



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:13 AM UTC

PDB ID : 1NO7 / pdb_00001no7
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.; Quioco, 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

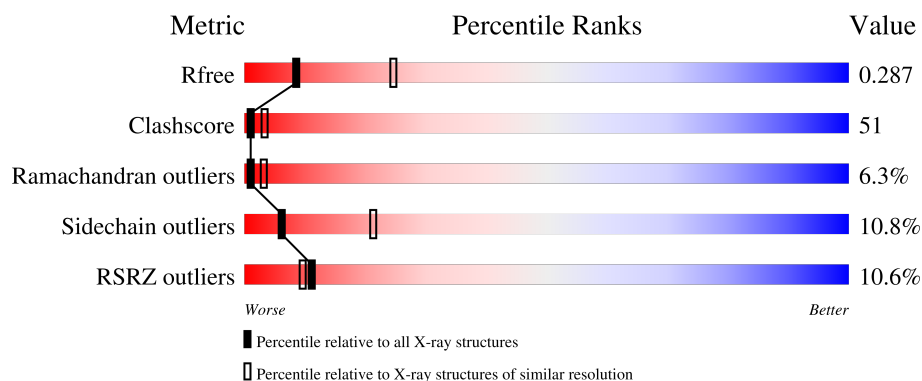
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	10% 29% 47% 13% • 10%
1	B	604	9% 30% 46% 12% • 12%

2 Entry composition

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.

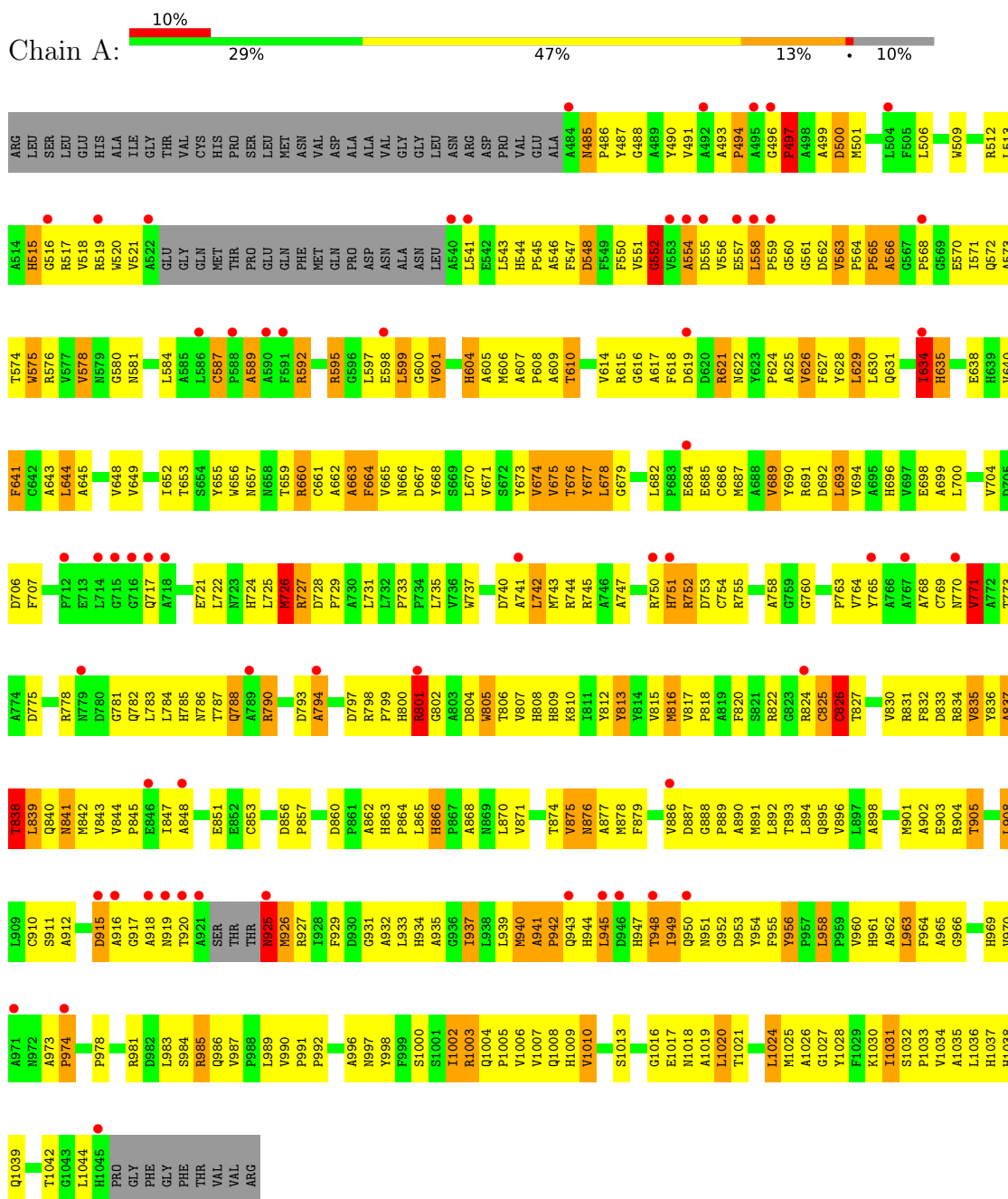
- Molecule 1 is a protein called Major capsid protein.

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

3 Residue-property plots

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 B:



4 Data and refinement statistics

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 47.09 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.3 (47.09-2.90) 91.4 (47.09-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.29 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.84	10/4235 (0.2%)	1.39	49/5798 (0.8%)
1	B	0.70	9/4169 (0.2%)	1.31	46/5704 (0.8%)
All	All	0.77	19/8404 (0.2%)	1.35	95/11502 (0.8%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	GLY	C-N	-25.63	0.95	1.33
1	A	800	HIS	CB-CG	-20.51	1.21	1.50
1	B	800	HIS	CB-CG	-20.10	1.22	1.50
1	A	555	ASP	C-N	-10.93	1.11	1.33
1	B	801	ARG	CB-CG	-10.41	1.21	1.52
1	A	794	ALA	N-CA	-8.52	1.35	1.46
1	A	920	THR	C-N	-7.50	1.22	1.33
1	A	676	THR	C-N	-6.89	1.22	1.33
1	B	842	MET	SD-CE	5.89	1.94	1.79
1	A	799	PRO	C-N	-5.80	1.26	1.33
1	A	678	LEU	C-N	5.75	1.42	1.33
1	B	676	THR	C-N	-5.64	1.24	1.33
1	B	794	ALA	N-CA	-5.61	1.39	1.46
1	A	801	ARG	C-O	5.53	1.29	1.23
1	A	726	MET	SD-CE	5.33	1.92	1.79
1	B	891	MET	SD-CE	5.29	1.92	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	925	ASN	C-N	-5.05	1.27	1.33
1	B	799	PRO	C-N	-5.04	1.27	1.33
1	B	794	ALA	CA-C	-5.04	1.47	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	554	ALA	N-CA-C	33.33	147.30	110.97
1	A	554	ALA	N-CA-C	33.32	147.29	110.97
1	A	800	HIS	CA-CB-CG	24.41	138.21	113.80
1	B	800	HIS	CA-CB-CG	23.77	137.57	113.80
1	A	677	TYR	N-CA-C	22.41	145.28	114.12
1	B	677	TYR	N-CA-C	18.78	140.22	114.12
1	A	677	TYR	CB-CA-C	-12.81	87.86	109.38
1	A	552	GLY	CA-C-N	12.80	139.06	122.93
1	A	552	GLY	C-N-CA	12.80	139.06	122.93
1	A	555	ASP	CA-C-N	12.26	140.09	121.71
1	A	555	ASP	C-N-CA	12.26	140.09	121.71
1	B	677	TYR	CB-CG-CD1	11.88	138.61	120.80
1	B	677	TYR	CB-CG-CD2	-11.80	103.10	120.80
1	A	677	TYR	CB-CG-CD1	11.72	138.38	120.80
1	B	677	TYR	CB-CA-C	-11.67	89.78	109.38
1	A	677	TYR	CB-CG-CD2	-11.54	103.49	120.80
1	B	800	HIS	CB-CG-CD2	10.90	145.37	131.20
1	A	800	HIS	CB-CG-CD2	10.51	144.86	131.20
1	A	920	THR	CA-C-N	-9.73	104.18	121.70
1	A	920	THR	C-N-CA	-9.73	104.18	121.70
1	A	677	TYR	CA-CB-CG	9.72	131.40	113.90
1	A	918	ALA	N-CA-C	-9.71	102.52	114.75
1	B	800	HIS	CB-CG-ND1	-9.52	108.42	122.70
1	A	678	LEU	N-CA-CB	-9.41	94.59	110.49
1	B	677	TYR	CA-CB-CG	9.30	130.65	113.90
1	A	771	VAL	N-CA-C	-9.17	104.21	113.47
1	A	555	ASP	CA-C-O	-9.11	109.03	119.05
1	B	555	ASP	CA-C-O	-9.07	109.07	119.05
1	A	800	HIS	CB-CG-ND1	-8.66	109.71	122.70
1	B	941	ALA	N-CA-C	-8.61	100.23	110.13
1	A	941	ALA	N-CA-C	-8.59	100.25	110.13
1	A	925	ASN	N-CA-C	8.33	134.31	111.00
1	B	801	ARG	CA-CB-CG	7.92	129.94	114.10
1	A	948	THR	N-CA-C	7.81	119.79	111.28
1	B	678	LEU	N-CA-CB	-7.75	97.40	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	771	VAL	N-CA-C	-7.61	105.14	113.43
1	B	1016	GLY	N-CA-C	-7.55	104.02	112.33
1	A	919	ASN	N-CA-C	-7.52	103.56	112.89
1	A	925	ASN	CA-CB-CG	-7.47	105.13	112.60
1	A	1016	GLY	N-CA-C	-7.09	104.53	112.33
1	B	615	ARG	N-CA-C	-6.92	103.43	110.97
1	B	593	ASP	N-CA-C	-6.74	103.63	110.97
1	B	866	HIS	N-CA-C	-6.72	101.60	110.07
1	A	866	HIS	N-CA-C	-6.69	101.63	109.93
1	A	554	ALA	O-C-N	6.63	128.93	122.03
1	B	554	ALA	O-C-N	6.59	128.89	122.03
1	B	552	GLY	CA-C-N	6.38	131.81	122.94
1	B	552	GLY	C-N-CA	6.38	131.81	122.94
1	A	496	GLY	CA-C-N	6.22	127.61	119.84
1	A	496	GLY	C-N-CA	6.22	127.61	119.84
1	B	587	CYS	CA-C-N	6.10	126.06	119.78
1	B	587	CYS	C-N-CA	6.10	126.06	119.78
1	A	752	ARG	N-CA-C	-5.94	98.15	110.80
1	B	556	VAL	N-CA-C	5.82	117.16	108.54
1	B	485	ASN	CA-C-N	5.74	126.50	120.12
1	B	485	ASN	C-N-CA	5.74	126.50	120.12
1	B	589	ALA	N-CA-C	-5.72	104.73	110.97
1	B	575	TRP	N-CA-C	5.67	118.66	108.17
1	B	675	VAL	N-CA-C	-5.67	106.94	111.81
1	B	555	ASP	O-C-N	5.65	129.30	122.35
1	A	485	ASN	CA-C-N	5.62	126.86	119.84
1	A	485	ASN	C-N-CA	5.62	126.86	119.84
1	A	634	ILE	CB-CA-C	-5.58	102.14	111.29
1	A	663	ALA	N-CA-C	5.57	117.05	110.97
1	B	799	PRO	O-C-N	-5.55	116.50	123.21
1	A	587	CYS	CA-C-N	5.54	125.48	119.78
1	A	587	CYS	C-N-CA	5.54	125.48	119.78
1	A	675	VAL	N-CA-C	-5.52	106.42	111.67
1	A	826	CYS	N-CA-C	5.51	117.47	108.55
1	B	496	GLY	CA-C-N	5.50	126.72	119.84
1	B	496	GLY	C-N-CA	5.50	126.72	119.84
1	A	589	ALA	N-CA-C	-5.45	104.99	111.03
1	A	554	ALA	CB-CA-C	-5.44	102.59	110.96
1	B	554	ALA	CB-CA-C	-5.42	102.62	110.96
1	B	641	PHE	N-CA-C	-5.40	105.50	111.71
1	B	768	ALA	N-CA-C	5.34	116.27	108.14
1	B	926	MET	N-CA-C	-5.34	99.39	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	799	PRO	O-C-N	-5.33	116.77	123.21
1	B	725	LEU	N-CA-C	5.33	116.89	111.14
1	B	664	PHE	N-CA-C	5.31	119.27	112.26
1	A	813	TYR	N-CA-C	5.29	117.13	111.36
1	A	956	TYR	CA-C-N	5.23	125.15	119.76
1	A	956	TYR	C-N-CA	5.23	125.15	119.76
1	B	811	ILE	CB-CA-C	-5.21	105.21	111.88
1	B	911	SER	N-CA-C	5.17	115.16	107.88
1	A	575	TRP	N-CA-C	5.16	117.11	108.23
1	B	1003	ARG	N-CA-C	5.10	118.27	110.36
1	A	641	PHE	N-CA-C	-5.09	105.73	111.28
1	A	768	ALA	N-CA-C	5.09	115.87	108.14
1	B	1034	VAL	CB-CA-C	-5.08	105.37	111.88
1	A	801	ARG	O-C-N	-5.08	116.12	122.11
1	B	830	VAL	N-CA-C	5.07	115.89	108.53
1	B	940	MET	N-CA-C	5.07	121.60	110.80
1	A	664	PHE	N-CA-C	5.03	119.56	111.81
1	B	663	ALA	N-CA-C	5.02	116.44	110.97

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	426	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4058	0	3932	409	0
All	All	8179	0	7918	828	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 51.

All (828) 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:926:MET:HE3	1:B:926:MET:HA	1.23	1.15
1:A:618:PHE:HA	1:A:940:MET:HE3	1.24	1.14
1:B:618:PHE:HA	1:B:940:MET:HE3	1.16	1.08
1:A:610:THR:HG22	1:A:689:VAL:HA	1.37	1.07
1:A:949:ILE:HD12	1:A:949:ILE:H	1.20	1.03
1:A:606:MET:HE1	1:A:816:MET:HE1	1.40	1.02
1:B:606:MET:HE1	1:B:816:MET:HE1	1.41	1.00
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:788:GLN:HE21	1:B:794:ALA:HA	1.28	0.95
1:A:726:MET:HE2	1:A:726:MET:HA	1.47	0.94
1:B:726:MET:HA	1:B:726:MET:HE2	1.49	0.94
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: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:B:926:MET:HA	1:B:926:MET:CE	2.02	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:B:618:PHE:HA	1:B:940:MET:CE	2.03	0.86
1:A:787:THR:O	1:A:801:ARG:NH2	2.08	0.86
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

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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:618:PHE:CA	1:B:940:MET:HE3	2.07	0.82
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: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: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
1:B:630:LEU:O	1:B:634:ILE:HG13	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:597:LEU:C	1:A:597:LEU:HD13	2.16	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:606:MET:HE2	1:A:696:HIS:CD2	2.28	0.68
1:A:997:ASN:HD21	1:A:1004:GLN:H	1.40	0.68
1:A:606:MET:CE	1:A:816:MET:HE1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:597:LEU:HD13	1:B:597:LEU:C	2.19	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:A:841:ASN:O	1:A:841:ASN:CG	2.39	0.66
1:B:816:MET:HE3	1:B:816:MET:HA	1.77	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:B:606:MET:HE2	1:B:696:HIS:CD2	2.32	0.65
1:B:898:ALA:HA	1:B:901:MET:HE3	1.78	0.64
1:A:499:ALA:HB2	1:A:956:TYR:CE2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:674:VAL:O	1:A:687:MET:HE1	2.00	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:617:ALA:C	1:B:940:MET:HE1	2.25	0.62
1:B:626:VAL:HA	1:B:629:LEU:HD13	1.82	0.62
1:A:830:VAL:HB	1:A:832:PHE:CE1	2.35	0.61
1:B:983:LEU:C	1:B:983:LEU:HD13	2.26	0.61
1:B:1034:VAL:O	1:B:1037:HIS:HB3	1.99	0.61
1:B:986:GLN:HG3	1:B:987:VAL:HG23	1.83	0.61
1:A:815:VAL:C	1:A:818:PRO:HD2	2.26	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:A:983:LEU:HD13	1:A:983:LEU:C	2.26	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:1009:HIS:CD2	1:B:1013:SER:HB2	2.37	0.60
1:A:816:MET:HE3	1:A:816:MET:HA	1.84	0.60
1:B:815:VAL:C	1:B:818:PRO:HD2	2.27	0.60
1:A:890:ALA:O	1:A:893:THR:OG1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:ASP:OD1	1:A:889:PRO:HD2	2.00	0.60
1:A:1000:SER:C	1:A:1002:ILE:H	2.09	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
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:606:MET:CE	1:B:816:MET:HE1	2.26	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:B:841:ASN:CG	1:B:841:ASN:O	2.43	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:617:ALA:C	1:A:940:MET:HE1	2.28	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:B:1000:SER:C	1:B:1002:ILE:H	2.09	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:726:MET:HA	1:A:726:MET:CE	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:804:ASP:HB3	1:B:808:HIS:CE1	2.40	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:A:1004:GLN:O	1:A:1005:PRO:C	2.49	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:1034:VAL:O	1:A:1037:HIS:HB3	2.05	0.56
1:B:743:MET:HE2	1:B:765:TYR:CD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:546:ALA:C	1:B:547:PHE:CD1	2.85	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:A:724:HIS:HD2	1:A:726:MET:H	1.55	0.54
1:A:581:ASN:ND2	1:A:1003:ARG:H	2.06	0.54
1:B:743:MET:HE2	1:B:765:TYR:CE2	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:ASN:C	1:B:485:ASN:HD22	2.16	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:A:1000:SER:C	1:A:1002:ILE:N	2.65	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
1:B:879:PHE:HE2	1:B:886:VAL:HG21	1.73	0.53
1:A:485:ASN:C	1:A:485:ASN:HD22	2.16	0.53
1:A:546:ALA:C	1:A:547:PHE:CD1	2.86	0.53
1:A:652:ILE:HG21	1:A:682:LEU:HD23	1.91	0.53
1:B:575:TRP:O	1:B:576:ARG:C	2.51	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: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:816:MET:HA	1:A:816:MET:CE	2.39	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:B:707:PHE:C	1:B:1042:THR:HG21	2.35	0.52
1:B:1000:SER:C	1:B:1002:ILE:N	2.64	0.52
1:A:597:LEU:C	1:A:597:LEU:CD1	2.83	0.52
1:A:497:PRO:HB2	1:A:500:ASP:HB2	1.91	0.52
1:A:606:MET:HE2	1:A:696:HIS:CG	2.44	0.52
1:A:629:LEU:HD12	1:A:629:LEU:N	2.11	0.52
1:A:758:ALA:C	1:A:760:GLY:H	2.16	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:B:893:THR:C	1:B:895:GLN:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:A:557:GLU:C	1:A:559:PRO:HD2	2.35	0.51
1:B:565:PRO:O	1:B:566:ALA:C	2.52	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:487:TYR:C	1:A:487:TYR:CD2	2.88	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:836:TYR:CE1	1:B:901:MET:HB2	2.46	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:A:565:PRO:O	1:A:566:ALA:C	2.54	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:804:ASP:O	1:B:805:TRP:C	2.54	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:A:743:MET:HE1	1:A:785:HIS:CD2	2.47	0.50
1:B:557:GLU:C	1:B:559:PRO:HD2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ARG:O	1:A:618:PHE:N	2.44	0.50
1:A:797:ASP:CG	1:A:798:ARG:H	2.19	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:915:ASP:CG	1:B:916:ALA:H	2.18	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:575:TRP:O	1:A:576:ARG:C	2.53	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:A:804:ASP:O	1:A:805:TRP:C	2.54	0.50
1:B:673:TYR:O	1:B:675:VAL:N	2.44	0.50
1:A:643:ALA:C	1:A:645:ALA:H	2.18	0.50
1:A:915:ASP:CG	1:A:916:ALA:H	2.18	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:663:ALA:N	1:B:690:TYR:HH	2.08	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:B:1004:GLN:O	1:B:1005:PRO:C	2.54	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
1:B:915:ASP:C	1:B:917:GLY:H	2.19	0.50
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:726:MET:HA	1:B:726:MET:CE	2.30	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:758:ALA:C	1:A:760:GLY:N	2.69	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:835:VAL:O	1:B:836:TYR:C	2.55	0.49
1:B:1031:ILE:O	1:B:1036:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:835:VAL:O	1:A:836:TYR:C	2.56	0.49
1:B:797:ASP:CG	1:B:798:ARG:H	2.21	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: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: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:B:673:TYR:C	1:B:675:VAL:N	2.69	0.49
1:A:915:ASP:C	1:A:917:GLY:H	2.21	0.48
1:B:487:TYR:C	1:B:487:TYR:CD2	2.91	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: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:500:ASP:O	1:B:501:MET:C	2.56	0.48
1:B:1026:ALA:C	1:B:1028:TYR:N	2.69	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: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:A:743:MET:HE1	1:A:785:HIS:NE2	2.29	0.48
1:B:597:LEU:HD13	1:B:597:LEU:O	2.13	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:A:673:TYR:C	1:A:675:VAL:N	2.70	0.48
1:A:1009:HIS:CD2	1:A:1009:HIS:C	2.91	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
1:B:673:TYR:C	1:B:675:VAL:H	2.22	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:512:ARG:NH2	1:B:563:VAL:HG12	2.29	0.48
1:B:617:ALA:C	1:B:940:MET:CE	2.86	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:696:HIS:C	1:A:698:GLU:N	2.71	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:597:LEU:C	1:B:597:LEU:CD1	2.87	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:643:ALA:C	1:B:645:ALA:H	2.22	0.47
1:A:615:ARG:O	1:A:616:GLY:C	2.57	0.47
1:B:515:HIS:ND1	1:B:516:GLY:N	2.63	0.47
1:B:606:MET:HE2	1:B:696:HIS:CG	2.50	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:670:LEU:O	1:A:671:VAL:C	2.56	0.47
1:A:743:MET:HE2	1:A:765:TYR:CD2	2.50	0.47
1:A:1039:GLN:HG2	1:A:1044:LEU:HD23	1.97	0.47
1:B:601:VAL:O	1:B:601:VAL:HG23	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:ALA:O	1:A:966:GLY:C	2.57	0.47
1:B:625:ALA:O	1:B:626:VAL:C	2.58	0.47
1:B:674:VAL:O	1:B:687:MET:HE1	2.15	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: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:B:1022:TYR:O	1:B:1023:ALA:C	2.59	0.46
1:B:871:VAL:O	1:B:874:THR:HB	2.15	0.46
1:B:893:THR:C	1:B:895:GLN:N	2.72	0.46
1:A:758:ALA:HA	1:A:908:LEU:HD12	1.98	0.46
1:A:833:ASP:O	1:A:834:ARG:C	2.58	0.46
1:A:837:ALA:C	1:A:839:LEU:N	2.74	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: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:A:618:PHE:CA	1:A:940:MET:CE	2.87	0.46
1:A:724:HIS:CD2	1:A:726:MET:H	2.33	0.46
1:A:625:ALA:O	1:A:626:VAL:C	2.58	0.46
1:A:724:HIS:HE1	1:A:1025:MET:O	1.99	0.46
1:A:546:ALA:O	1:A:575:TRP:HD1	1.99	0.46
1:A:888:GLY:O	1:A:892:LEU:HD23	2.16	0.46
1:A:961:HIS:C	1:A:990:VAL:HG21	2.41	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:721:GLU:OE1	1:A:729:PRO:HG3	2.16	0.45
1:A:742:LEU:HD12	1:A:908:LEU:HD21	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1009:HIS:CD2	1:B:1009:HIS:C	2.93	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:600:GLY:O	1:B:601:VAL:C	2.59	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:743:MET:HE1	1:B:785:HIS:NE2	2.31	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:A:652:ILE:HG21	1:A:682:LEU:CD2	2.46	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:486:PRO:O	1:B:487:TYR:C	2.57	0.45
1:B:656:TRP:CE2	1:B:686:CYS:HB2	2.51	0.45
1:B:618:PHE:N	1:B:940:MET:HE1	2.32	0.45
1:B:670:LEU:O	1:B:671:VAL:C	2.59	0.45
1:A:871:VAL:O	1:A:874:THR:HB	2.17	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: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
1:A:576:ARG:CA	1:A:1003:ARG:HH21	2.29	0.44
1:A:600:GLY:O	1:A:601:VAL:C	2.60	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ALA:HB2	1:A:560:GLY:HA2	1.98	0.44
1:A:926:MET:HE3	1:A:926:MET:HA	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: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: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:743:MET:HE1	1:B:785:HIS:CD2	2.52	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:B:911:SER:CB	1:B:929:PHE:CD1	2.99	0.44
1:A:778:ARG:HD2	1:A:903:GLU:CD	2.43	0.44
1:A:893:THR:C	1:A:895:GLN:H	2.26	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: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:B:778:ARG:HD2	1:B:903:GLU:CD	2.42	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
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:A:925:ASN:O	1:A:926:MET:C	2.59	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:758:ALA:C	1:B:760:GLY:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ALA:N	1:A:690:TYR:HH	2.16	0.43
1:A:830:VAL:CG2	1:A:937:ILE:HD12	2.48	0.43
1:B:837:ALA:C	1:B:839:LEU:N	2.76	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:618:PHE:CA	1:B:940:MET:CE	2.83	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:778:ARG:HH11	1:A:903:GLU:CD	2.27	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: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:673:TYR:C	1:A:675:VAL:H	2.26	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: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
1:B:744:ARG:NH2	1:B:802:GLY:C	2.77	0.42
1:A:984:SER:C	1:A:986:GLN:H	2.27	0.42
1:A:1038:HIS:O	1:A:1039:GLN:C	2.62	0.42
1:B:556:VAL:O	1:B:558:LEU:N	2.51	0.42
1:B:984:SER:C	1:B:986:GLN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:VAL:HG12	1:A:644:LEU:HD13	2.00	0.42
1:B:662:ALA:CB	1:B:665:VAL:CG1	2.96	0.42
1:B:674:VAL:O	1:B:674:VAL:HG12	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: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:A:887:ASP:OD1	1:A:887:ASP:C	2.62	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:607:ALA:O	1:A:608:PRO:C	2.62	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:B:485:ASN:C	1:B:485:ASN:ND2	2.77	0.42
1:B:961:HIS:O	1:B:962:ALA:C	2.62	0.42
1:B:967:ALA:HB1	1:B:985:ARG:NH1	2.34	0.42
1:B:742:LEU:HD11	1:B:908:LEU:HD21	2.01	0.42
1:B:758:ALA:C	1:B:760:GLY:N	2.78	0.42
1:B:940:MET:HE3	1:B:940:MET:HB3	1.87	0.42
1:B:1002:ILE:HD12	1:B:1028:TYR:CZ	2.55	0.42
1:A:485:ASN:C	1:A:485:ASN:ND2	2.77	0.42
1:A:648:VAL:O	1:A:649:VAL:C	2.61	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:750:ARG:C	1:A:752:ARG:H	2.26	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:511:GLN:O	1:B:512:ARG:C	2.63	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:A:733:PRO:HB3	1:A:810:LYS:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:VAL:O	1:A:1008:GLN:C	2.62	0.41
1:A:737:TRP:CZ3	1:A:935:ALA:HA	2.55	0.41
1:A:750:ARG:O	1:A:752:ARG:N	2.49	0.41
1:A:1006:VAL:O	1:A:1007:VAL:C	2.62	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:A:706:ASP:O	1:A:707:PHE:CD2	2.74	0.41
1:A:743:MET:HE2	1:A:765:TYR:CE2	2.55	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:778:ARG:HH11	1:B:903:GLU:CD	2.29	0.41
1:B:833:ASP:O	1:B:834:ARG:C	2.63	0.41
1:B:857:PRO:O	1:B:866:HIS:HA	2.21	0.41
1:B:891:MET:HE3	1:B:891:MET:HB2	1.66	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: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:A:1026:ALA:C	1:A:1028:TYR:N	2.73	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:744:ARG:NH2	1:A:802:GLY:C	2.79	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:A:1019:ALA:C	1:A:1021:THR:N	2.79	0.41
1:B:517:ARG:HD2	1:B:517:ARG:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PRO:O	1:A:487:TYR:C	2.63	0.41
1:A:548:ASP:HB2	1:A:574:THR:HG23	2.02	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
1:B:1019:ALA:C	1:B:1021:THR:N	2.78	0.41
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:607:ALA:O	1:B:608:PRO:C	2.64	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:1026:ALA:O	1:B:1027:GLY:C	2.64	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:991:PRO:HA	1:A:992:PRO:HD2	1.99	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:805:TRP:O	1:A:806:THR:C	2.63	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:707:PHE:C	1:A:1042:THR:HG21	2.45	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:893:THR:C	1:A:895:GLN:N	2.78	0.40
1:A:911:SER:O	1:A:912:ALA:HB2	2.21	0.40
1:A:950:GLN:C	1:A:952:GLY:H	2.30	0.40
1:A:1002:ILE:CD1	1:A:1028:TYR:OH	2.69	0.40
1:B:502:GLN:HG3	1:B:958:LEU:HA	2.03	0.40
1:B:696:HIS:C	1:B:698:GLU:N	2.79	0.40
1:B:726:MET:O	1:B:810:LYS:NZ	2.45	0.40
1:B:813:TYR:HA	1:B:817:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:965:ALA:O	1:B:966:GLY:C	2.64	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:A:745:ARG:C	1:A:747:ALA:N	2.77	0.40
1:B:696:HIS:O	1:B:699:ALA:N	2.53	0.40
1:B:1006:VAL:O	1:B:1007:VAL:C	2.64	0.40
1:A:584:LEU:HA	1:A:587:CYS:O	2.22	0.40
1:A:770:ASN:H	1:A:773:THR:HB	1.86	0.40
1:B:543:LEU:HD23	1:B:543:LEU:N	2.37	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
1:B:1024:LEU:O	1:B:1025:MET:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	3

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	HIS

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	369 (89%)	47 (11%)	5	19
1	B	409/467 (88%)	367 (90%)	42 (10%)	7	23
All	All	825/934 (88%)	736 (89%)	89 (11%)	6	21

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	494	PRO
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
1	A	599	LEU
1	A	610	THR
1	A	621	ARG
1	A	629	LEU
1	A	634	ILE
1	A	677	TYR
1	A	693	LEU
1	A	726	MET
1	A	727	ARG
1	A	731	LEU
1	A	742	LEU
1	A	771	VAL
1	A	783	LEU
1	A	788	GLN
1	A	790	ARG
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	963	LEU
1	A	970	VAL

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Mol	Chain	Res	Type
1	A	985	ARG
1	A	1003	ARG
1	A	1024	LEU
1	A	1031	ILE
1	B	494	PRO
1	B	497	PRO
1	B	543	LEU
1	B	548	ASP
1	B	558	LEU
1	B	562	ASP
1	B	563	VAL
1	B	578	VAL
1	B	592	ARG
1	B	595	ARG
1	B	599	LEU
1	B	621	ARG
1	B	677	TYR
1	B	693	LEU
1	B	726	MET
1	B	731	LEU
1	B	732	LEU
1	B	742	LEU
1	B	771	VAL
1	B	783	LEU
1	B	790	ARG
1	B	801	ARG
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	925	ASN
1	B	926	MET
1	B	937	ILE
1	B	958	LEU
1	B	970	VAL

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Mol	Chain	Res	Type
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 (51) 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
1	A	639	HIS
1	A	657	ASN
1	A	658	ASN
1	A	666	ASN
1	A	724	HIS
1	A	761	HIS
1	A	770	ASN
1	A	779	ASN
1	A	841	ASN
1	A	866	HIS
1	A	876	ASN
1	A	925	ASN
1	A	951	ASN
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	544	HIS
1	B	572	GLN
1	B	581	ASN
1	B	604	HIS

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Mol	Chain	Res	Type
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	761	HIS
1	B	770	ASN
1	B	779	ASN
1	B	786	ASN
1	B	841	ASN
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 oligosaccharides 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

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

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, 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%)	0.46	60 (11%) 10 9	8, 54, 122, 193	0
1	B	534/604 (88%)	0.56	54 (10%) 12 10	13, 58, 124, 166	0
All	All	1076/1208 (89%)	0.51	114 (10%) 11 9	8, 55, 124, 193	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1045	HIS	8.5
1	A	715	GLY	6.7
1	A	801	ARG	5.6
1	A	714	LEU	5.5
1	A	558	LEU	5.2
1	B	558	LEU	4.8
1	B	540	ALA	4.7
1	A	945	LEU	4.6
1	B	917	GLY	4.4
1	B	921	ALA	4.3
1	B	952	GLY	4.2
1	B	495	ALA	4.2
1	A	553	VAL	4.0
1	B	621	ARG	3.9
1	A	540	ALA	3.9
1	A	712	PRO	3.8
1	B	916	ALA	3.8
1	B	522	ALA	3.8
1	A	916	ALA	3.7
1	A	921	ALA	3.7
1	A	919	ASN	3.6
1	A	846	GLU	3.6
1	B	712	PRO	3.6
1	B	714	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	925	ASN	3.4
1	A	598	GLU	3.3
1	A	751	HIS	3.3
1	B	710	THR	3.3
1	B	770	ASN	3.2
1	A	554	ALA	3.2
1	B	517	ARG	3.2
1	A	522	ALA	3.2
1	A	765	TYR	3.2
1	A	770	ASN	3.2
1	A	1045	HIS	3.2
1	B	568	PRO	3.1
1	A	718	ALA	3.1
1	B	553	VAL	3.1
1	A	779	ASN	3.1
1	A	557	GLU	3.1
1	A	915	ASP	3.0
1	A	848	ALA	3.0
1	B	925	ASN	3.0
1	A	559	PRO	3.0
1	A	918	ALA	3.0
1	A	519	ARG	2.9
1	B	539	LEU	2.9
1	A	971	ALA	2.8
1	A	948	THR	2.8
1	A	591	PHE	2.8
1	B	698	GLU	2.7
1	A	886	VAL	2.7
1	B	944	HIS	2.7
1	A	920	THR	2.7
1	A	484	ALA	2.6
1	B	978	PRO	2.6
1	A	950	GLN	2.6
1	B	1041	LYS	2.5
1	B	519	ARG	2.5
1	A	586	LEU	2.5
1	B	920	THR	2.5
1	B	779	ASN	2.5
1	A	568	PRO	2.5
1	B	565	PRO	2.5
1	B	556	VAL	2.5
1	B	572	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	915	ASP	2.4
1	A	588	PRO	2.4
1	A	789	ALA	2.4
1	A	590	ALA	2.4
1	B	564	PRO	2.4
1	A	619	ASP	2.4
1	A	750	ARG	2.4
1	A	684	GLU	2.4
1	A	492	ALA	2.4
1	B	520	TRP	2.4
1	A	946	ASP	2.4
1	B	750	ARG	2.4
1	A	794	ALA	2.4
1	B	1040	LEU	2.4
1	A	555	ASP	2.3
1	B	886	VAL	2.3
1	B	848	ALA	2.3
1	A	943	GLN	2.3
1	B	773	THR	2.3
1	B	516	GLY	2.3
1	B	715	GLY	2.3
1	A	495	ALA	2.3
1	B	749	ASP	2.3
1	A	717	GLN	2.3
1	A	634	ILE	2.3
1	B	769	CYS	2.3
1	B	803	ALA	2.2
1	B	751	HIS	2.2
1	B	995	GLY	2.2
1	A	541	LEU	2.2
1	A	741	ALA	2.2
1	A	516	GLY	2.1
1	B	716	GLY	2.1
1	A	767	ALA	2.1
1	A	824	ARG	2.1
1	B	559	PRO	2.1
1	B	824	ARG	2.1
1	B	634	ILE	2.1
1	B	846	GLU	2.1
1	A	496	GLY	2.1
1	A	716	GLY	2.1
1	B	850	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	741	ALA	2.1
1	A	974	PRO	2.0
1	A	504	LEU	2.0
1	B	801	ARG	2.0
1	B	680	GLY	2.0
1	B	711	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.