



Full wwPDB X-ray Structure Validation Report i

Jun 17, 2024 – 11:14 PM EDT

PDB ID : 5YZV
Title : Biophysical and structural characterization of the thermostable WD40 domain of a prokaryotic protein, Thermomonospora curvata PkwA
Authors : Li, D.Y.; Shen, C.; Du, Y.; Qiao, F.F.; Kong, T.; Yuan, L.R.; Zhang, D.L.; Wu, X.H.; Wu, Y.D.
Deposited on : 2017-12-15
Resolution : 2.60 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) : 1.13
EDS : 2.37.1
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) : 2.37.1

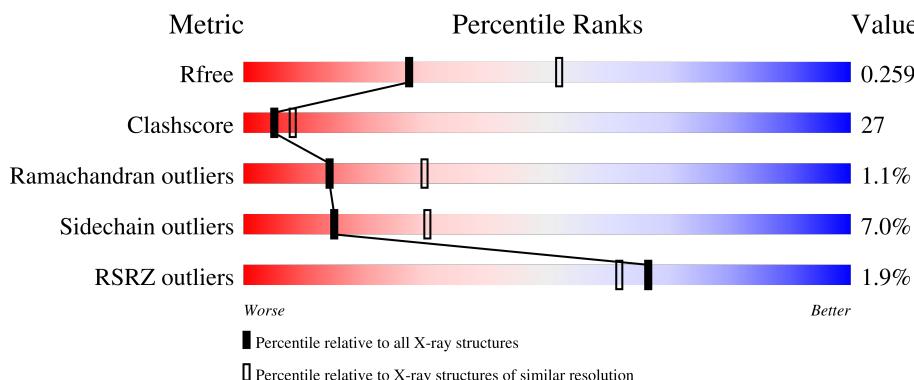
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

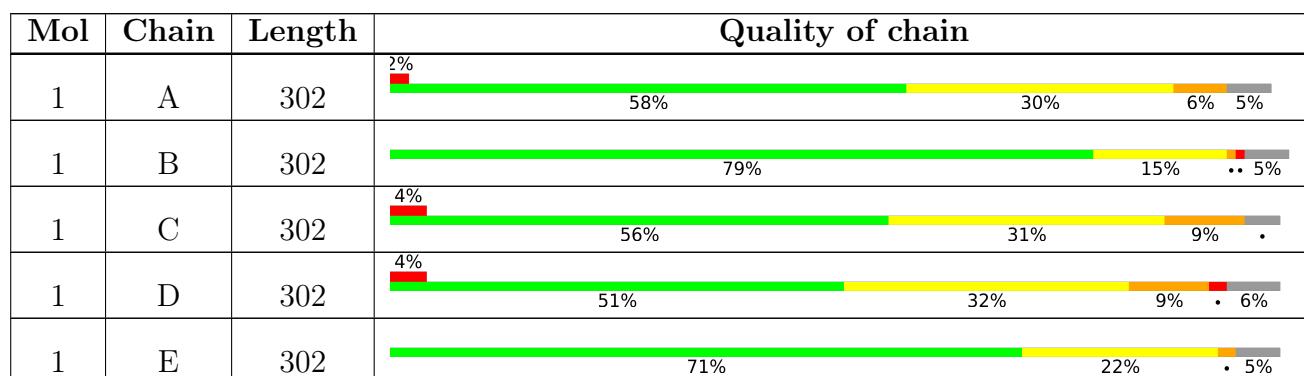
The reported resolution of this entry is 2.60 Å.

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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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.



2 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 10922 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 Probable serine/threonine-protein kinase PkwA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total 2124	C 1325	N 369	O 427	S 3	0	0	0
1	B	288	Total 2154	C 1341	N 377	O 433	S 3	0	0	0
1	C	290	Total 2152	C 1341	N 373	O 435	S 3	0	0	0
1	D	284	Total 2111	C 1319	N 364	O 425	S 3	0	0	0
1	E	288	Total 2151	C 1340	N 376	O 432	S 3	0	0	0

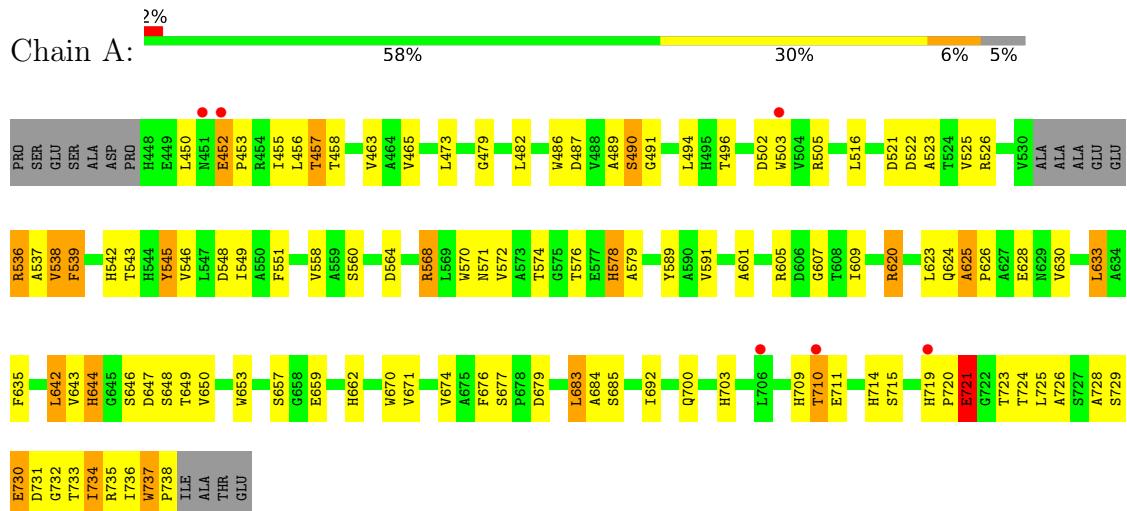
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	44	Total O 44 44	0	0
2	C	44	Total O 44 44	0	0
2	D	42	Total O 42 42	0	0
2	E	43	Total O 43 43	0	0

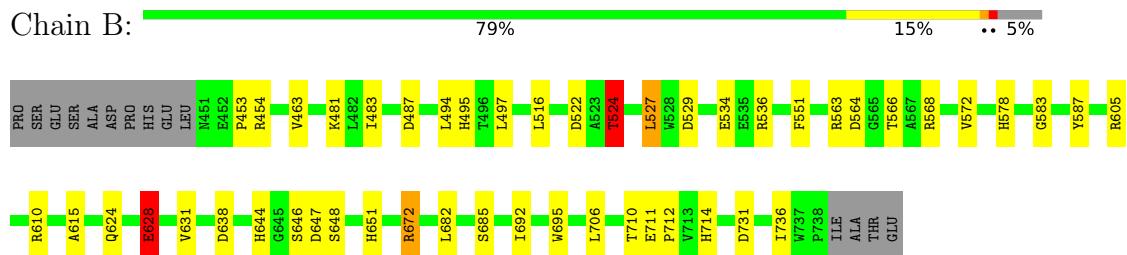
3 Residue-property plots [\(i\)](#)

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.

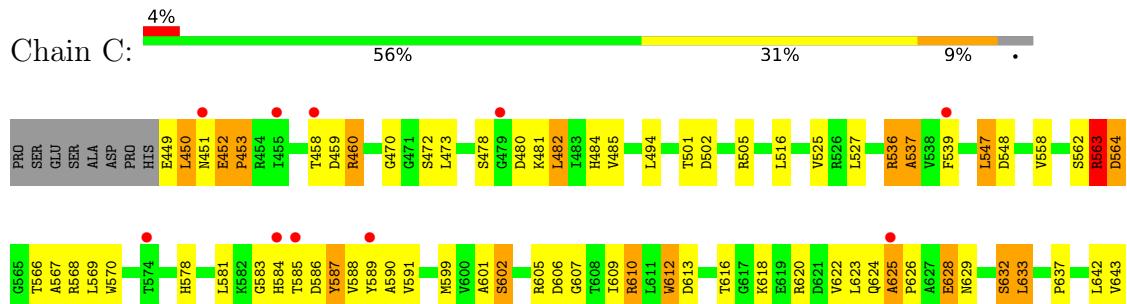
- Molecule 1: Probable serine/threonine-protein kinase PkwA



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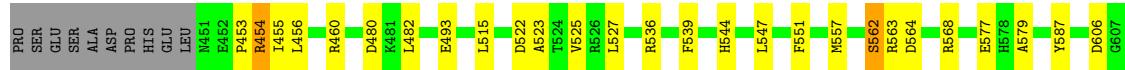




- Molecule 1: Probable serine/threonine-protein kinase PkwA



- Molecule 1: Probable serine/threonine-protein kinase PkwA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.69 Å 107.26 Å 110.27 Å 78.77° 89.33° 88.91°	Depositor
Resolution (Å)	50.01 – 2.60 44.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.01-2.60) 87.3 (44.05-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	3.62 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R , R_{free}	0.225 , 0.259 0.230 , 0.259	Depositor DCC
R_{free} test set	2895 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l 0.013 for -h,l,k 0.118 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10922	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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 [\(i\)](#)

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	1.14	7/2178 (0.3%)	1.12	5/2981 (0.2%)
1	B	1.03	2/2209 (0.1%)	1.04	6/3022 (0.2%)
1	C	1.12	9/2207 (0.4%)	1.15	16/3022 (0.5%)
1	D	1.21	10/2165 (0.5%)	1.16	11/2964 (0.4%)
1	E	1.01	2/2206 (0.1%)	1.01	7/3018 (0.2%)
All	All	1.10	30/10965 (0.3%)	1.10	45/15007 (0.3%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	453	PRO	N-CA	12.93	1.69	1.47
1	D	539	PHE	CB-CG	-8.56	1.36	1.51
1	C	649	THR	CB-CG2	-8.28	1.25	1.52
1	D	540	GLU	CG-CD	-7.67	1.40	1.51
1	D	727	SER	CB-OG	7.21	1.51	1.42
1	B	524	THR	CB-CG2	-6.87	1.29	1.52
1	A	491	GLY	N-CA	-6.75	1.35	1.46
1	C	628	GLU	CG-CD	-6.56	1.42	1.51
1	C	647	ASP	CB-CG	6.25	1.64	1.51
1	D	548	ASP	CB-CG	-6.17	1.38	1.51
1	C	460	ARG	CG-CD	-6.16	1.36	1.51
1	A	536	ARG	CA-C	-6.08	1.37	1.52
1	D	685	SER	CB-OG	-5.92	1.34	1.42
1	B	628	GLU	CD-OE2	5.90	1.32	1.25
1	D	539	PHE	CA-C	-5.87	1.37	1.52
1	A	538	VAL	CA-CB	-5.77	1.42	1.54
1	D	574	THR	CB-CG2	-5.68	1.33	1.52
1	C	452	GLU	C-N	5.67	1.45	1.34
1	C	612	TRP	CG-CD1	-5.65	1.28	1.36
1	D	455	ILE	CA-CB	-5.62	1.42	1.54
1	E	562	SER	CB-OG	-5.52	1.35	1.42
1	A	574	THR	CB-CG2	-5.45	1.34	1.52
1	E	454	ARG	CA-CB	-5.30	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	454	ARG	CA-CB	-5.23	1.42	1.53
1	A	576	THR	CB-CG2	-5.22	1.35	1.52
1	A	490	SER	CA-CB	-5.21	1.45	1.52
1	C	733	THR	CB-CG2	-5.19	1.35	1.52
1	D	456	LEU	CA-CB	-5.12	1.42	1.53
1	A	721	GLU	CD-OE1	-5.09	1.20	1.25
1	C	537	ALA	N-CA	-5.09	1.36	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	610	ARG	NE-CZ-NH1	-13.24	113.68	120.30
1	C	453	PRO	CA-N-CD	-10.29	97.10	111.50
1	D	460	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	C	610	ARG	NE-CZ-NH2	8.77	124.69	120.30
1	E	454	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	D	540	GLU	OE1-CD-OE2	7.65	132.48	123.30
1	B	605	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	B	536	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	C	647	ASP	CB-CG-OD2	6.90	124.51	118.30
1	C	669	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	682	LEU	CA-CB-CG	6.56	130.40	115.30
1	A	538	VAL	CA-CB-CG2	-6.23	101.55	110.90
1	D	539	PHE	CB-CA-C	-6.23	97.95	110.40
1	D	459	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	E	568	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	E	620	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	E	515	LEU	CB-CG-CD1	6.08	121.33	111.00
1	D	568	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	B	672	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	E	618	LYS	CD-CE-NZ	-5.93	98.06	111.70
1	C	516	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	547	LEU	CB-CG-CD2	5.69	120.67	111.00
1	A	578	HIS	CB-CA-C	-5.58	99.23	110.40
1	C	505	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	B	610	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	452	GLU	C-N-CD	5.56	140.07	128.40
1	C	563	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	620	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	C	564	ASP	CB-CA-C	-5.38	99.64	110.40
1	C	647	ASP	OD1-CG-OD2	-5.33	113.18	123.30
1	D	538	VAL	CA-CB-CG2	-5.32	102.92	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ARG	CB-CA-C	-5.26	99.88	110.40
1	A	568	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	B	454	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	538	VAL	CB-CA-C	-5.20	101.52	111.40
1	C	536	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	605	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	D	457	THR	CA-CB-CG2	-5.10	105.26	112.40
1	D	471	GLY	C-N-CA	5.09	134.42	121.70
1	E	456	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	C	449	GLU	C-N-CA	5.02	134.26	121.70
1	C	449	GLU	O-C-N	5.01	130.72	122.70
1	C	672	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	E	557	MET	CG-SD-CE	-5.01	92.18	100.20
1	C	647	ASP	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2124	0	1969	151	0
1	B	2154	0	2013	29	0
1	C	2152	0	1995	167	0
1	D	2111	0	1963	172	0
1	E	2151	0	2009	46	0
2	A	57	0	0	3	0
2	B	44	0	0	0	0
2	C	44	0	0	4	0
2	D	42	0	0	0	0
2	E	43	0	0	0	0
All	All	10922	0	9949	559	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 27.

All (559) 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:452:GLU:HG2	1:A:453:PRO:CD	1.31	1.57
1:C:453:PRO:N	1:C:453:PRO:CA	1.69	1.34
1:A:452:GLU:CG	1:A:453:PRO:CD	2.13	1.27
1:A:452:GLU:CG	1:A:453:PRO:HD3	1.64	1.24
1:C:605:ARG:HG3	1:C:629:ASN:ND2	1.60	1.16
1:C:694:LEU:HD21	1:C:725:LEU:CD2	1.77	1.15
1:D:453:PRO:C	1:D:454:ARG:HD2	1.70	1.11
1:D:662:HIS:HB3	1:D:700:GLN:OE1	1.49	1.10
1:D:662:HIS:HB3	1:D:700:GLN:CD	1.71	1.09
1:C:643:VAL:HG21	1:C:683:LEU:HD11	1.35	1.06
1:A:456:LEU:O	1:A:457:THR:HG23	1.55	1.05
1:C:694:LEU:HD21	1:C:725:LEU:HD21	1.32	1.04
1:A:643:VAL:HG21	1:A:683:LEU:HD11	1.39	1.02
1:C:605:ARG:HG3	1:C:629:ASN:HD21	1.25	1.02
1:C:599:MET:HE2	1:C:620:ARG:HD3	1.42	0.98
1:A:452:GLU:CG	1:A:453:PRO:HD2	1.94	0.98
1:B:487:ASP:HB2	1:B:494:LEU:HD11	1.43	0.97
1:D:571:ASN:HB2	1:D:578:HIS:HE1	1.31	0.94
1:C:628:GLU:HG2	1:C:629:ASN:H	1.33	0.93
1:C:451:ASN:O	1:C:738:PRO:HD2	1.69	0.90
1:D:650:VAL:HG12	1:D:664:PHE:HB2	1.54	0.90
1:C:643:VAL:HG21	1:C:683:LEU:CD1	2.02	0.89
1:D:643:VAL:HG12	1:D:652:LEU:HD23	1.55	0.88
1:C:599:MET:CE	1:C:620:ARG:HD3	2.03	0.88
1:C:451:ASN:O	1:C:738:PRO:CD	2.22	0.87
1:C:692:ILE:CG1	1:C:706:LEU:HB2	2.04	0.87
1:A:452:GLU:CB	1:A:453:PRO:HD2	2.04	0.87
1:C:450:LEU:CB	1:C:704:THR:HG21	2.05	0.86
1:C:599:MET:CE	1:C:620:ARG:CD	2.54	0.86
1:D:461:GLU:HG3	1:D:503:TRP:HH2	1.40	0.85
1:A:607:GLY:O	1:A:626:PRO:HG2	1.77	0.84
1:D:453:PRO:CD	1:D:736:ILE:HG13	2.06	0.84
1:D:650:VAL:CG1	1:D:664:PHE:HB2	2.10	0.81
1:C:599:MET:HE2	1:C:620:ARG:CD	2.10	0.81
1:A:452:GLU:HB3	1:A:453:PRO:HD2	1.63	0.81
1:C:460:ARG:HD2	1:C:478:SER:OG	1.81	0.81
1:A:643:VAL:HG11	1:A:683:LEU:HD21	1.61	0.80
1:D:542:HIS:CE1	1:D:568:ARG:HH21	1.99	0.80
1:A:643:VAL:HG21	1:A:683:LEU:CD1	2.10	0.80
1:D:451:ASN:ND2	1:D:451:ASN:O	2.14	0.80
1:A:456:LEU:O	1:A:457:THR:CG2	2.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:ASN:HB2	1:D:578:HIS:CE1	2.16	0.80
1:C:616:THR:HG23	1:C:618:LYS:HB2	1.62	0.79
1:D:460:ARG:HG2	1:D:461:GLU:H	1.47	0.79
1:B:615:ALA:HB1	1:C:719:HIS:HE2	1.47	0.79
1:C:482:LEU:HD13	1:C:484:HIS:NE2	1.98	0.79
1:C:699:ALA:O	1:C:700:GLN:HB3	1.82	0.79
1:C:711:GLU:HG2	1:C:712:PRO:HD2	1.64	0.79
1:D:699:ALA:O	1:D:700:GLN:HB2	1.82	0.79
1:D:708:GLY:O	1:D:709:HIS:HB2	1.82	0.78
1:C:607:GLY:O	1:C:626:PRO:HG2	1.84	0.77
1:D:454:ARG:HD2	1:D:454:ARG:N	1.93	0.77
1:D:453:PRO:HD2	1:D:736:ILE:HG13	1.65	0.77
1:A:452:GLU:CB	1:A:453:PRO:CD	2.58	0.77
1:A:490:SER:O	1:A:490:SER:OG	1.98	0.77
1:A:626:PRO:HB3	1:A:644:HIS:NE2	1.99	0.77
1:E:455:ILE:N	1:E:455:ILE:HD12	2.00	0.76
1:C:723:THR:HG23	1:C:724:THR:HG23	1.67	0.76
1:A:526:ARG:NH1	1:A:539:PHE:HE2	1.83	0.76
1:A:643:VAL:HG23	1:A:676:PHE:CE2	2.21	0.76
1:A:450:LEU:O	1:A:738:PRO:HD3	1.86	0.76
1:D:715:SER:OG	1:D:728:ALA:HB3	1.84	0.76
1:D:539:PHE:CD1	1:D:539:PHE:N	2.49	0.75
1:A:625:ALA:N	1:A:626:PRO:HD2	2.01	0.75
1:D:643:VAL:HG13	1:D:676:PHE:CZ	2.20	0.75
1:D:643:VAL:HG12	1:D:652:LEU:CD2	2.17	0.74
1:C:587:TYR:CE1	1:C:605:ARG:HD3	2.23	0.73
1:C:664:PHE:CD1	1:C:700:GLN:CG	2.72	0.73
1:C:609:ILE:HD11	1:C:644:HIS:HB2	1.70	0.73
1:C:548:ASP:OD2	1:C:591:VAL:N	2.20	0.73
1:D:566:THR:OG1	1:D:568:ARG:NH1	2.22	0.73
1:D:538:VAL:HG12	1:D:539:PHE:N	2.02	0.72
1:C:450:LEU:CB	1:C:704:THR:CG2	2.68	0.72
1:A:538:VAL:HG12	1:A:539:PHE:N	2.04	0.72
1:A:571:ASN:HB2	1:A:578:HIS:NE2	2.04	0.72
1:D:643:VAL:HG13	1:D:676:PHE:CE2	2.23	0.72
1:C:599:MET:HE1	1:C:620:ARG:CD	2.19	0.72
1:D:457:THR:HG22	1:D:486:TRP:HH2	1.54	0.72
1:C:599:MET:HE1	1:C:620:ARG:HD2	1.71	0.72
1:D:650:VAL:HG13	1:D:664:PHE:CD2	2.24	0.72
1:C:570:TRP:HA	1:C:578:HIS:HB3	1.70	0.72
1:C:664:PHE:CD1	1:C:700:GLN:HG2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ARG:NH1	1:A:539:PHE:CE2	2.58	0.71
1:C:711:GLU:CG	1:C:712:PRO:HD2	2.20	0.71
1:C:599:MET:CE	1:C:620:ARG:HD2	2.19	0.71
1:A:643:VAL:HG23	1:A:676:PHE:CZ	2.25	0.71
1:D:454:ARG:N	1:D:454:ARG:CD	2.51	0.71
1:E:644:HIS:HD2	1:E:653:TRP:HE1	1.39	0.71
1:C:599:MET:HE2	1:C:620:ARG:HH11	1.55	0.71
1:D:711:GLU:HB2	1:D:729:SER:OG	1.90	0.70
1:D:607:GLY:O	1:D:626:PRO:HG2	1.91	0.70
1:A:568:ARG:HG2	1:A:568:ARG:HH21	1.55	0.70
1:A:564:ASP:OD2	1:A:568:ARG:NH1	2.20	0.70
1:B:564:ASP:OD1	1:B:566:THR:HG22	1.92	0.70
1:A:542:HIS:CE1	1:A:568:ARG:HG3	2.26	0.70
1:D:626:PRO:HB3	1:D:644:HIS:NE2	2.06	0.69
1:D:460:ARG:CZ	1:D:503:TRP:HZ2	2.04	0.69
1:D:454:ARG:HG3	1:D:735:ARG:HG3	1.74	0.69
1:D:538:VAL:CG1	1:D:539:PHE:N	2.56	0.69
1:D:644:HIS:HB3	1:D:653:TRP:HE1	1.57	0.69
1:A:452:GLU:HG2	1:A:453:PRO:HD3	0.70	0.69
1:C:626:PRO:HB3	1:C:644:HIS:NE2	2.07	0.69
1:D:457:THR:CG2	1:D:486:TRP:HH2	2.06	0.69
1:D:625:ALA:N	1:D:626:PRO:HD2	2.07	0.68
1:A:455:ILE:HB	1:A:734:ILE:HB	1.75	0.68
1:A:643:VAL:CG1	1:A:683:LEU:HD21	2.23	0.68
1:B:487:ASP:CB	1:B:494:LEU:HD11	2.23	0.68
1:C:453:PRO:HD3	1:C:738:PRO:HD3	1.75	0.68
1:A:648:SER:O	1:A:649:THR:HG23	1.93	0.68
1:C:673:ALA:HB1	2:C:834:HOH:O	1.93	0.68
1:D:719:HIS:ND1	1:D:721:GLU:HG2	2.09	0.68
1:A:719:HIS:CE1	1:A:721:GLU:HG3	2.29	0.67
1:C:703:HIS:O	1:C:704:THR:OG1	2.11	0.67
1:D:452:GLU:N	1:D:452:GLU:OE1	2.28	0.67
1:C:644:HIS:HB3	1:C:653:TRP:HE1	1.60	0.67
1:A:542:HIS:HE1	1:A:568:ARG:HG2	1.59	0.67
1:A:450:LEU:O	1:A:738:PRO:CD	2.43	0.66
1:C:703:HIS:ND1	1:E:577:GLU:OE1	2.28	0.66
1:D:450:LEU:O	1:D:738:PRO:HD2	1.95	0.66
1:C:692:ILE:CD1	1:C:706:LEU:HD12	2.25	0.66
1:D:712:PRO:CD	1:D:730:GLU:HG3	2.25	0.66
1:A:542:HIS:CE1	1:A:568:ARG:CG	2.79	0.65
1:A:607:GLY:O	1:A:626:PRO:CG	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:THR:CG2	1:D:486:TRP:CH2	2.79	0.65
1:B:628:GLU:HB3	1:B:646:SER:OG	1.96	0.65
1:C:731:ASP:OD1	1:C:733:THR:HG22	1.96	0.65
1:D:457:THR:HG23	1:D:458:THR:N	2.12	0.65
1:C:625:ALA:N	1:C:626:PRO:HD2	2.10	0.65
1:A:628:GLU:HB2	1:A:647:ASP:HB2	1.79	0.65
1:B:615:ALA:CB	1:C:719:HIS:HE2	2.09	0.64
1:D:712:PRO:HD2	1:D:730:GLU:HG3	1.77	0.64
1:C:480:ASP:HB2	1:C:482:LEU:CD1	2.26	0.64
1:D:650:VAL:HG13	1:D:664:PHE:HD2	1.61	0.64
1:D:662:HIS:CB	1:D:700:GLN:CD	2.59	0.64
1:A:457:THR:HG1	1:A:486:TRP:HH2	1.44	0.64
1:D:456:LEU:O	1:D:457:THR:HB	1.97	0.64
1:D:650:VAL:CG1	1:D:664:PHE:HD2	2.10	0.64
1:C:536:ARG:HG2	1:C:537:ALA:H	1.62	0.64
1:B:494:LEU:N	1:B:494:LEU:HD12	2.12	0.63
1:A:589:TYR:CE2	1:A:605:ARG:HG3	2.33	0.63
1:C:480:ASP:HB2	1:C:482:LEU:HD11	1.79	0.63
1:C:689:ASP:OD1	1:C:691:THR:HG22	1.98	0.63
1:D:537:ALA:O	1:D:539:PHE:HE1	1.80	0.63
1:A:709:HIS:O	1:A:710:THR:OG1	2.12	0.63
1:C:563:ARG:HG2	1:C:587:TYR:HD2	1.63	0.63
1:D:450:LEU:HD12	1:D:450:LEU:H	1.64	0.63
1:A:560:SER:HG	1:A:570:TRP:HZ3	1.46	0.62
1:A:457:THR:OG1	1:A:486:TRP:HH2	1.82	0.62
1:C:451:ASN:O	1:C:738:PRO:HD3	2.00	0.62
1:C:470:GLY:HA3	2:C:838:HOH:O	1.99	0.62
1:E:454:ARG:C	1:E:455:ILE:HD12	2.19	0.62
1:C:602:SER:HB2	1:C:612:TRP:HZ3	1.65	0.62
1:C:643:VAL:CG1	1:C:683:LEU:HD21	2.29	0.62
1:A:455:ILE:C	1:A:456:LEU:HG	2.19	0.62
1:D:652:LEU:HD12	1:D:700:GLN:NE2	2.15	0.62
1:D:735:ARG:NH1	1:D:735:ARG:HB2	2.15	0.62
1:C:692:ILE:HG12	1:C:706:LEU:HB2	1.80	0.61
1:C:664:PHE:CD1	1:C:700:GLN:HG3	2.35	0.61
1:C:692:ILE:CD1	1:C:706:LEU:HB2	2.31	0.61
1:C:692:ILE:CG2	1:C:713:VAL:HG11	2.29	0.61
1:C:602:SER:HB2	1:C:612:TRP:CZ3	2.35	0.61
1:A:601:ALA:CB	1:A:642:LEU:HD11	2.31	0.61
1:D:455:ILE:C	1:D:456:LEU:HG	2.20	0.61
1:D:526:ARG:NH1	1:D:539:PHE:HE2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:GLU:N	1:D:452:GLU:CD	2.54	0.61
1:C:605:ARG:HG3	1:C:629:ASN:CG	2.20	0.60
1:A:538:VAL:CG1	1:A:539:PHE:N	2.63	0.60
1:C:692:ILE:HD11	1:C:706:LEU:HB2	1.82	0.60
1:D:538:VAL:C	1:D:539:PHE:CD1	2.74	0.60
1:E:647:ASP:HB2	1:E:670:TRP:CZ3	2.36	0.60
1:A:560:SER:CB	1:A:570:TRP:HZ3	2.14	0.60
1:D:457:THR:HG21	1:D:486:TRP:CH2	2.36	0.60
1:C:628:GLU:HG2	1:C:629:ASN:N	2.08	0.60
1:D:619:GLU:OE2	1:D:622:VAL:CG2	2.50	0.59
1:C:568:ARG:HB3	1:C:578:HIS:CD2	2.36	0.59
1:C:694:LEU:CD2	1:C:725:LEU:HD21	2.21	0.59
1:D:542:HIS:NE2	1:D:570:TRP:HH2	1.99	0.59
1:D:601:ALA:HB2	1:D:642:LEU:HD11	1.84	0.59
1:B:711:GLU:HG3	1:B:731:ASP:HB3	1.83	0.59
1:D:460:ARG:CZ	1:D:503:TRP:CZ2	2.86	0.59
1:A:473:LEU:HD11	1:A:494:LEU:CD2	2.32	0.59
1:C:480:ASP:HB2	1:C:482:LEU:HG	1.85	0.59
1:C:587:TYR:CD1	1:C:605:ARG:HD3	2.38	0.59
1:C:649:THR:HG21	1:C:651:HIS:CE1	2.37	0.59
1:D:455:ILE:HB	1:D:734:ILE:HB	1.84	0.59
1:D:539:PHE:N	1:D:539:PHE:HD1	2.01	0.59
1:D:457:THR:HG22	1:D:486:TRP:CH2	2.37	0.58
1:A:542:HIS:HE1	1:A:568:ARG:CG	2.15	0.58
1:D:451:ASN:HD22	1:D:451:ASN:C	2.06	0.58
1:A:648:SER:C	1:A:649:THR:HG23	2.24	0.57
1:C:616:THR:CG2	1:C:618:LYS:HB2	2.34	0.57
1:E:689:ASP:O	1:E:690:ARG:HB2	2.04	0.57
1:A:537:ALA:O	1:A:539:PHE:CE1	2.57	0.57
1:B:463:VAL:HG12	1:B:714:HIS:HD2	1.69	0.57
1:A:730:GLU:HB3	2:A:837:HOH:O	2.04	0.57
1:C:589:TYR:OH	1:C:629:ASN:ND2	2.37	0.57
1:D:574:THR:OG1	1:D:576:THR:HG23	2.04	0.57
1:D:460:ARG:CG	1:D:461:GLU:H	2.15	0.57
1:A:456:LEU:O	1:A:457:THR:CB	2.52	0.57
1:C:481:LYS:HD3	1:C:481:LYS:N	2.20	0.57
1:C:670:TRP:CZ3	1:D:545:TYR:OH	2.45	0.57
1:D:712:PRO:CG	1:D:730:GLU:HG3	2.35	0.57
1:D:661:LEU:O	1:D:662:HIS:HB2	2.04	0.57
1:A:537:ALA:O	1:A:539:PHE:HE1	1.87	0.56
1:C:590:ALA:HB1	1:C:633:LEU:HD22	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:MET:CE	1:C:620:ARG:HH11	2.18	0.56
1:C:664:PHE:HD1	1:C:700:GLN:HG3	1.70	0.56
1:E:647:ASP:O	1:E:648:SER:HB2	2.05	0.56
1:A:560:SER:OG	1:A:570:TRP:HZ3	1.88	0.56
1:A:453:PRO:HD2	1:A:736:ILE:CG2	2.35	0.56
1:C:584:HIS:O	1:C:585:THR:HG22	2.06	0.56
1:E:631:VAL:HG11	1:E:672:ARG:HG2	1.86	0.56
1:D:558:VAL:HG23	1:D:572:VAL:HG12	1.87	0.56
1:B:578:HIS:CE1	1:C:472:SER:HB2	2.41	0.56
1:C:586:ASP:HB3	1:C:605:ARG:HB3	1.87	0.56
1:C:616:THR:HG23	1:C:618:LYS:CB	2.35	0.56
1:A:536:ARG:CA	1:A:536:ARG:HE	2.18	0.56
1:A:542:HIS:HD1	1:A:568:ARG:CZ	2.19	0.56
1:A:625:ALA:N	1:A:626:PRO:CD	2.69	0.56
1:D:643:VAL:HG11	1:D:683:LEU:CD2	2.36	0.56
1:C:480:ASP:HB2	1:C:482:LEU:CG	2.35	0.56
1:C:481:LYS:HD2	1:C:502:ASP:HA	1.88	0.56
1:C:536:ARG:CG	1:C:537:ALA:H	2.18	0.56
1:C:643:VAL:HG22	1:C:652:LEU:HD12	1.88	0.56
1:A:589:TYR:HE2	1:A:605:ARG:HG3	1.70	0.56
1:D:453:PRO:O	1:D:454:ARG:HD2	2.06	0.56
1:A:715:SER:OG	1:A:728:ALA:HB3	2.06	0.55
1:C:632:SER:HB3	1:C:674:VAL:HG22	1.87	0.55
1:C:643:VAL:CG2	1:C:683:LEU:HD21	2.37	0.55
1:C:692:ILE:HG13	1:C:706:LEU:HD12	1.88	0.55
1:A:568:ARG:HG2	1:A:568:ARG:NH2	2.22	0.55
1:C:563:ARG:HG2	1:C:587:TYR:CD2	2.40	0.55
1:C:584:HIS:HB3	1:C:606:ASP:OD2	2.06	0.55
1:C:724:THR:HB	1:C:737:TRP:O	2.07	0.55
1:D:453:PRO:CD	1:D:453:PRO:O	2.55	0.55
1:D:479:GLY:HA2	1:D:503:TRP:CD2	2.42	0.55
1:D:547:LEU:HD11	1:D:587:TYR:CD2	2.41	0.55
1:A:536:ARG:CA	1:A:536:ARG:NE	2.68	0.55
1:A:539:PHE:N	1:A:539:PHE:CD1	2.73	0.55
1:A:724:THR:CG2	1:A:736:ILE:HG12	2.37	0.55
1:B:631:VAL:HG11	1:B:672:ARG:HG2	1.89	0.54
1:D:452:GLU:HB2	1:D:453:PRO:HD3	1.89	0.54
1:D:558:VAL:CG2	1:D:572:VAL:HG12	2.36	0.54
1:D:657:SER:HB3	1:D:659:GLU:HG2	1.89	0.54
1:D:712:PRO:HG2	1:D:730:GLU:HG3	1.89	0.54
1:C:481:LYS:HD2	1:C:502:ASP:CA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:HIS:ND1	1:C:578:HIS:N	2.56	0.54
1:E:480:ASP:OD2	1:E:482:LEU:HD12	2.06	0.54
1:A:463:VAL:HG12	1:A:714:HIS:HD2	1.72	0.54
1:A:560:SER:HB2	1:A:570:TRP:HZ3	1.70	0.54
1:A:650:VAL:CG2	1:A:671:VAL:HG11	2.38	0.54
1:C:650:VAL:HB	1:C:664:PHE:HB2	1.88	0.54
1:D:650:VAL:CG1	1:D:664:PHE:CD2	2.88	0.54
1:A:643:VAL:CG2	1:A:676:PHE:CE2	2.90	0.54
1:A:650:VAL:HG22	1:A:671:VAL:HG11	1.90	0.54
1:A:724:THR:HG22	1:A:725:LEU:N	2.23	0.54
1:C:460:ARG:O	1:C:732:GLY:HA2	2.07	0.54
1:C:601:ALA:HA	1:C:610:ARG:O	2.08	0.54
1:D:539:PHE:C	1:D:540:GLU:HG2	2.26	0.54
1:A:456:LEU:O	1:A:457:THR:OG1	2.26	0.54
1:E:644:HIS:CD2	1:E:653:TRP:HE1	2.23	0.54
1:D:625:ALA:N	1:D:626:PRO:CD	2.72	0.53
1:D:628:GLU:HB2	1:D:647:ASP:HB2	1.91	0.53
1:A:465:VAL:HG13	1:A:728:ALA:HB2	1.90	0.53
1:A:589:TYR:HE2	1:A:605:ARG:CG	2.21	0.53
1:D:520:SER:O	1:D:546:VAL:HG23	2.07	0.53
1:A:526:ARG:CZ	1:A:539:PHE:HE2	2.20	0.53
1:A:536:ARG:NE	1:A:536:ARG:HA	2.23	0.53
1:A:711:GLU:HB2	1:A:730:GLU:OE1	2.08	0.53
1:A:729:SER:OG	1:A:733:THR:OG1	2.26	0.53
1:D:661:LEU:HD23	1:D:700:GLN:HE21	1.73	0.53
1:C:569:LEU:N	1:C:569:LEU:HD12	2.23	0.53
1:C:460:ARG:CD	1:C:478:SER:OG	2.55	0.53
1:D:707:GLU:HB3	1:D:709:HIS:CD2	2.44	0.53
1:C:563:ARG:HA	1:C:587:TYR:HB3	1.91	0.53
1:E:643:VAL:HG11	1:E:683:LEU:HD11	1.91	0.53
1:D:643:VAL:HG11	1:D:683:LEU:CD1	2.38	0.53
1:D:717:ALA:O	1:D:725:LEU:HD12	2.09	0.53
1:E:643:VAL:HG21	1:E:683:LEU:HD21	1.91	0.53
1:A:560:SER:HB2	1:A:570:TRP:CZ3	2.44	0.52
1:D:568:ARG:HB2	1:D:568:ARG:NH2	2.24	0.52
1:C:643:VAL:HG11	1:C:683:LEU:HD21	1.91	0.52
1:D:542:HIS:CD2	1:D:546:VAL:HG13	2.45	0.52
1:A:643:VAL:CG2	1:A:676:PHE:CZ	2.93	0.52
1:E:609:ILE:HB	1:E:623:LEU:HB2	1.92	0.52
1:A:542:HIS:CE1	1:A:568:ARG:NH2	2.78	0.52
1:D:560:SER:HB2	1:D:570:TRP:HZ3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:GLU:C	1:A:721:GLU:OE1	2.48	0.52
1:C:692:ILE:HG22	1:C:713:VAL:HG11	1.92	0.52
1:E:716:VAL:HG13	1:E:725:LEU:HD11	1.92	0.52
1:A:711:GLU:CB	1:A:730:GLU:OE1	2.58	0.52
1:C:651:HIS:CE1	2:C:802:HOH:O	2.62	0.52
1:D:461:GLU:OE2	1:D:730:GLU:CG	2.58	0.52
1:D:657:SER:CB	1:D:659:GLU:HG2	2.40	0.52
1:A:601:ALA:HB2	1:A:642:LEU:HD11	1.91	0.52
1:C:589:TYR:HE2	1:C:629:ASN:HB3	1.75	0.51
1:D:450:LEU:O	1:D:737:TRP:HB3	2.10	0.51
1:C:536:ARG:HG2	1:C:537:ALA:N	2.25	0.51
1:D:623:LEU:HB3	1:D:653:TRP:CE3	2.45	0.51
1:E:692:ILE:HD12	1:E:727:SER:HB3	1.92	0.51
1:C:482:LEU:HD13	1:C:484:HIS:CD2	2.45	0.51
1:C:567:ALA:HB3	1:C:581:LEU:HB2	1.92	0.51
1:D:461:GLU:CG	1:D:503:TRP:HH2	2.19	0.51
1:A:644:HIS:CE1	1:A:646:SER:HB2	2.46	0.51
1:C:460:ARG:HD3	1:C:480:ASP:CG	2.31	0.51
1:C:562:SER:N	1:C:588:VAL:HG23	2.25	0.51
1:D:456:LEU:O	1:D:457:THR:CB	2.59	0.51
1:A:452:GLU:HG2	1:A:453:PRO:N	2.16	0.51
1:C:692:ILE:HG13	1:C:706:LEU:HB2	1.89	0.51
1:D:724:THR:HG23	1:D:737:TRP:O	2.11	0.51
1:D:735:ARG:HB2	1:D:735:ARG:HH11	1.75	0.51
1:A:609:ILE:HD12	1:A:630:VAL:HG21	1.92	0.50
1:A:579:ALA:HB2	2:A:834:HOH:O	2.10	0.50
1:C:652:LEU:HD21	1:C:697:VAL:HG13	1.93	0.50
1:A:723:THR:O	1:A:738:PRO:HA	2.11	0.50
1:C:643:VAL:CG2	1:C:683:LEU:HD11	2.25	0.50
1:C:605:ARG:CG	1:C:629:ASN:ND2	2.54	0.50
1:D:506:ALA:CB	1:D:548:ASP:HA	2.42	0.50
1:D:624:GLN:O	1:D:625:ALA:HB2	2.12	0.50
1:E:610:ARG:HG2	1:E:622:VAL:HG22	1.92	0.50
1:A:473:LEU:HD11	1:A:494:LEU:HD22	1.93	0.50
1:D:652:LEU:HB2	1:D:700:GLN:HE22	1.76	0.50
1:D:548:ASP:OD2	1:D:591:VAL:HG22	2.11	0.50
1:D:643:VAL:HG11	1:D:683:LEU:HD22	1.93	0.50
1:A:737:TRP:N	1:A:737:TRP:CD1	2.80	0.50
1:C:613:ASP:OD2	1:C:616:THR:HG22	2.12	0.50
1:E:527:LEU:HD13	1:E:539:PHE:HE2	1.76	0.50
1:C:643:VAL:HG21	1:C:683:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:LEU:O	1:C:536:ARG:HB3	2.11	0.49
1:D:542:HIS:CE1	1:D:568:ARG:NH2	2.74	0.49
1:A:625:ALA:H	1:A:626:PRO:HD2	1.77	0.49
1:C:643:VAL:HG21	1:C:683:LEU:CD2	2.42	0.49
1:C:682:LEU:HD23	1:C:695:TRP:O	2.12	0.49
1:A:568:ARG:HB2	1:A:570:TRP:CZ3	2.48	0.49
1:D:537:ALA:O	1:D:539:PHE:CE1	2.63	0.49
1:D:600:VAL:HG23	1:D:614:VAL:HG12	1.94	0.49
1:E:656:ALA:O	1:E:657:SER:CB	2.60	0.49
1:A:545:TYR:H	1:A:545:TYR:HD1	1.54	0.49
1:D:453:PRO:HD2	1:D:453:PRO:O	2.13	0.49
1:C:458:THR:OG1	1:C:460:ARG:NH1	2.46	0.49
1:C:664:PHE:HD1	1:C:700:GLN:CG	2.21	0.49
1:A:662:HIS:ND1	1:A:700:GLN:HB3	2.28	0.49
1:D:456:LEU:C	1:D:457:THR:HG22	2.31	0.49
1:D:526:ARG:CZ	1:D:539:PHE:HE2	2.25	0.49
1:D:643:VAL:HG21	1:D:683:LEU:HD11	1.95	0.49
1:A:545:TYR:CD1	1:A:545:TYR:N	2.72	0.49
1:A:609:ILE:HG22	1:A:623:LEU:HD12	1.94	0.49
1:C:625:ALA:N	1:C:626:PRO:CD	2.75	0.49
1:A:526:ARG:CZ	1:A:539:PHE:CE2	2.95	0.48
1:B:563:ARG:NH2	1:B:587:TYR:OH	2.46	0.48
1:C:692:ILE:HG13	1:C:706:LEU:CG	2.42	0.48
1:B:644:HIS:CE1	1:B:651:HIS:HB2	2.48	0.48
1:D:545:TYR:H	1:D:545:TYR:HD1	1.56	0.48
1:B:453:PRO:CB	1:B:736:ILE:O	2.61	0.48
1:D:662:HIS:HB3	1:D:700:GLN:NE2	2.24	0.48
1:C:673:ALA:CB	2:C:834:HOH:O	2.56	0.48
1:D:545:TYR:CD1	1:D:545:TYR:N	2.78	0.48
1:A:453:PRO:CB	2:A:857:HOH:O	2.62	0.48
1:C:591:VAL:C	1:C:633:LEU:HD21	2.34	0.48
1:C:601:ALA:O	1:C:633:LEU:HD11	2.14	0.48
1:A:548:ASP:HB3	1:A:591:VAL:HG22	1.95	0.47
1:A:644:HIS:O	1:A:650:VAL:HG13	2.14	0.47
1:A:724:THR:HG21	1:A:736:ILE:HG12	1.96	0.47
1:E:563:ARG:NH2	1:E:587:TYR:OH	2.46	0.47
1:C:525:VAL:HB	1:C:539:PHE:HB2	1.95	0.47
1:A:677:SER:OG	1:A:679:ASP:OD1	2.28	0.47
1:C:649:THR:CG2	1:C:651:HIS:CE1	2.98	0.47
1:D:453:PRO:HG3	1:D:736:ILE:HD11	1.97	0.47
1:D:623:LEU:HD13	1:D:653:TRP:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:VAL:HG11	1:D:683:LEU:HD13	1.97	0.47
1:A:479:GLY:HA3	1:A:503:TRP:CE3	2.50	0.47
1:C:485:VAL:HG13	1:C:494:LEU:HB2	1.95	0.47
1:C:674:VAL:HA	1:C:684:ALA:O	2.14	0.47
1:E:692:ILE:HD13	1:E:713:VAL:HG11	1.96	0.47
1:A:463:VAL:HG11	1:A:505:ARG:NH1	2.30	0.47
1:C:692:ILE:CG1	1:C:706:LEU:HD12	2.44	0.47
1:D:460:ARG:NH2	1:D:503:TRP:HZ2	2.13	0.47
1:E:626:PRO:O	1:E:627:ALA:HB3	2.15	0.47
1:E:692:ILE:HB	1:E:706:LEU:HB2	1.96	0.47
1:D:451:ASN:HA	1:D:737:TRP:HA	1.97	0.47
1:E:719:HIS:CE1	1:E:721:GLU:HG2	2.50	0.47
1:D:724:THR:HG22	1:D:725:LEU:N	2.31	0.46
1:A:479:GLY:CA	1:A:503:TRP:CE3	2.98	0.46
1:A:644:HIS:HB3	1:A:653:TRP:HE1	1.80	0.46
1:A:730:GLU:HG2	1:A:731:ASP:HB2	1.97	0.46
1:D:623:LEU:HD13	1:D:653:TRP:HB3	1.97	0.46
1:D:704:THR:HG22	1:D:705:THR:N	2.31	0.46
1:C:685:SER:OG	1:C:695:TRP:NE1	2.44	0.46
1:A:522:ASP:O	1:A:523:ALA:HB3	2.15	0.46
1:E:547:LEU:HD11	1:E:563:ARG:HG3	1.98	0.46
1:A:473:LEU:HD11	1:A:494:LEU:HD21	1.97	0.46
1:C:536:ARG:CG	1:C:537:ALA:N	2.79	0.46
1:C:562:SER:O	1:C:588:VAL:HG22	2.16	0.46
1:E:616:THR:OG1	1:E:618:LYS:HB2	2.16	0.46
1:B:587:TYR:N	1:B:587:TYR:CD1	2.84	0.46
1:C:644:HIS:ND1	1:C:651:HIS:HB2	2.31	0.46
1:D:726:ALA:HA	1:D:735:ARG:O	2.15	0.46
1:D:455:ILE:C	1:D:456:LEU:CG	2.80	0.46
1:D:542:HIS:CD2	1:D:546:VAL:CG1	2.99	0.46
1:C:625:ALA:HB3	1:C:653:TRP:HH2	1.80	0.46
1:D:563:ARG:CB	1:D:587:TYR:CZ	2.98	0.46
1:E:562:SER:OG	1:E:564:ASP:OD1	2.34	0.46
1:C:692:ILE:HD12	1:C:706:LEU:HD12	1.97	0.45
1:D:542:HIS:ND1	1:D:568:ARG:NH2	2.63	0.45
1:D:650:VAL:HG13	1:D:664:PHE:HB2	1.97	0.45
1:E:536:ARG:O	1:E:536:ARG:HG2	2.15	0.45
1:A:624:GLN:O	1:A:625:ALA:HB2	2.16	0.45
1:A:657:SER:OG	1:A:659:GLU:HG2	2.16	0.45
1:C:539:PHE:HE2	1:C:558:VAL:HG11	1.81	0.45
1:A:458:THR:HG22	1:A:732:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:GLU:OE1	1:A:723:THR:HB	2.16	0.45
1:C:569:LEU:N	1:C:569:LEU:CD1	2.79	0.45
1:C:583:GLY:O	1:C:585:THR:N	2.49	0.45
1:D:737:TRP:CD1	1:D:737:TRP:N	2.85	0.45
1:A:456:LEU:C	1:A:457:THR:HG23	2.28	0.45
1:A:457:THR:OG1	1:A:486:TRP:CH2	2.67	0.45
1:C:568:ARG:HB3	1:C:578:HIS:HD2	1.78	0.45
1:C:609:ILE:HB	1:C:623:LEU:HB2	1.98	0.45
1:D:719:HIS:CE1	1:D:721:GLU:HG2	2.51	0.45
1:E:527:LEU:HB3	1:E:536:ARG:HD3	1.98	0.45
1:E:628:GLU:HB3	1:E:646:SER:OG	2.16	0.45
1:B:711:GLU:HB3	1:B:712:PRO:HD2	1.97	0.45
1:D:616:THR:O	1:D:618:LYS:N	2.47	0.45
1:D:696:ASP:O	1:D:700:GLN:N	2.49	0.45
1:C:458:THR:O	1:C:459:ASP:HB2	2.17	0.45
1:D:461:GLU:OE2	1:D:730:GLU:CB	2.64	0.45
1:D:644:HIS:CB	1:D:653:TRP:HE1	2.27	0.45
1:A:620:ARG:HD2	1:A:620:ARG:HA	1.81	0.45
1:B:711:GLU:HB3	1:B:712:PRO:CD	2.47	0.45
1:C:688:ASP:HA	1:C:712:PRO:HB3	1.98	0.45
1:D:451:ASN:HB3	1:D:737:TRP:CE3	2.52	0.45
1:D:570:TRP:NE1	1:D:577:GLU:HB2	2.32	0.45
1:A:609:ILE:HG13	1:A:633:LEU:HD11	1.99	0.45
1:D:712:PRO:HG2	1:D:730:GLU:CG	2.46	0.45
1:A:719:HIS:HB2	1:A:724:THR:HB	1.99	0.45
1:A:724:THR:CG2	1:A:725:LEU:N	2.79	0.45
1:B:487:ASP:N	1:B:494:LEU:CD1	2.80	0.45
1:C:649:THR:HG21	1:C:651:HIS:HE1	1.81	0.45
1:B:483:ILE:HB	1:B:497:LEU:HB2	1.99	0.44
1:C:637:PRO:HG3	1:C:678:PRO:O	2.16	0.44
1:D:457:THR:CG2	1:D:458:THR:N	2.79	0.44
1:D:460:ARG:NE	1:D:503:TRP:HZ2	2.16	0.44
1:A:685:SER:O	1:A:692:ILE:HA	2.17	0.44
1:C:547:LEU:HD12	1:C:589:TYR:HD1	1.82	0.44
1:E:455:ILE:N	1:E:455:ILE:CD1	2.70	0.44
1:A:455:ILE:C	1:A:456:LEU:CG	2.82	0.44
1:B:685:SER:O	1:B:692:ILE:HA	2.18	0.44
1:D:502:ASP:HB3	1:D:521:ASP:HB2	2.00	0.44
1:D:652:LEU:HB2	1:D:700:GLN:NE2	2.33	0.44
1:E:711:GLU:HG2	1:E:731:ASP:HB3	2.00	0.44
1:A:551:PHE:CE1	1:A:558:VAL:CG2	3.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:CG	1:A:568:ARG:NH2	2.80	0.44
1:A:662:HIS:HB2	1:A:700:GLN:HG2	2.00	0.44
1:D:699:ALA:O	1:D:700:GLN:CB	2.60	0.43
1:E:525:VAL:HB	1:E:539:PHE:HB2	1.99	0.43
1:A:482:LEU:HD22	1:A:496:THR:CG2	2.48	0.43
1:A:536:ARG:HE	1:A:536:ARG:HA	1.80	0.43
1:E:631:VAL:O	1:E:631:VAL:HG12	2.16	0.43
1:E:662:HIS:CG	1:E:663:THR:N	2.86	0.43
1:A:450:LEU:O	1:A:738:PRO:HD2	2.17	0.43
1:D:609:ILE:HD11	1:D:630:VAL:HG11	2.00	0.43
1:A:539:PHE:N	1:A:539:PHE:HD1	2.15	0.43
1:A:719:HIS:CG	1:A:720:PRO:HD2	2.53	0.43
1:C:460:ARG:HD3	1:C:480:ASP:OD2	2.18	0.43
1:C:501:THR:HG22	1:C:501:THR:O	2.18	0.43
1:C:605:ARG:CG	1:C:629:ASN:HD21	2.12	0.43
1:D:571:ASN:OD1	1:D:574:THR:HG22	2.18	0.43
1:A:674:VAL:HA	1:A:684:ALA:O	2.18	0.43
1:D:619:GLU:OE2	1:D:622:VAL:HG22	2.16	0.43
1:D:538:VAL:CG1	1:D:539:PHE:H	2.30	0.43
1:D:631:VAL:HG12	1:D:631:VAL:O	2.19	0.43
1:A:558:VAL:HG23	1:A:572:VAL:HG22	2.00	0.43
1:D:454:ARG:HG3	1:D:735:ARG:CG	2.47	0.43
1:E:454:ARG:CA	1:E:455:ILE:HD12	2.49	0.43
1:C:460:ARG:HD3	1:C:480:ASP:OD1	2.18	0.43
1:E:726:ALA:HA	1:E:735:ARG:O	2.19	0.43
1:D:589:TYR:CE1	1:D:605:ARG:HG3	2.54	0.43
1:D:600:VAL:HG23	1:D:614:VAL:CG1	2.48	0.43
1:A:482:LEU:HD22	1:A:496:THR:HG21	2.01	0.42
1:A:625:ALA:HB3	1:A:653:TRP:HH2	1.84	0.42
1:A:542:HIS:HD1	1:A:568:ARG:NH2	2.16	0.42
1:E:664:PHE:HB3	1:E:695:TRP:CZ3	2.54	0.42
1:D:471:GLY:HA3	1:D:472:SER:CB	2.49	0.42
1:D:598:SER:O	1:D:614:VAL:HG22	2.19	0.42
1:A:479:GLY:HA2	1:A:503:TRP:CD2	2.55	0.42
1:B:647:ASP:O	1:B:648:SER:HB2	2.20	0.42
1:C:482:LEU:HD12	1:C:482:LEU:O	2.19	0.42
1:C:664:PHE:CE1	1:C:700:GLN:CG	3.02	0.42
1:D:647:ASP:CB	1:D:670:TRP:HD1	2.33	0.42
1:D:487:ASP:OD2	1:D:490:SER:HB3	2.19	0.42
1:E:647:ASP:HB2	1:E:670:TRP:CH2	2.55	0.42
1:A:542:HIS:ND1	1:A:568:ARG:NH2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:GLU:HG3	1:E:579:ALA:HB1	2.00	0.42
1:D:462:ALA:O	1:D:728:ALA:HB1	2.19	0.42
1:A:589:TYR:CD2	1:A:605:ARG:HG3	2.54	0.42
1:A:647:ASP:OD1	1:A:670:TRP:CD2	2.73	0.42
1:D:461:GLU:OE2	1:D:730:GLU:HA	2.19	0.42
1:A:487:ASP:CG	1:A:489:ALA:O	2.58	0.42
1:A:726:ALA:HA	1:A:735:ARG:O	2.20	0.42
1:B:494:LEU:N	1:B:494:LEU:CD1	2.81	0.42
1:A:452:GLU:HB3	1:A:736:ILE:CG2	2.49	0.42
1:B:494:LEU:HD12	1:B:494:LEU:H	1.81	0.42
1:B:566:THR:HG21	1:B:568:ARG:HH21	1.84	0.42
1:C:480:ASP:CB	1:C:482:LEU:HG	2.48	0.42
1:C:624:GLN:O	1:C:625:ALA:HB2	2.20	0.42
1:E:453:PRO:CB	1:E:736:ILE:O	2.68	0.42
1:E:522:ASP:O	1:E:523:ALA:HB3	2.19	0.42
1:A:502:ASP:HB3	1:A:521:ASP:HB2	2.02	0.41
1:B:527:LEU:HD12	1:B:527:LEU:HA	1.92	0.41
1:C:692:ILE:HD11	1:C:706:LEU:CB	2.48	0.41
1:D:560:SER:CB	1:D:570:TRP:HZ3	2.33	0.41
1:D:602:SER:CA	1:D:633:LEU:HD21	2.50	0.41
1:D:609:ILE:HB	1:D:623:LEU:HB2	2.02	0.41
1:A:453:PRO:HG2	1:A:736:ILE:HG21	2.02	0.41
1:A:525:VAL:HG23	1:A:546:VAL:HG21	2.02	0.41
1:C:719:HIS:ND1	1:C:721:GLU:HG2	2.34	0.41
1:C:733:THR:HG21	1:C:735:ARG:HH21	1.86	0.41
1:A:453:PRO:HD2	1:A:736:ILE:HG21	2.03	0.41
1:A:609:ILE:CD1	1:A:630:VAL:HG21	2.50	0.41
1:D:644:HIS:O	1:D:650:VAL:HA	2.21	0.41
1:B:529:ASP:HB3	1:B:534:GLU:HG2	2.02	0.41
1:C:607:GLY:O	1:C:626:PRO:CG	2.64	0.41
1:E:606:ASP:OD1	1:E:608:THR:OG1	2.25	0.41
1:B:692:ILE:HB	1:B:706:LEU:HB2	2.02	0.41
1:C:450:LEU:CB	1:C:704:THR:HG23	2.50	0.41
1:C:692:ILE:HG13	1:C:706:LEU:CB	2.50	0.41
1:D:675:ALA:O	1:D:683:LEU:HD12	2.20	0.41
1:E:736:ILE:HD13	1:E:736:ILE:HG21	1.89	0.41
1:B:522:ASP:OD1	1:B:524:THR:HB	2.20	0.41
1:B:682:LEU:HD23	1:B:695:TRP:O	2.20	0.41
1:C:539:PHE:HB3	1:C:570:TRP:CZ3	2.56	0.41
1:D:542:HIS:HE1	1:D:568:ARG:HH21	1.61	0.41
1:D:692:ILE:HB	1:D:706:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:662:HIS:CD2	1:E:663:THR:N	2.89	0.41
1:A:458:THR:HG22	1:A:732:GLY:CA	2.50	0.41
1:C:473:LEU:CD2	1:C:494:LEU:CD1	2.99	0.41
1:D:568:ARG:HH21	1:D:568:ARG:HB2	1.86	0.41
1:C:562:SER:O	1:C:588:VAL:CG2	2.69	0.41
1:D:589:TYR:CE1	1:D:605:ARG:HD3	2.56	0.41
1:A:646:SER:OG	1:A:647:ASP:N	2.53	0.41
1:C:711:GLU:HG3	1:C:712:PRO:HD2	2.02	0.41
1:D:547:LEU:HD11	1:D:587:TYR:HD2	1.83	0.41
1:D:554:ASP:OD2	1:D:556:SER:OG	2.39	0.41
1:D:644:HIS:CE1	1:D:646:SER:HB2	2.55	0.41
1:A:455:ILE:O	1:A:456:LEU:HD23	2.20	0.41
1:C:646:SER:OG	1:C:647:ASP:N	2.54	0.41
1:C:647:ASP:HB3	1:C:670:TRP:CD1	2.56	0.41
1:D:685:SER:O	1:D:692:ILE:HA	2.21	0.41
1:C:706:LEU:HB3	1:C:737:TRP:CZ3	2.56	0.40
1:C:473:LEU:HD22	1:C:494:LEU:HD12	2.03	0.40
1:E:460:ARG:HG3	1:E:480:ASP:HB3	2.02	0.40
1:A:452:GLU:HB3	1:A:736:ILE:HG23	2.04	0.40
1:D:625:ALA:HB3	1:D:653:TRP:HH2	1.85	0.40
1:D:650:VAL:HG23	1:D:674:VAL:HG11	2.04	0.40
1:E:699:ALA:O	1:E:700:GLN:HB2	2.22	0.40
1:A:456:LEU:C	1:A:457:THR:OG1	2.60	0.40
1:A:644:HIS:HE1	1:A:649:THR:O	2.05	0.40
1:C:643:VAL:HG12	1:C:674:VAL:HG21	2.03	0.40
1:D:572:VAL:HG23	1:D:573:ALA:N	2.36	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	282/302 (93%)	268 (95%)	10 (4%)	4 (1%)	11 22
1	B	286/302 (95%)	273 (96%)	12 (4%)	1 (0%)	41 64
1	C	288/302 (95%)	270 (94%)	15 (5%)	3 (1%)	15 32
1	D	280/302 (93%)	258 (92%)	15 (5%)	7 (2%)	5 9
1	E	286/302 (95%)	273 (96%)	12 (4%)	1 (0%)	41 64
All	All	1422/1510 (94%)	1342 (94%)	64 (4%)	16 (1%)	14 30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	452	GLU
1	A	625	ALA
1	C	625	ALA
1	D	453	PRO
1	D	457	THR
1	D	625	ALA
1	A	457	THR
1	A	710	THR
1	B	583	GLY
1	D	472	SER
1	D	709	HIS
1	E	657	SER
1	D	617	GLY
1	C	450	LEU
1	C	648	SER
1	D	452	GLU

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	219/235 (93%)	204 (93%)	15 (7%)	16 32
1	B	223/235 (95%)	212 (95%)	11 (5%)	25 48
1	C	221/235 (94%)	202 (91%)	19 (9%)	10 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	219/235 (93%)	195 (89%)	24 (11%)	6 11
1	E	222/235 (94%)	214 (96%)	8 (4%)	35 61
All	All	1104/1175 (94%)	1027 (93%)	77 (7%)	15 30

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	516	LEU
1	A	539	PHE
1	A	543	THR
1	A	545	TYR
1	A	549	ILE
1	A	633	LEU
1	A	635	PHE
1	A	642	LEU
1	A	644	HIS
1	A	683	LEU
1	A	703	HIS
1	A	721	GLU
1	A	730	GLU
1	A	734	ILE
1	A	737	TRP
1	B	481	LYS
1	B	495	HIS
1	B	516	LEU
1	B	524	THR
1	B	527	LEU
1	B	551	PHE
1	B	572	VAL
1	B	624	GLN
1	B	628	GLU
1	B	638	ASP
1	B	710	THR
1	C	452	GLU
1	C	482	LEU
1	C	563	ARG
1	C	564	ASP
1	C	566	THR
1	C	587	TYR
1	C	602	SER
1	C	622	VAL

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Mol	Chain	Res	Type
1	C	632	SER
1	C	633	LEU
1	C	642	LEU
1	C	644	HIS
1	C	651	HIS
1	C	676	PHE
1	C	683	LEU
1	C	685	SER
1	C	711	GLU
1	C	725	LEU
1	C	737	TRP
1	D	450	LEU
1	D	451	ASN
1	D	453	PRO
1	D	472	SER
1	D	501	THR
1	D	516	LEU
1	D	539	PHE
1	D	544	HIS
1	D	545	TYR
1	D	546	VAL
1	D	554	ASP
1	D	578	HIS
1	D	582	LYS
1	D	616	THR
1	D	633	LEU
1	D	635	PHE
1	D	642	LEU
1	D	644	HIS
1	D	648	SER
1	D	703	HIS
1	D	710	THR
1	D	735	ARG
1	D	736	ILE
1	D	737	TRP
1	E	493	GLU
1	E	544	HIS
1	E	551	PHE
1	E	613	ASP
1	E	644	HIS
1	E	646	SER
1	E	685	SER

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Mol	Chain	Res	Type
1	E	692	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	544	HIS
1	A	703	HIS
1	A	714	HIS
1	B	629	ASN
1	B	651	HIS
1	C	495	HIS
1	C	629	ASN
1	C	651	HIS
1	D	544	HIS
1	D	578	HIS
1	D	651	HIS
1	D	700	GLN
1	D	709	HIS
1	E	644	HIS

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	286/302 (94%)	0.03	6 (2%) 63 58	19, 37, 68, 101	0
1	B	288/302 (95%)	-0.30	0 100 100	20, 36, 60, 79	0
1	C	290/302 (96%)	0.07	11 (3%) 40 33	19, 38, 69, 93	0
1	D	284/302 (94%)	0.06	11 (3%) 39 32	22, 40, 69, 92	0
1	E	288/302 (95%)	-0.30	0 100 100	23, 40, 61, 85	0
All	All	1436/1510 (95%)	-0.09	28 (1%) 66 62	19, 38, 67, 101	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	585	THR	4.2
1	A	710	THR	3.9
1	D	700	GLN	3.5
1	A	452	GLU	3.3
1	A	451	ASN	3.2
1	A	503	TRP	3.2
1	D	503	TRP	3.0
1	D	710	THR	3.0
1	C	589	TYR	2.9
1	D	730	GLU	2.7
1	D	495	HIS	2.6
1	D	452	GLU	2.6
1	C	584	HIS	2.5
1	C	458	THR	2.5
1	C	539	PHE	2.5
1	C	451	ASN	2.4
1	C	479	GLY	2.4
1	C	692	ILE	2.4
1	D	560	SER	2.4
1	A	719	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	714	HIS	2.3
1	C	625	ALA	2.3
1	C	574	THR	2.3
1	D	719	HIS	2.1
1	A	706	LEU	2.1
1	C	455	ILE	2.0
1	D	731	ASP	2.0
1	D	664	PHE	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.