:HIS:CE1	1:B:612:ALA:HB1	2.50	0.46
1:B:804:ASP:O	1:B:805:TRP:C	2.54	0.46
1:A:724:HIS:CD2	1:A:726:MET:H	2.33	0.46
1:B:915:ASP:CG	1:B:916:ALA:H	2.18	0.46
1:A:724:HIS:HE1	1:A:1025:MET:O	1.99	0.46
1:B:557:GLU:C	1:B:559:PRO:HD2	2.36	0.46
1:A:546:ALA:O	1:A:575:TRP:HD1	1.99	0.46
1:A:643:ALA:C	1:A:645:ALA:H	2.18	0.46
1:A:797:ASP:CG	1:A:798:ARG:H	2.19	0.46
1:A:888:GLY:O	1:A:892:LEU:HD23	2.16	0.46
1:B:584:LEU:HA	1:B:587:CYS:O	2.15	0.46
1:B:629:LEU:H	1:B:629:LEU:CD1	2.18	0.46
1:A:512:ARG:CZ	1:A:563:VAL:HG12	2.46	0.45
1:A:575:TRP:O	1:A:576:ARG:C	2.53	0.45
1:A:721:GLU:OE1	1:A:729:PRO:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:LEU:HD12	1:A:908:LEU:HD21	1.98	0.45
1:A:758:ALA:C	1:A:760:GLY:N	2.69	0.45
1:A:804:ASP:O	1:A:805:TRP:C	2.54	0.45
1:B:490:TYR:CG	1:B:564:PRO:HG3	2.51	0.45
1:B:724:HIS:CD2	1:B:726:MET:H	2.34	0.45
1:A:494:PRO:HB2	1:A:760:GLY:CA	2.46	0.45
1:A:707:PHE:HA	1:A:1042:THR:HG21	1.98	0.45
1:B:663:ALA:N	1:B:690:TYR:HH	2.14	0.45
1:A:674:VAL:O	1:A:687:MET:HE1	2.16	0.45
1:A:678:LEU:CD1	1:A:682:LEU:HD11	2.46	0.45
1:A:758:ALA:O	1:A:760:GLY:N	2.50	0.45
1:A:764:VAL:CG1	1:A:782:GLN:HA	2.47	0.45
1:A:812:TYR:O	1:A:816:MET:HB2	2.17	0.45
1:B:678:LEU:CB	1:B:682:LEU:HD11	2.46	0.45
1:B:959:PRO:HB3	1:B:964:PHE:O	2.16	0.45
1:B:1024:LEU:O	1:B:1028:TYR:HD2	1.99	0.45
1:A:753:ASP:OD1	1:A:755:ARG:NH1	2.50	0.45
1:A:866:HIS:HD2	1:A:868:ALA:HB3	1.82	0.45
1:B:577:VAL:O	1:B:1031:ILE:HB	2.17	0.45
1:B:635:HIS:HD1	1:B:635:HIS:N	2.08	0.45
1:B:961:HIS:ND1	1:B:963:LEU:HB2	2.31	0.45
1:A:662:ALA:HB3	1:A:665:VAL:HG13	1.98	0.45
1:B:915:ASP:C	1:B:917:GLY:H	2.19	0.45
1:B:1004:GLN:O	1:B:1005:PRO:C	2.54	0.45
1:A:652:ILE:HG21	1:A:682:LEU:CD2	2.46	0.45
1:A:743:MET:HE3	1:A:785:HIS:CE1	2.52	0.45
1:A:875:VAL:O	1:A:879:PHE:HD1	2.00	0.45
1:A:1032:SER:HB2	1:A:1033:PRO:HD2	1.97	0.45
1:B:542:GLU:HG3	1:B:542:GLU:O	2.17	0.45
1:B:725:LEU:O	1:B:728:ASP:HB3	2.16	0.45
1:A:595:ARG:O	1:A:599:LEU:HB2	2.17	0.45
1:B:656:TRP:CE2	1:B:686:CYS:HB2	2.51	0.45
1:A:871:VAL:O	1:A:874:THR:HB	2.17	0.45
1:A:915:ASP:CG	1:A:916:ALA:H	2.18	0.45
1:B:673:TYR:C	1:B:675:VAL:N	2.69	0.45
1:A:724:HIS:CD2	1:A:725:LEU:N	2.85	0.45
1:A:879:PHE:CE2	1:A:886:VAL:HG21	2.52	0.45
1:A:939:LEU:O	1:A:969:HIS:CE1	2.65	0.45
1:B:835:VAL:O	1:B:836:TYR:C	2.55	0.45
1:B:860:ASP:OD1	1:B:862:ALA:HB3	2.17	0.45
1:B:867:PRO:HA	1:B:870:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ARG:CA	1:A:1003:ARG:HH21	2.29	0.44
1:A:836:TYR:CE1	1:A:901:MET:HB2	2.51	0.44
1:A:874:THR:O	1:A:877:ALA:N	2.50	0.44
1:A:653:THR:HG22	1:A:657:ASN:ND2	2.28	0.44
1:A:835:VAL:O	1:A:836:TYR:C	2.56	0.44
1:B:674:VAL:HG11	1:B:690:TYR:CD2	2.52	0.44
1:B:875:VAL:HG23	1:B:879:PHE:HE1	1.79	0.44
1:A:493:ALA:HB2	1:A:560:GLY:HA2	1.98	0.44
1:A:1036:LEU:HD13	1:A:1036:LEU:HA	1.63	0.44
1:B:733:PRO:HB3	1:B:810:LYS:HG3	1.98	0.44
1:B:797:ASP:CG	1:B:798:ARG:H	2.21	0.44
1:B:1026:ALA:C	1:B:1028:TYR:N	2.69	0.44
1:A:490:TYR:CG	1:A:564:PRO:HG3	2.53	0.44
1:A:782:GLN:H	1:A:904:ARG:NH2	2.06	0.44
1:B:617:ALA:C	1:B:940:MET:CE	2.86	0.44
1:B:656:TRP:CZ2	1:B:660:ARG:NH2	2.85	0.44
1:B:911:SER:O	1:B:912:ALA:HB2	2.18	0.44
1:B:1036:LEU:HD13	1:B:1036:LEU:HA	1.58	0.44
1:A:512:ARG:HE	1:A:563:VAL:CG1	2.30	0.44
1:A:728:ASP:HA	1:A:729:PRO:HD2	1.79	0.44
1:B:487:TYR:C	1:B:487:TYR:CD2	2.91	0.44
1:B:830:VAL:CG2	1:B:937:ILE:HD12	2.48	0.44
1:B:839:LEU:HD22	1:B:894:LEU:HD13	1.98	0.44
1:A:509:TRP:O	1:A:513:LEU:HG	2.17	0.44
1:A:755:ARG:HH11	1:A:927:ARG:NH2	2.14	0.44
1:A:915:ASP:C	1:A:917:GLY:H	2.21	0.44
1:B:911:SER:CB	1:B:929:PHE:CD1	2.99	0.44
1:A:1020:LEU:HD11	1:A:1024:LEU:HD11	1.99	0.44
1:B:644:LEU:H	1:B:644:LEU:CD1	2.29	0.44
1:A:509:TRP:CZ2	1:A:564:PRO:HD3	2.53	0.44
1:A:845:PRO:CG	1:A:862:ALA:O	2.66	0.44
1:B:500:ASP:O	1:B:501:MET:C	2.56	0.44
1:B:1026:ALA:O	1:B:1028:TYR:N	2.51	0.44
1:A:554:ALA:HB2	1:A:568:PRO:O	2.18	0.43
1:A:570:GLU:HG3	1:A:571:ILE:N	2.31	0.43
1:A:743:MET:SD	1:A:797:ASP:O	2.76	0.43
1:A:841:ASN:HD21	1:A:874:THR:HA	1.83	0.43
1:B:548:ASP:O	1:B:573:ALA:HA	2.18	0.43
1:B:614:VAL:HG21	1:B:693:LEU:HD11	1.98	0.43
1:A:652:ILE:HA	1:A:663:ALA:HB2	2.00	0.43
1:A:674:VAL:HG11	1:A:690:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:LEU:O	1:A:728:ASP:HB3	2.18	0.43
1:A:827:THR:HG23	1:A:964:PHE:HB2	1.99	0.43
1:B:584:LEU:HD23	1:B:587:CYS:O	2.17	0.43
1:B:630:LEU:HD23	1:B:630:LEU:HA	1.85	0.43
1:B:939:LEU:O	1:B:969:HIS:HE1	2.00	0.43
1:A:543:LEU:N	1:A:543:LEU:HD23	2.34	0.43
1:A:673:TYR:C	1:A:675:VAL:N	2.70	0.43
1:A:830:VAL:CG2	1:A:937:ILE:HD12	2.48	0.43
1:A:1009:HIS:CD2	1:A:1009:HIS:C	2.91	0.43
1:B:499:ALA:HB2	1:B:956:TYR:CZ	2.54	0.43
1:B:575:TRP:HZ2	1:B:1031:ILE:HG22	1.82	0.43
1:B:765:TYR:CD1	1:B:765:TYR:N	2.84	0.43
1:B:893:THR:O	1:B:895:GLN:N	2.52	0.43
1:A:1002:ILE:HG13	1:A:1006:VAL:HG21	1.99	0.43
1:B:570:GLU:HG3	1:B:571:ILE:N	2.33	0.43
1:B:830:VAL:HG22	1:B:937:ILE:HD12	2.01	0.43
1:A:962:ALA:N	1:A:990:VAL:HG21	2.33	0.43
1:B:743:MET:HG3	1:B:765:TYR:HE2	1.83	0.43
1:B:893:THR:C	1:B:895:GLN:N	2.72	0.43
1:A:841:ASN:O	1:A:841:ASN:ND2	2.51	0.43
1:A:931:GLY:O	1:A:932:ALA:HB2	2.18	0.43
1:A:944:HIS:HB3	1:A:947:HIS:CD2	2.53	0.43
1:B:541:LEU:HD12	1:B:541:LEU:N	2.34	0.43
1:B:847:ILE:HD13	1:B:853:CYS:HA	2.00	0.43
1:A:764:VAL:O	1:A:782:GLN:HA	2.18	0.43
1:A:927:ARG:HH11	1:A:927:ARG:HB2	1.83	0.43
1:A:1002:ILE:HD12	1:A:1028:TYR:CZ	2.54	0.43
1:B:741:ALA:O	1:B:745:ARG:HB2	2.19	0.43
1:A:687:MET:HG3	1:A:691:ARG:NE	2.33	0.43
1:A:740:ASP:OD1	1:A:801:ARG:N	2.48	0.43
1:A:745:ARG:NH1	1:A:754:CYS:HB3	2.34	0.43
1:A:857:PRO:HB3	1:A:863:HIS:CE1	2.54	0.43
1:A:927:ARG:HH11	1:A:927:ARG:CB	2.32	0.43
1:B:597:LEU:C	1:B:597:LEU:CD1	2.87	0.43
1:B:678:LEU:CB	1:B:682:LEU:CD1	2.97	0.43
1:B:764:VAL:CG1	1:B:782:GLN:HA	2.49	0.43
1:B:848:ALA:O	1:B:851:GLU:HB2	2.19	0.43
1:B:984:SER:HA	1:B:989:LEU:HD21	2.01	0.43
1:A:830:VAL:HG22	1:A:955:PHE:HD2	1.84	0.42
1:A:835:VAL:HA	1:A:954:TYR:HD2	1.84	0.42
1:A:1030:LYS:HB2	1:A:1035:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:ALA:C	1:B:645:ALA:H	2.22	0.42
1:A:615:ARG:O	1:A:616:GLY:C	2.57	0.42
1:B:556:VAL:O	1:B:558:LEU:N	2.51	0.42
1:A:640:VAL:HG12	1:A:644:LEU:HD13	2.00	0.42
1:A:663:ALA:N	1:A:690:TYR:HH	2.17	0.42
1:B:662:ALA:CB	1:B:665:VAL:CG1	2.96	0.42
1:B:674:VAL:HG12	1:B:674:VAL:O	2.19	0.42
1:B:857:PRO:HB3	1:B:863:HIS:CE1	2.53	0.42
1:A:544:HIS:CE1	1:A:545:PRO:HD2	2.54	0.42
1:A:670:LEU:O	1:A:671:VAL:C	2.56	0.42
1:A:875:VAL:HG23	1:A:879:PHE:HE1	1.82	0.42
1:B:485:ASN:HD22	1:B:486:PRO:HD2	1.84	0.42
1:B:578:VAL:HB	1:B:1027:GLY:O	2.18	0.42
1:B:724:HIS:HE1	1:B:1025:MET:O	2.02	0.42
1:B:831:ARG:CZ	1:B:834:ARG:HG3	2.49	0.42
1:B:647:LEU:O	1:B:647:LEU:HD12	2.19	0.42
1:B:753:ASP:O	1:B:927:ARG:NH2	2.53	0.42
1:A:635:HIS:HD1	1:A:635:HIS:H	1.65	0.42
1:A:765:TYR:CD1	1:A:765:TYR:N	2.86	0.42
1:A:965:ALA:O	1:A:966:GLY:C	2.57	0.42
1:B:967:ALA:HB1	1:B:985:ARG:NH1	2.34	0.42
1:B:625:ALA:O	1:B:626:VAL:C	2.58	0.42
1:B:726:MET:O	1:B:810:LYS:NZ	2.45	0.42
1:B:742:LEU:HD11	1:B:908:LEU:HD21	2.01	0.42
1:B:1002:ILE:HD12	1:B:1028:TYR:CZ	2.55	0.42
1:A:1003:ARG:H	1:A:1003:ARG:HG2	1.53	0.42
1:B:721:GLU:HG2	1:B:729:PRO:CD	2.50	0.42
1:A:512:ARG:CZ	1:A:564:PRO:HD2	2.49	0.42
1:A:664:PHE:CD1	1:A:664:PHE:N	2.87	0.42
1:A:945:LEU:HD12	1:A:945:LEU:N	2.32	0.42
1:B:615:ARG:O	1:B:618:PHE:N	2.52	0.42
1:B:626:VAL:CG2	1:B:878:MET:HB3	2.39	0.42
1:B:709:LEU:HB2	1:B:1038:HIS:CE1	2.55	0.42
1:B:875:VAL:CG2	1:B:879:PHE:HE1	2.32	0.42
1:B:1019:ALA:O	1:B:1021:THR:N	2.52	0.42
1:A:1017:GLU:OE2	1:A:1017:GLU:N	2.52	0.42
1:B:640:VAL:HG12	1:B:644:LEU:HD13	2.01	0.42
1:B:650:GLN:OE1	1:B:886:VAL:HA	2.20	0.42
1:B:673:TYR:C	1:B:675:VAL:H	2.22	0.42
1:A:733:PRO:HB3	1:A:810:LYS:CG	2.50	0.41
1:A:737:TRP:CZ3	1:A:935:ALA:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ARG:O	1:A:752:ARG:N	2.49	0.41
1:B:509:TRP:O	1:B:513:LEU:HG	2.21	0.41
1:B:812:TYR:O	1:B:816:MET:HB2	2.20	0.41
1:B:1022:TYR:O	1:B:1023:ALA:C	2.59	0.41
1:A:706:ASP:O	1:A:707:PHE:CD2	2.74	0.41
1:A:822:ARG:HA	1:A:1010:VAL:CG1	2.50	0.41
1:A:875:VAL:CG2	1:A:879:PHE:HE1	2.33	0.41
1:A:945:LEU:HA	1:A:950:GLN:HG2	2.02	0.41
1:B:734:PRO:HD3	1:B:814:TYR:CZ	2.54	0.41
1:B:857:PRO:O	1:B:866:HIS:HA	2.21	0.41
1:B:1003:ARG:H	1:B:1003:ARG:HG2	1.54	0.41
1:B:1020:LEU:HD11	1:B:1024:LEU:HD11	2.02	0.41
1:A:668:TYR:HD2	1:A:809:HIS:CE1	2.37	0.41
1:A:830:VAL:HG22	1:A:937:ILE:HD12	2.02	0.41
1:A:833:ASP:O	1:A:834:ARG:C	2.58	0.41
1:A:837:ALA:C	1:A:839:LEU:N	2.74	0.41
1:A:925:ASN:O	1:A:926:MET:C	2.59	0.41
1:B:678:LEU:HD13	1:B:682:LEU:HD11	2.02	0.41
1:A:627:PHE:N	1:A:627:PHE:CD1	2.88	0.41
1:A:630:LEU:HD23	1:A:630:LEU:HA	1.76	0.41
1:A:807:VAL:O	1:A:810:LYS:N	2.54	0.41
1:A:1002:ILE:HD12	1:A:1028:TYR:HE1	1.81	0.41
1:B:567:GLY:HA3	1:B:568:PRO:HD2	1.89	0.41
1:B:628:TYR:HB3	1:B:955:PHE:CE1	2.56	0.41
1:B:664:PHE:CD1	1:B:664:PHE:N	2.89	0.41
1:B:717:GLN:HE22	1:B:752:ARG:NH1	2.19	0.41
1:A:933:LEU:HD21	1:A:958:LEU:CD2	2.51	0.41
1:B:604:HIS:CD2	1:B:696:HIS:ND1	2.78	0.41
1:B:752:ARG:HD2	1:B:752:ARG:HA	1.88	0.41
1:B:755:ARG:HH11	1:B:927:ARG:NH2	2.18	0.41
1:A:541:LEU:N	1:A:541:LEU:HD12	2.35	0.41
1:A:584:LEU:HD23	1:A:587:CYS:O	2.21	0.41
1:A:624:PRO:HG2	1:A:627:PHE:CD2	2.55	0.41
1:A:775:ASP:OD2	1:A:778:ARG:HB3	2.21	0.41
1:B:517:ARG:HD2	1:B:517:ARG:HA	1.78	0.41
1:A:548:ASP:HB2	1:A:574:THR:HG23	2.02	0.41
1:A:625:ALA:O	1:A:626:VAL:C	2.58	0.41
1:A:961:HIS:C	1:A:990:VAL:HG21	2.41	0.41
1:B:742:LEU:HD12	1:B:908:LEU:HD21	2.03	0.41
1:B:766:ALA:HB3	1:B:784:LEU:HD23	2.03	0.41
1:B:933:LEU:HD11	1:B:958:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:HD23	1:A:571:ILE:HD11	2.02	0.41
1:A:595:ARG:HH11	1:A:595:ARG:CB	2.34	0.41
1:A:700:LEU:HD21	1:A:1021:THR:CG2	2.50	0.41
1:A:721:GLU:HG2	1:A:729:PRO:CD	2.50	0.41
1:A:831:ARG:CZ	1:A:834:ARG:HG3	2.51	0.41
1:B:544:HIS:HA	1:B:545:PRO:HD3	1.85	0.41
1:B:623:TYR:HA	1:B:624:PRO:HD2	1.85	0.41
1:B:708:THR:HG22	1:B:709:LEU:N	2.36	0.41
1:B:733:PRO:HD3	1:B:810:LYS:HD2	2.03	0.41
1:B:817:VAL:HB	1:B:818:PRO:CD	2.44	0.41
1:B:1009:HIS:CD2	1:B:1009:HIS:C	2.93	0.41
1:A:550:PHE:CE2	1:A:998:TYR:HB3	2.57	0.41
1:A:607:ALA:HB1	1:A:608:PRO:HD2	2.03	0.41
1:A:696:HIS:C	1:A:698:GLU:N	2.71	0.41
1:A:991:PRO:HA	1:A:992:PRO:HD2	1.99	0.41
1:B:600:GLY:O	1:B:601:VAL:C	2.59	0.41
1:B:721:GLU:HG2	1:B:729:PRO:HD3	2.02	0.41
1:A:641:PHE:CE2	1:A:673:TYR:HB3	2.55	0.40
1:A:1009:HIS:HD2	1:A:1013:SER:HB2	1.82	0.40
1:B:671:VAL:HG11	1:B:693:LEU:HD23	2.03	0.40
1:B:817:VAL:CB	1:B:818:PRO:HD3	2.44	0.40
1:B:875:VAL:O	1:B:879:PHE:HD1	2.04	0.40
1:B:1039:GLN:HG2	1:B:1044:LEU:CD2	2.51	0.40
1:A:787:THR:HB	1:A:801:ARG:NH2	2.21	0.40
1:A:813:TYR:HA	1:A:817:VAL:CG2	2.51	0.40
1:A:820:PHE:CE2	1:A:1017:GLU:HG2	2.56	0.40
1:A:911:SER:O	1:A:912:ALA:HB2	2.21	0.40
1:A:1002:ILE:CD1	1:A:1028:TYR:OH	2.69	0.40
1:A:1026:ALA:C	1:A:1028:TYR:N	2.73	0.40
1:B:502:GLN:HG3	1:B:958:LEU:HA	2.03	0.40
1:B:813:TYR:HA	1:B:817:VAL:CG2	2.51	0.40
1:A:512:ARG:HH21	1:A:563:VAL:HG12	1.85	0.40
1:A:578:VAL:HG11	1:A:1028:TYR:HA	2.03	0.40
1:A:662:ALA:CB	1:A:665:VAL:CG1	2.99	0.40
1:A:696:HIS:HE2	1:A:1021:THR:CG2	2.17	0.40
1:A:754:CYS:HA	1:A:911:SER:O	2.20	0.40
1:B:544:HIS:ND1	1:B:545:PRO:CD	2.83	0.40
1:A:721:GLU:HG2	1:A:729:PRO:HD3	2.04	0.40
1:B:486:PRO:O	1:B:487:TYR:C	2.57	0.40
1:B:696:HIS:O	1:B:699:ALA:N	2.53	0.40
1:A:584:LEU:HA	1:A:587:CYS:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ASN:H	1:A:773:THR:HB	1.86	0.40
1:A:785:HIS:CG	1:A:785:HIS:O	2.75	0.40
1:B:543:LEU:HD23	1:B:543:LEU:N	2.37	0.40
1:B:670:LEU:O	1:B:671:VAL:C	2.59	0.40
1:B:743:MET:SD	1:B:797:ASP:O	2.80	0.40
1:B:903:GLU:HG3	1:B:904:ARG:H	1.85	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	536/604 (89%)	379 (71%)	122 (23%)	35 (6%)	1 3
1	B	524/604 (87%)	367 (70%)	125 (24%)	32 (6%)	1 4
All	All	1060/1208 (88%)	746 (70%)	247 (23%)	67 (6%)	1 4

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	HIS
1	A	660	ARG
1	A	837	ALA
1	B	660	ARG
1	B	837	ALA
1	A	497	PRO
1	A	674	VAL
1	A	751	HIS
1	A	838	THR
1	B	497	PRO
1	B	501	MET
1	B	635	HIS

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Mol	Chain	Res	Type
1	B	674	VAL
1	B	751	HIS
1	B	838	THR
1	B	1020	LEU
1	A	501	MET
1	A	515	HIS
1	A	566	ALA
1	A	805	TRP
1	A	870	LEU
1	A	940	MET
1	B	506	LEU
1	B	515	HIS
1	B	546	ALA
1	B	566	ALA
1	B	805	TRP
1	B	870	LEU
1	B	915	ASP
1	B	934	HIS
1	B	940	MET
1	A	604	HIS
1	A	609	ALA
1	A	644	LEU
1	A	915	ASP
1	A	934	HIS
1	A	945	LEU
1	A	1020	LEU
1	B	604	HIS
1	B	679	GLY
1	B	894	LEU
1	B	965	ALA
1	A	506	LEU
1	A	565	PRO
1	A	601	VAL
1	A	679	GLY
1	A	684	GLU
1	A	974	PRO
1	B	565	PRO
1	B	974	PRO
1	A	685	GLU
1	A	689	VAL
1	A	825	CYS
1	A	835	VAL

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Mol	Chain	Res	Type
1	B	601	VAL
1	B	626	VAL
1	B	689	VAL
1	B	916	ALA
1	A	626	VAL
1	B	835	VAL
1	B	624	PRO
1	A	634	ILE
1	A	942	PRO
1	A	1002	ILE
1	B	545	PRO
1	A	1010	VAL
1	B	568	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	416/467 (89%)	372 (89%)	44 (11%)	6 20
1	B	409/467 (88%)	371 (91%)	38 (9%)	9 27
All	All	825/934 (88%)	743 (90%)	82 (10%)	8 24

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	485	ASN
1	A	497	PRO
1	A	500	ASP
1	A	548	ASP
1	A	558	LEU
1	A	562	ASP
1	A	563	VAL
1	A	578	VAL
1	A	592	ARG
1	A	595	ARG

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Mol	Chain	Res	Type
1	A	599	LEU
1	A	621	ARG
1	A	666	ASN
1	A	677	TYR
1	A	693	LEU
1	A	726	MET
1	A	727	ARG
1	A	731	LEU
1	A	762	ASP
1	A	771	VAL
1	A	779	ASN
1	A	783	LEU
1	A	790	ARG
1	A	804	ASP
1	A	816	MET
1	A	826	CYS
1	A	838	THR
1	A	839	LEU
1	A	841	ASN
1	A	856	ASP
1	A	865	LEU
1	A	875	VAL
1	A	876	ASN
1	A	905	THR
1	A	908	LEU
1	A	925	ASN
1	A	926	MET
1	A	937	ILE
1	A	949	ILE
1	A	958	LEU
1	A	985	ARG
1	A	1003	ARG
1	A	1024	LEU
1	A	1031	ILE
1	B	485	ASN
1	B	500	ASP
1	B	548	ASP
1	B	558	LEU
1	B	562	ASP
1	B	592	ARG
1	B	595	ARG
1	B	599	LEU

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Mol	Chain	Res	Type
1	B	621	ARG
1	B	677	TYR
1	B	726	MET
1	B	727	ARG
1	B	731	LEU
1	B	762	ASP
1	B	771	VAL
1	B	779	ASN
1	B	783	LEU
1	B	790	ARG
1	B	801	ARG
1	B	804	ASP
1	B	816	MET
1	B	826	CYS
1	B	838	THR
1	B	839	LEU
1	B	841	ASN
1	B	856	ASP
1	B	865	LEU
1	B	875	VAL
1	B	876	ASN
1	B	905	THR
1	B	908	LEU
1	B	926	MET
1	B	937	ILE
1	B	958	LEU
1	B	985	ARG
1	B	1003	ARG
1	B	1024	LEU
1	B	1031	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	485	ASN
1	A	503	GLN
1	A	507	ASN
1	A	572	GLN
1	A	581	ASN
1	A	604	HIS
1	A	622	ASN
1	A	631	GLN

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Mol	Chain	Res	Type
1	A	639	HIS
1	A	657	ASN
1	A	658	ASN
1	A	666	ASN
1	A	717	GLN
1	A	724	HIS
1	A	779	ASN
1	A	841	ASN
1	A	866	HIS
1	A	876	ASN
1	A	925	ASN
1	A	944	HIS
1	A	947	HIS
1	A	969	HIS
1	A	986	GLN
1	A	997	ASN
1	A	1018	ASN
1	A	1037	HIS
1	A	1039	GLN
1	B	485	ASN
1	B	503	GLN
1	B	507	ASN
1	B	572	GLN
1	B	581	ASN
1	B	604	HIS
1	B	631	GLN
1	B	639	HIS
1	B	657	ASN
1	B	658	ASN
1	B	666	ASN
1	B	724	HIS
1	B	779	ASN
1	B	786	ASN
1	B	841	ASN
1	B	866	HIS
1	B	876	ASN
1	B	986	GLN
1	B	997	ASN
1	B	1018	ASN
1	B	1037	HIS
1	B	1039	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	555:ASP	C	556:VAL	N	1.11
1	A	552:GLY	C	553:VAL	N	0.95

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	542/604 (89%)	-0.24	16 (2%)	50	45	8, 54, 122, 193	0
1	B	534/604 (88%)	-0.21	10 (1%)	66	65	13, 58, 124, 166	0
All	All	1076/1208 (89%)	-0.23	26 (2%)	59	56	8, 55, 124, 193	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	714	LEU	7.4
1	A	715	GLY	5.7
1	B	565	PRO	5.4
1	B	714	LEU	4.9
1	A	716	GLY	4.5
1	B	1045	HIS	4.1
1	B	558	LEU	3.9
1	A	919	ASN	3.9
1	A	558	LEU	3.7
1	A	568	PRO	3.6
1	A	565	PRO	3.6
1	A	712	PRO	3.5
1	B	564	PRO	3.4
1	A	564	PRO	3.2
1	B	566	ALA	3.1
1	A	566	ALA	2.8
1	B	556	VAL	2.7
1	A	553	VAL	2.4
1	B	712	PRO	2.4
1	A	918	ALA	2.4
1	A	541	LEU	2.4
1	B	916	ALA	2.3
1	B	517	ARG	2.2
1	A	515	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	751	HIS	2.0
1	A	554	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.