



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:03 PM EDT

PDB ID : 4N9N / pdb_00004n9n
Title : Crystal Structure of Saccharomyces cerevisiae Upc2 Transcription Factor fused with T4 Lysozyme
Authors : Yang, H.; Im, Y.J.
Deposited on : 2013-10-21
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
Mogul : 2022.3.0, CSD as543be (2022)
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

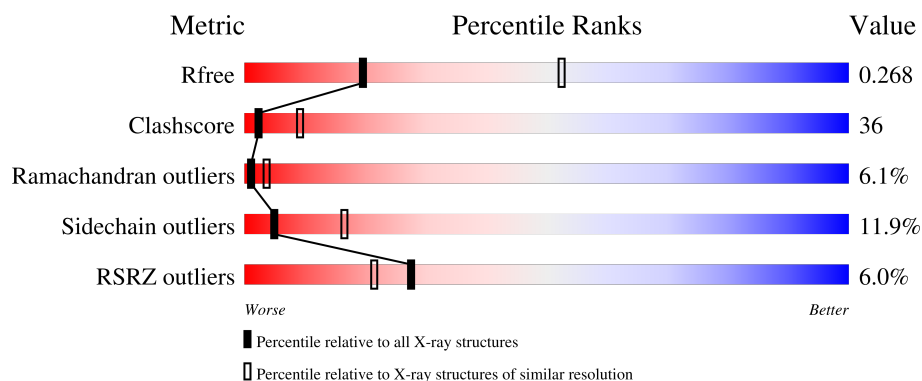
1 Overall quality at a glance

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	438	4% 41% 44% 11% ..
1	B	438	7% 41% 43% 13% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6829 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 Sterol uptake control protein 2, Lysozyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	Se	0	0	0
			3400	2182	577	628	2	11			
1	B	428	Total	C	N	O	S	Se	0	0	0
			3400	2182	577	628	2	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	594	GLY	-	expression tag	UNP Q12151
A	595	SER	-	expression tag	UNP Q12151
A	596	HIS	-	expression tag	UNP Q12151
A	597	MSE	-	expression tag	UNP Q12151
A	715	VAL	-	linker	UNP Q12151
A	716	ASP	-	linker	UNP Q12151
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	724	VAL	-	linker	UNP Q12151
A	725	ASP	-	linker	UNP Q12151
B	594	GLY	-	expression tag	UNP Q12151
B	595	SER	-	expression tag	UNP Q12151
B	596	HIS	-	expression tag	UNP Q12151
B	597	MSE	-	expression tag	UNP Q12151
B	715	VAL	-	linker	UNP Q12151
B	716	ASP	-	linker	UNP Q12151
B	1054	THR	CYS	engineered mutation	UNP P00720
B	1097	ALA	CYS	engineered mutation	UNP P00720
B	724	VAL	-	linker	UNP Q12151
B	725	ASP	-	linker	UNP Q12151

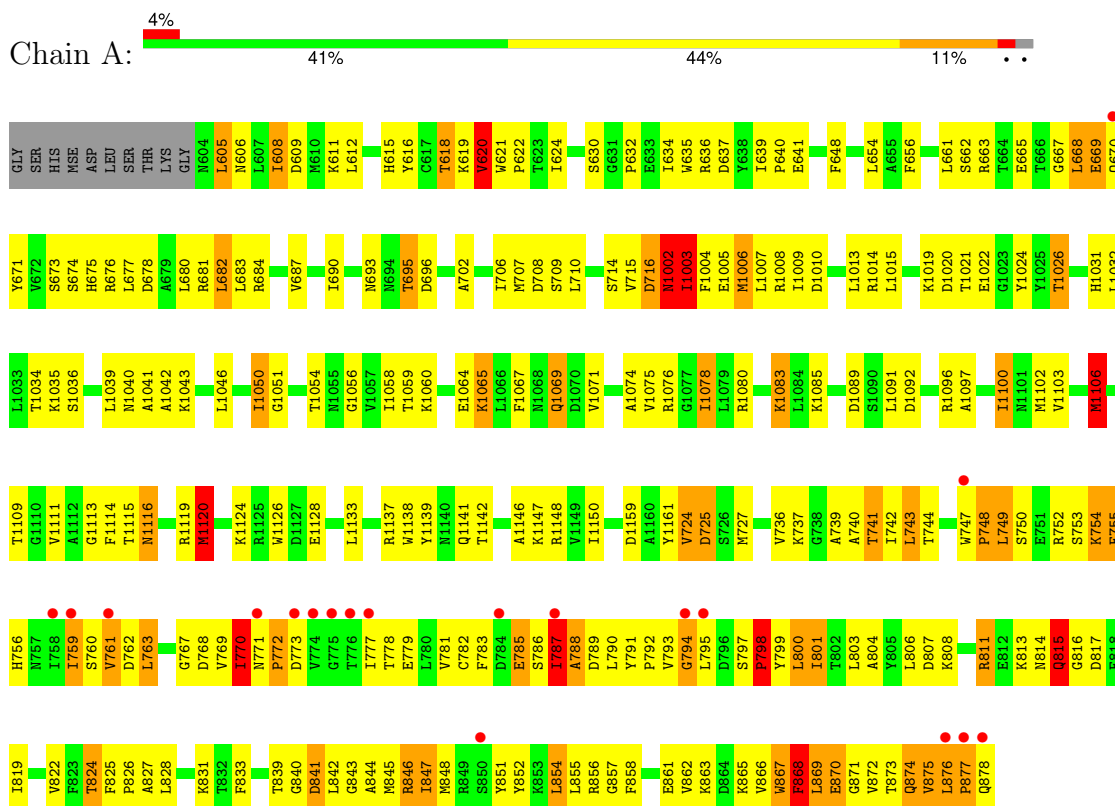
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total 21	O 21	0	0
2	B	8	Total 8	O 8	0	0

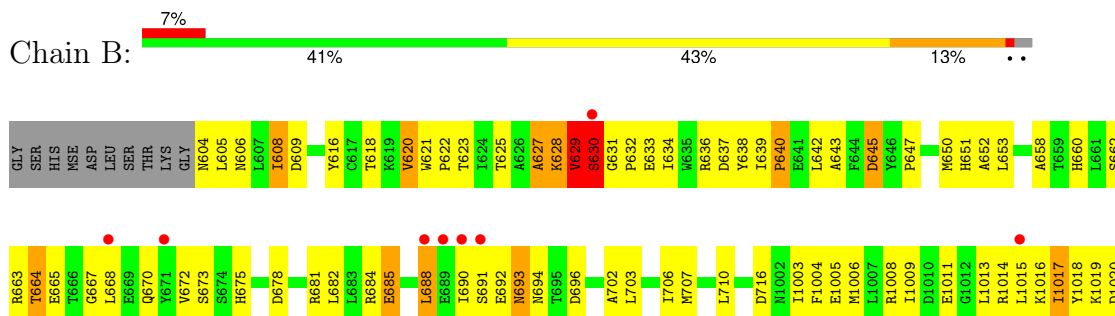
3 Residue-property plots

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: Sterol uptake control protein 2, Lysozyme



- Molecule 1: Sterol uptake control protein 2, Lysozyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	67.17Å 67.17Å 257.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.17 – 2.90 58.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (58.17-2.90) 99.8 (58.17-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.272 0.249 , 0.268	Depositor DCC
R_{free} test set	1442 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.062 for h,-h-k,-l 0.042 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6829	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.45	4/3460 (0.1%)	0.99	17/4678 (0.4%)
1	B	0.45	5/3460 (0.1%)	0.99	17/4678 (0.4%)
All	All	0.45	9/6920 (0.1%)	0.99	34/9356 (0.4%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1106	MSE	SE-CE	-5.85	1.77	1.95
1	A	1120	MSE	SE-CE	-5.60	1.78	1.95
1	A	1006	MSE	SE-CE	-5.51	1.78	1.95
1	B	1102	MSE	SE-CE	-5.37	1.79	1.95
1	B	1106	MSE	CG-SE	-5.32	1.79	1.95
1	A	1106	MSE	CG-SE	-5.22	1.79	1.95
1	B	1120	MSE	SE-CE	-5.19	1.79	1.95
1	B	1006	MSE	SE-CE	-5.03	1.80	1.95
1	A	1120	MSE	CG-SE	-5.02	1.80	1.95

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	766	LEU	N-CA-C	-10.55	95.79	110.35
1	B	629	VAL	N-CA-C	-9.91	97.61	111.89
1	B	620	VAL	N-CA-C	8.93	118.87	110.74
1	A	1003	ILE	N-CA-C	-8.58	102.47	110.53
1	A	869	LEU	N-CA-C	-7.92	103.18	112.92
1	B	645	ASP	N-CA-C	-7.26	98.48	110.17
1	B	813	LYS	N-CA-C	-6.89	100.60	110.59
1	B	638	TYR	N-CA-C	6.75	118.29	111.07
1	B	839	THR	N-CA-C	-6.63	104.91	114.12
1	B	735	HIS	N-CA-C	-6.54	103.77	111.03
1	A	620	VAL	N-CA-C	6.37	118.33	111.58
1	B	631	GLY	N-CA-C	-6.29	99.51	112.34
1	A	1041	ALA	N-CA-C	-6.21	104.59	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1091	LEU	N-CA-C	5.86	119.64	110.32
1	A	788	ALA	N-CA-C	-5.72	105.40	112.38
1	A	1002	ASN	N-CA-C	-5.71	105.97	113.17
1	A	1065	LYS	N-CA-C	-5.68	104.30	111.11
1	A	759	ILE	N-CA-C	-5.61	104.08	111.09
1	B	765	ASP	N-CA-C	5.40	117.04	108.67
1	B	869	LEU	N-CA-C	-5.40	106.70	113.72
1	A	783	PHE	N-CA-C	-5.38	100.99	109.50
1	B	1026	THR	N-CA-C	5.35	115.19	108.45
1	A	1010	ASP	N-CA-C	5.35	118.02	111.82
1	B	769	VAL	N-CA-C	-5.34	105.29	110.42
1	A	1069	GLN	N-CA-C	-5.24	105.57	111.28
1	B	630	SER	N-CA-C	5.22	121.92	110.80
1	A	755	PHE	N-CA-C	-5.17	106.65	113.17
1	B	786	SER	N-CA-C	-5.16	106.68	112.87
1	A	870	GLU	N-CA-C	-5.11	105.41	111.69
1	A	1142	THR	CA-C-N	5.10	124.27	118.97
1	A	1142	THR	C-N-CA	5.10	124.27	118.97
1	B	1035	LYS	N-CA-C	-5.06	105.84	111.36
1	B	1105	GLN	N-CA-C	5.06	116.60	111.14
1	A	845	MSE	N-CA-C	-5.03	105.90	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3400	0	3432	242	0
1	B	3400	0	3432	246	0
2	A	21	0	0	0	0
2	B	8	0	0	0	0
All	All	6829	0	6864	488	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (488) 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:715:VAL:HG12	1:A:716:ASP:OD2	1.40	1.18
1:A:846:ARG:HG3	1:A:846:ARG:HH11	1.04	1.18
1:B:797:SER:HB2	1:B:798:PRO:HA	1.11	1.09
1:B:825:PHE:HE2	1:B:848:MSE:HE1	1.24	1.00
1:B:1024:TYR:HB3	1:B:1035:LYS:HA	1.44	0.97
1:B:797:SER:HB2	1:B:798:PRO:CA	1.95	0.97
1:A:616:TYR:HA	1:A:620:VAL:CG1	1.96	0.95
1:B:856:ARG:HE	1:B:873:THR:HG21	1.32	0.95
1:B:848:MSE:HA	1:B:848:MSE:HE2	1.47	0.94
1:B:1106:MSE:HE1	1:B:1114:PHE:HE2	1.31	0.93
1:B:759:ILE:HD12	1:B:760:SER:N	1.84	0.93
1:B:636:ARG:HG2	1:B:637:ASP:OD2	1.68	0.92
1:A:695:THR:HG21	1:A:749:LEU:HD22	1.50	0.91
1:B:797:SER:CB	1:B:798:PRO:HA	1.98	0.90
1:B:1008:ARG:HG3	1:B:1008:ARG:HH11	1.39	0.88
1:A:791:TYR:HB3	1:A:792:PRO:HA	1.57	0.87
1:B:628:LYS:HE3	1:B:816:GLY:N	1.89	0.87
1:A:606:ASN:OD1	1:A:608:ILE:HG23	1.73	0.87
1:B:678:ASP:O	1:B:682:LEU:HD23	1.73	0.87
1:B:1146:ALA:O	1:B:1150:ILE:HG12	1.73	0.86
1:A:618:THR:HG22	1:A:619:LYS:HG3	1.54	0.86
1:B:825:PHE:CE2	1:B:848:MSE:HE1	2.11	0.86
1:A:815:GLN:HG3	1:A:858:PHE:HE1	1.39	0.85
1:A:616:TYR:HA	1:A:620:VAL:HG13	1.56	0.85
1:B:855:LEU:HD12	1:B:872:VAL:HG21	1.58	0.85
1:A:1040:ASN:HA	1:A:1043:LYS:HG2	1.59	0.85
1:A:1146:ALA:O	1:A:1150:ILE:HG12	1.77	0.84
1:A:695:THR:HG21	1:A:749:LEU:CD2	2.06	0.84
1:A:1106:MSE:HE1	1:A:1114:PHE:HE2	1.42	0.83
1:A:630:SER:OG	1:A:634:ILE:HG21	1.77	0.83
1:B:856:ARG:HE	1:B:873:THR:CG2	1.90	0.83
1:A:1089:ASP:HA	1:A:1096:ARG:HH21	1.44	0.81
1:A:846:ARG:HG3	1:A:846:ARG:NH1	1.84	0.81
1:B:634:ILE:O	1:B:639:ILE:HG12	1.81	0.79
1:A:825:PHE:HB3	1:A:826:PRO:HD3	1.64	0.79
1:B:813:LYS:O	1:B:814:ASN:HB3	1.82	0.78
1:B:1083:LYS:O	1:B:1083:LYS:HE2	1.83	0.78
1:B:747:TRP:HD1	1:B:759:ILE:HD13	1.48	0.78
1:B:1027:ILE:HG23	1:B:1031:HIS:HB3	1.65	0.77
1:B:832:THR:O	1:B:836:LEU:HD23	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:MSE:HE1	1:B:1114:PHE:CE2	2.17	0.77
1:B:1025:TYR:HB2	1:B:1034:THR:HG22	1.67	0.76
1:A:702:ALA:O	1:A:706:ILE:HG12	1.85	0.76
1:B:1004:PHE:HA	1:B:1067:PHE:CE2	2.20	0.76
1:A:797:SER:HB2	1:A:798:PRO:HD2	1.67	0.76
1:A:846:ARG:HH11	1:A:846:ARG:CG	1.92	0.76
1:A:844:ALA:HA	1:A:847:ILE:HD11	1.68	0.75
1:A:1106:MSE:HE1	1:A:1114:PHE:CE2	2.21	0.75
1:A:744:THR:HA	1:A:747:TRP:CE3	2.21	0.75
1:A:791:TYR:HA	1:A:793:VAL:H	1.52	0.75
1:A:1050:ILE:HG22	1:A:1051:GLY:H	1.51	0.75
1:B:707:MSE:HE3	1:B:868:PHE:CZ	2.21	0.74
1:A:1137:ARG:O	1:A:1141:GLN:HG2	1.88	0.74
1:B:1011:GLU:OE1	1:B:1029:ILE:HG22	1.88	0.74
1:B:1116:ASN:O	1:B:1120:MSE:HG3	1.89	0.73
1:B:874:GLN:CD	1:B:874:GLN:H	1.94	0.73
1:A:744:THR:HG22	1:A:747:TRP:CZ3	2.24	0.72
1:B:1029:ILE:H	1:B:1029:ILE:HD12	1.54	0.72
1:B:729:PRO:O	1:B:731:ALA:N	2.22	0.72
1:A:630:SER:HB3	1:A:635:TRP:NE1	2.06	0.71
1:A:814:ASN:O	1:A:816:GLY:N	2.23	0.71
1:B:1145:ARG:O	1:B:1149:VAL:HG23	1.89	0.71
1:B:784:ASP:O	1:B:785:GLU:HB2	1.91	0.71
1:B:767:GLY:O	1:B:768:ASP:HB2	1.90	0.71
1:A:706:ILE:HD13	1:A:739:ALA:HB3	1.72	0.71
1:B:1008:ARG:HG3	1:B:1008:ARG:NH1	2.03	0.71
1:A:630:SER:HB3	1:A:635:TRP:HE1	1.56	0.70
1:A:737:LYS:O	1:A:741:THR:HG22	1.92	0.70
1:B:812:GLU:HG3	1:B:821:ARG:HD2	1.74	0.70
1:A:668:LEU:O	1:A:670:GLN:N	2.25	0.69
1:B:694:ASN:HD21	1:B:696:ASP:HB2	1.57	0.69
1:B:796:ASP:O	1:B:797:SER:CB	2.41	0.69
1:A:673:SER:O	1:A:677:LEU:HD23	1.94	0.68
1:A:1040:ASN:HA	1:A:1043:LYS:CG	2.24	0.68
1:A:707:MSE:HA	1:A:710:LEU:HD12	1.76	0.67
1:B:690:ILE:O	1:B:692:GLU:N	2.25	0.67
1:A:761:VAL:HG13	1:A:762:ASP:N	2.10	0.67
1:B:1106:MSE:HE2	1:B:1111:VAL:HA	1.75	0.67
1:A:608:ILE:HG12	1:A:671:TYR:CE2	2.30	0.67
1:A:1015:LEU:HD12	1:A:1058:ILE:O	1.95	0.66
1:A:1089:ASP:HA	1:A:1096:ARG:NH2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:ASP:HA	1:B:724:VAL:HG23	1.77	0.66
1:B:632:PRO:O	1:B:636:ARG:HB3	1.95	0.66
1:A:770:ILE:O	1:A:772:PRO:HD3	1.96	0.66
1:A:1026:THR:HG22	1:A:1031:HIS:C	2.21	0.66
1:A:843:GLY:O	1:A:846:ARG:HB2	1.96	0.66
1:A:706:ILE:CD1	1:A:739:ALA:HB3	2.26	0.65
1:A:1120:MSE:HE2	1:A:1128:GLU:HB3	1.77	0.65
1:B:856:ARG:HG3	1:B:873:THR:HB	1.77	0.65
1:B:867:TRP:C	1:B:869:LEU:H	2.04	0.65
1:B:856:ARG:NE	1:B:873:THR:HG21	2.11	0.65
1:B:628:LYS:HE3	1:B:816:GLY:CA	2.27	0.65
1:A:605:LEU:N	1:A:605:LEU:CD2	2.59	0.65
1:A:872:VAL:HG13	1:A:873:THR:HG23	1.78	0.64
1:B:796:ASP:O	1:B:797:SER:HB3	1.97	0.64
1:B:867:TRP:O	1:B:869:LEU:N	2.29	0.64
1:B:1078:ILE:HD11	1:B:1103:VAL:HG21	1.79	0.64
1:A:1092:ASP:O	1:A:1096:ARG:HG3	1.97	0.64
1:B:606:ASN:ND2	1:B:609:ASP:CG	2.56	0.64
1:B:628:LYS:C	1:B:630:SER:N	2.48	0.64
1:B:872:VAL:O	1:B:873:THR:C	2.41	0.64
1:B:848:MSE:HA	1:B:848:MSE:CE	2.25	0.63
1:A:714:SER:HA	1:A:1002:ASN:HD21	1.62	0.63
1:B:658:ALA:HB1	1:B:672:VAL:HG22	1.80	0.63
1:A:632:PRO:O	1:A:636:ARG:HB3	1.98	0.63
1:A:1005:GLU:OE2	1:A:1008:ARG:NH1	2.32	0.63
1:B:1027:ILE:HG13	1:B:1028:GLY:N	2.13	0.63
1:B:670:GLN:OE1	1:B:670:GLN:HA	1.99	0.62
1:A:759:ILE:O	1:A:760:SER:HB2	2.00	0.62
1:B:651:HIS:CD2	1:B:675:HIS:HD2	2.17	0.62
1:B:1074:ALA:O	1:B:1078:ILE:HG12	1.99	0.61
1:B:628:LYS:HG2	1:B:816:GLY:HA2	1.82	0.61
1:A:1074:ALA:O	1:A:1078:ILE:HG12	1.99	0.61
1:B:1101:ASN:HD21	1:B:1145:ARG:HH21	1.49	0.61
1:A:1120:MSE:HE2	1:A:1128:GLU:C	2.24	0.61
1:A:814:ASN:C	1:A:816:GLY:H	2.09	0.61
1:A:606:ASN:HB3	1:A:609:ASP:HB2	1.82	0.61
1:B:1013:LEU:HD12	1:B:1014:ARG:H	1.65	0.60
1:A:661:LEU:HD23	1:A:668:LEU:HD11	1.83	0.60
1:A:715:VAL:CG1	1:A:716:ASP:OD2	2.33	0.60
1:B:670:GLN:C	1:B:672:VAL:H	2.07	0.60
1:B:877:PRO:O	1:B:878:GLN:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:PHE:HB3	1:A:682:LEU:HB3	1.82	0.60
1:A:815:GLN:HG3	1:A:858:PHE:CE1	2.28	0.60
1:B:685:GLU:O	1:B:688:LEU:HB3	2.01	0.60
1:B:690:ILE:C	1:B:692:GLU:H	2.09	0.60
1:B:797:SER:CB	1:B:798:PRO:CA	2.64	0.60
1:B:759:ILE:HD12	1:B:760:SER:H	1.63	0.60
1:B:1137:ARG:O	1:B:1141:GLN:HG2	2.00	0.60
1:A:791:TYR:CB	1:A:792:PRO:HA	2.24	0.60
1:A:866:VAL:HG12	1:A:867:TRP:O	2.01	0.60
1:B:1116:ASN:HA	1:B:1119:ARG:NH2	2.17	0.59
1:B:684:ARG:HE	1:B:684:ARG:HA	1.67	0.59
1:A:833:PHE:CE2	1:A:848:MSE:HE3	2.37	0.59
1:A:715:VAL:C	1:A:716:ASP:OD2	2.46	0.59
1:A:867:TRP:O	1:A:869:LEU:N	2.32	0.59
1:A:852:TYR:HE2	1:A:856:ARG:HH12	1.48	0.59
1:B:703:LEU:O	1:B:707:MSE:HG3	2.02	0.59
1:A:873:THR:O	1:A:874:GLN:HB2	2.02	0.59
1:B:1101:ASN:ND2	1:B:1145:ARG:HH21	2.02	0.58
1:A:1046:LEU:HD23	1:A:1056:GLY:HA2	1.84	0.58
1:A:1120:MSE:CE	1:A:1128:GLU:HB3	2.34	0.58
1:B:1029:ILE:HD13	1:B:1067:PHE:HB2	1.86	0.58
1:B:1159:ASP:O	1:B:724:VAL:HG23	2.02	0.57
1:A:714:SER:O	1:A:1002:ASN:OD1	2.22	0.57
1:A:695:THR:CG2	1:A:749:LEU:HD22	2.31	0.57
1:A:876:LEU:H	1:A:876:LEU:HD12	1.69	0.57
1:B:628:LYS:C	1:B:630:SER:H	2.08	0.57
1:B:866:VAL:HG23	1:B:867:TRP:O	2.04	0.57
1:A:608:ILE:O	1:A:612:LEU:HG	2.05	0.57
1:B:1005:GLU:OE1	1:B:727:MSE:HA	2.04	0.57
1:B:1014:ARG:HG3	1:B:1016:LYS:HE3	1.87	0.57
1:B:1016:LYS:O	1:B:1027:ILE:HD12	2.04	0.57
1:B:1029:ILE:CD1	1:B:1067:PHE:HB2	2.35	0.57
1:B:845:MSE:HE3	1:B:849:ARG:HH12	1.70	0.57
1:B:874:GLN:CD	1:B:874:GLN:N	2.59	0.57
1:A:696:ASP:OD1	1:A:753:SER:HB2	2.04	0.57
1:B:606:ASN:ND2	1:B:609:ASP:OD2	2.38	0.57
1:A:798:PRO:O	1:A:799:TYR:HB2	2.05	0.56
1:B:670:GLN:C	1:B:672:VAL:N	2.62	0.56
1:B:777:ILE:HA	1:B:794:GLY:HA2	1.86	0.56
1:B:1092:ASP:OD1	1:B:1094:VAL:HG23	2.06	0.56
1:A:1076:ARG:O	1:A:1080:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ARG:HG2	1:A:637:ASP:OD2	2.07	0.55
1:A:759:ILE:HD12	1:A:761:VAL:O	2.06	0.55
1:B:651:HIS:HD2	1:B:675:HIS:CD2	2.24	0.55
1:B:1027:ILE:CG2	1:B:1031:HIS:HB3	2.36	0.55
1:A:608:ILE:HG12	1:A:671:TYR:CZ	2.41	0.55
1:A:630:SER:HB3	1:A:635:TRP:CD1	2.41	0.55
1:B:1005:GLU:O	1:B:1009:ILE:HG12	2.06	0.55
1:A:611:LYS:HE3	1:A:661:LEU:HD21	1.89	0.55
1:A:791:TYR:HB3	1:A:792:PRO:CA	2.35	0.54
1:B:747:TRP:HD1	1:B:759:ILE:CD1	2.20	0.54
1:B:1159:ASP:HA	1:B:724:VAL:CG2	2.38	0.54
1:A:605:LEU:HD23	1:A:605:LEU:H	1.72	0.54
1:A:786:SER:O	1:A:787:ILE:HG13	2.07	0.54
1:B:667:GLY:C	1:B:668:LEU:HG	2.31	0.54
1:B:844:ALA:O	1:B:847:ILE:HG13	2.07	0.54
1:A:767:GLY:HA2	1:A:770:ILE:HD11	1.88	0.54
1:A:637:ASP:O	1:A:641:GLU:HG2	2.07	0.54
1:A:876:LEU:HD12	1:A:876:LEU:N	2.23	0.54
1:B:847:ILE:CD1	1:B:848:MSE:HE3	2.37	0.54
1:B:1045:GLU:HG2	1:B:1048:LYS:HZ2	1.73	0.54
1:B:1144:ASN:HB3	1:B:1148:ARG:HH12	1.73	0.54
1:A:687:VAL:HG22	1:A:690:ILE:HD11	1.90	0.53
1:A:1046:LEU:O	1:A:1050:ILE:HG12	2.08	0.53
1:A:803:LEU:HD21	1:A:847:ILE:HG21	1.91	0.53
1:A:1139:TYR:OH	1:A:1147:LYS:HE2	2.08	0.53
1:B:1013:LEU:HD12	1:B:1014:ARG:N	2.23	0.53
1:A:676:ARG:NH2	1:A:709:SER:OG	2.41	0.53
1:B:848:MSE:O	1:B:851:TYR:HB3	2.09	0.53
1:A:872:VAL:O	1:A:872:VAL:HG22	2.09	0.53
1:B:1005:GLU:HB3	1:B:727:MSE:HB3	1.91	0.53
1:B:814:ASN:C	1:B:816:GLY:H	2.17	0.53
1:A:667:GLY:O	1:A:668:LEU:C	2.52	0.52
1:A:1133:LEU:HB2	1:A:1150:ILE:HD12	1.91	0.52
1:B:625:THR:HG23	1:B:630:SER:HB2	1.91	0.52
1:B:777:ILE:CD1	1:B:777:ILE:N	2.72	0.52
1:B:791:TYR:HA	1:B:792:PRO:C	2.34	0.52
1:A:877:PRO:HG2	1:A:878:GLN:H	1.75	0.52
1:B:877:PRO:CD	1:B:878:GLN:H	2.22	0.52
1:B:759:ILE:CD1	1:B:760:SER:N	2.66	0.52
1:A:760:SER:O	1:A:761:VAL:HB	2.09	0.52
1:B:1065:LYS:O	1:B:1069:GLN:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:LEU:O	1:A:1042:ALA:HB3	2.09	0.52
1:B:651:HIS:CD2	1:B:675:HIS:CD2	2.97	0.52
1:B:1125:ARG:O	1:B:1126:TRP:C	2.53	0.52
1:A:791:TYR:HA	1:A:793:VAL:N	2.22	0.52
1:A:797:SER:HB2	1:A:798:PRO:CD	2.39	0.52
1:B:842:LEU:O	1:B:846:ARG:HG3	2.11	0.51
1:A:630:SER:OG	1:A:634:ILE:CG2	2.54	0.51
1:B:658:ALA:CB	1:B:672:VAL:HG22	2.40	0.51
1:A:636:ARG:NH1	1:A:637:ASP:OD1	2.44	0.51
1:A:792:PRO:O	1:A:793:VAL:C	2.52	0.51
1:A:654:LEU:HD12	1:A:675:HIS:NE2	2.25	0.51
1:B:1094:VAL:HG21	1:B:1156:GLY:O	2.10	0.51
1:A:842:LEU:HD12	1:A:842:LEU:O	2.09	0.51
1:A:624:ILE:HD11	1:A:656:PHE:HE2	1.76	0.51
1:B:608:ILE:HD13	1:B:608:ILE:C	2.36	0.51
1:B:628:LYS:CG	1:B:628:LYS:O	2.57	0.51
1:B:777:ILE:N	1:B:777:ILE:HD12	2.25	0.51
1:A:750:SER:C	1:A:752:ARG:H	2.17	0.51
1:A:750:SER:C	1:A:752:ARG:N	2.69	0.51
1:A:814:ASN:HD22	1:A:817:ASP:H	1.58	0.51
1:A:844:ALA:HA	1:A:847:ILE:CD1	2.36	0.51
1:B:867:TRP:C	1:B:869:LEU:N	2.69	0.51
1:A:1019:LYS:HA	1:A:1024:TYR:O	2.11	0.51
1:A:749:LEU:O	1:A:756:HIS:ND1	2.44	0.50
1:B:814:ASN:CG	1:B:814:ASN:O	2.53	0.50
1:A:791:TYR:CD2	1:A:793:VAL:HG23	2.47	0.50
1:B:636:ARG:O	1:B:640:PRO:HG2	2.11	0.50
1:B:833:PHE:CZ	1:B:847:ILE:HD11	2.47	0.50
1:B:847:ILE:HD12	1:B:848:MSE:HE3	1.93	0.50
1:B:694:ASN:ND2	1:B:696:ASP:HB2	2.26	0.50
1:A:621:TRP:CG	1:A:622:PRO:HD3	2.47	0.50
1:A:792:PRO:C	1:A:794:GLY:N	2.69	0.50
1:A:866:VAL:C	1:A:867:TRP:O	2.53	0.50
1:B:739:ALA:C	1:B:741:THR:N	2.68	0.50
1:A:608:ILE:HD11	1:A:668:LEU:HD22	1.94	0.50
1:A:761:VAL:HG22	1:A:762:ASP:H	1.76	0.50
1:A:858:PHE:O	1:A:862:VAL:HG23	2.11	0.50
1:A:868:PHE:CD1	1:A:868:PHE:C	2.89	0.50
1:B:1047:ASP:OD2	1:B:1047:ASP:N	2.42	0.50
1:A:616:TYR:CD1	1:A:616:TYR:C	2.89	0.50
1:A:1002:ASN:HB2	1:A:727:MSE:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:ALA:O	1:B:628:LYS:HB2	2.12	0.50
1:A:1161:TYR:CB	1:A:727:MSE:HE3	2.41	0.49
1:A:789:ASP:HB3	1:A:846:ARG:NH2	2.27	0.49
1:B:608:ILE:HG23	1:B:609:ASP:N	2.27	0.49
1:B:706:ILE:HD11	1:B:740:ALA:HA	1.93	0.49
1:A:1089:ASP:CA	1:A:1096:ARG:HH21	2.22	0.49
1:A:857:GLY:O	1:A:861:GLU:HG3	2.12	0.49
1:B:1045:GLU:HG2	1:B:1048:LYS:NZ	2.28	0.49
1:B:1085:LYS:HB3	1:B:1086:PRO:HD3	1.95	0.49
1:B:1143:PRO:O	1:B:1147:LYS:HG3	2.12	0.49
1:A:767:GLY:HA2	1:A:770:ILE:CD1	2.42	0.49
1:A:811:ARG:NH1	1:A:811:ARG:HG2	2.27	0.49
1:B:1076:ARG:O	1:B:1080:ARG:HD2	2.12	0.49
1:A:777:ILE:HG23	1:A:794:GLY:HA2	1.95	0.49
1:B:1029:ILE:HD12	1:B:1029:ILE:N	2.24	0.49
1:A:618:THR:HG22	1:A:619:LYS:CG	2.34	0.48
1:A:874:GLN:O	1:A:875:VAL:C	2.55	0.48
1:B:1034:THR:HG23	1:B:1034:THR:O	2.12	0.48
1:B:640:PRO:O	1:B:643:ALA:HB3	2.13	0.48
1:B:1045:GLU:O	1:B:1046:LEU:C	2.55	0.48
1:B:606:ASN:HD21	1:B:609:ASP:CG	2.20	0.48
1:B:629:VAL:O	1:B:630:SER:O	2.31	0.48
1:A:799:TYR:O	1:A:803:LEU:HD23	2.13	0.48
1:A:831:LYS:HB3	1:A:831:LYS:HE2	1.61	0.48
1:B:621:TRP:CG	1:B:622:PRO:HD3	2.49	0.48
1:B:739:ALA:C	1:B:741:THR:H	2.20	0.48
1:A:1124:LYS:HG2	1:A:1126:TRP:CZ2	2.48	0.48
1:A:605:LEU:N	1:A:605:LEU:HD23	2.28	0.48
1:A:1026:THR:HG22	1:A:1031:HIS:O	2.14	0.48
1:A:695:THR:HG21	1:A:749:LEU:HD21	1.94	0.47
1:B:636:ARG:NH1	1:B:637:ASP:OD2	2.47	0.47
1:B:1027:ILE:HG22	1:B:1031:HIS:O	2.14	0.47
1:B:1043:LYS:O	1:B:1044:SER:HB2	2.13	0.47
1:A:1065:LYS:O	1:A:1069:GLN:HG3	2.15	0.47
1:B:738:GLY:O	1:B:739:ALA:HB2	2.14	0.47
1:B:1033:LEU:HD13	1:B:1046:LEU:HB2	1.95	0.47
1:B:759:ILE:O	1:B:760:SER:HB3	2.13	0.47
1:A:1059:THR:O	1:A:1060:LYS:C	2.57	0.47
1:B:856:ARG:HB2	1:B:873:THR:CB	2.44	0.47
1:A:1003:ILE:HG23	1:A:1004:PHE:H	1.80	0.47
1:B:642:LEU:O	1:B:645:ASP:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:TYR:O	1:A:725:ASP:N	2.47	0.47
1:B:1005:GLU:HB3	1:B:727:MSE:CB	2.45	0.47
1:B:856:ARG:CG	1:B:873:THR:HB	2.42	0.47
1:B:651:HIS:HD2	1:B:675:HIS:HD2	1.59	0.47
1:B:805:TYR:CE1	1:B:828:LEU:HD13	2.49	0.47
1:A:661:LEU:HD23	1:A:668:LEU:CD1	2.44	0.47
1:A:683:LEU:HD13	1:A:742:ILE:CD1	2.45	0.47
1:A:1002:ASN:O	1:A:1006:MSE:N	2.42	0.47
1:B:1009:ILE:HD12	1:B:726:SER:HB3	1.96	0.47
1:B:1118:LEU:O	1:B:1119:ARG:C	2.58	0.47
1:A:785:GLU:C	1:A:787:ILE:N	2.73	0.47
1:B:1034:THR:CG2	1:B:1042:ALA:HB2	2.45	0.47
1:A:797:SER:O	1:A:798:PRO:O	2.32	0.46
1:A:1083:LYS:HZ3	1:A:1115:THR:HG22	1.80	0.46
1:A:824:THR:HG23	1:A:828:LEU:HD12	1.96	0.46
1:A:769:VAL:HG22	1:A:769:VAL:O	2.14	0.46
1:A:740:ALA:O	1:A:743:LEU:HB2	2.14	0.46
1:A:747:TRP:HZ2	1:A:763:LEU:HD12	1.81	0.46
1:B:706:ILE:HD11	1:B:740:ALA:CA	2.45	0.46
1:A:616:TYR:HA	1:A:620:VAL:HG11	1.92	0.46
1:A:768:ASP:OD1	1:A:808:LYS:NZ	2.49	0.46
1:A:874:GLN:C	1:A:876:LEU:HG	2.41	0.46
1:A:615:HIS:CD2	1:A:661:LEU:HB2	2.51	0.46
1:A:1003:ILE:HG23	1:A:1004:PHE:N	2.31	0.46
1:A:1003:ILE:O	1:A:1006:MSE:HB3	2.15	0.46
1:A:793:VAL:C	1:A:795:LEU:H	2.24	0.46
1:B:1008:ARG:HH12	1:B:1013:LEU:HD23	1.80	0.46
1:B:1019:LYS:HE3	1:B:1023:GLY:O	2.16	0.46
1:B:1114:PHE:O	1:B:1116:ASN:N	2.48	0.46
1:A:1085:LYS:NZ	1:A:1089:ASP:OD2	2.49	0.45
1:A:811:ARG:HG2	1:A:811:ARG:HH11	1.81	0.45
1:B:759:ILE:CD1	1:B:760:SER:H	2.27	0.45
1:B:1054:THR:O	1:B:1056:GLY:N	2.49	0.45
1:B:1015:LEU:HD22	1:B:1058:ILE:O	2.16	0.45
1:B:1117:SER:O	1:B:1118:LEU:C	2.60	0.45
1:A:1102:MSE:HE3	1:A:1138:TRP:CZ3	2.52	0.45
1:A:840:GLY:O	1:A:842:LEU:N	2.49	0.45
1:A:636:ARG:HG2	1:A:636:ARG:HH11	1.81	0.45
1:A:841:ASP:OD2	1:A:841:ASP:C	2.60	0.45
1:A:740:ALA:HB3	1:A:827:ALA:HB2	1.98	0.45
1:A:748:PRO:HB3	1:A:762:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1019:LYS:HA	1:B:1025:TYR:HA	1.99	0.45
1:A:1026:THR:CG2	1:A:1032:LEU:HA	2.46	0.45
1:A:846:ARG:NH1	1:A:846:ARG:CG	2.61	0.45
1:A:714:SER:O	1:A:715:VAL:C	2.57	0.45
1:A:770:ILE:HG13	1:A:771:ASN:H	1.82	0.45
1:B:1159:ASP:C	1:B:724:VAL:HG23	2.41	0.45
1:B:706:ILE:HD11	1:B:740:ALA:HB2	1.98	0.45
1:B:710:LEU:HD21	1:B:732:TRP:CZ3	2.51	0.45
1:B:785:GLU:C	1:B:787:ILE:H	2.25	0.45
1:B:805:TYR:CD1	1:B:828:LEU:HD13	2.52	0.45
1:B:820:LEU:O	1:B:824:THR:HB	2.17	0.45
1:B:850:SER:O	1:B:854:LEU:HD13	2.16	0.45
1:A:678:ASP:OD1	1:A:681:ARG:NH1	2.50	0.45
1:B:1087:VAL:HG21	1:B:1118:LEU:HB3	1.98	0.45
1:A:615:HIS:CG	1:A:661:LEU:HD13	2.52	0.44
1:A:819:ILE:O	1:A:822:VAL:HB	2.17	0.44
1:B:1041:ALA:O	1:B:1045:GLU:HB2	2.17	0.44
1:B:736:VAL:O	1:B:737:LYS:C	2.59	0.44
1:B:742:ILE:O	1:B:746:VAL:HG13	2.17	0.44
1:A:681:ARG:NH2	1:A:682:LEU:HD11	2.33	0.44
1:B:739:ALA:O	1:B:741:THR:N	2.50	0.44
1:B:759:ILE:HD12	1:B:760:SER:CA	2.46	0.44
1:B:809:LEU:O	1:B:812:GLU:HB2	2.17	0.44
1:B:815:GLN:HA	1:B:818:PHE:HB3	1.99	0.44
1:A:814:ASN:C	1:A:816:GLY:N	2.74	0.44
1:B:1046:LEU:C	1:B:1046:LEU:HD12	2.42	0.44
1:B:874:GLN:O	1:B:875:VAL:HB	2.18	0.44
1:A:669:GLU:C	1:A:669:GLU:CD	2.86	0.44
1:A:806:LEU:HD11	1:A:851:TYR:HA	1.99	0.44
1:B:731:ALA:HB1	1:B:735:HIS:CE1	2.53	0.44
1:A:804:ALA:O	1:A:808:LYS:HG3	2.18	0.44
1:B:682:LEU:HD22	1:B:682:LEU:N	2.32	0.44
1:B:692:GLU:O	1:B:693:ASN:C	2.61	0.44
1:B:1046:LEU:HG	1:B:1047:ASP:N	2.33	0.44
1:A:706:ILE:HG23	1:A:736:VAL:HG13	2.00	0.43
1:A:867:TRP:CE3	1:A:868:PHE:N	2.84	0.43
1:A:707:MSE:HE2	1:A:868:PHE:CZ	2.53	0.43
1:A:789:ASP:HB3	1:A:846:ARG:HH22	1.80	0.43
1:B:814:ASN:ND2	1:B:816:GLY:H	2.16	0.43
1:B:785:GLU:C	1:B:787:ILE:N	2.73	0.43
1:A:754:LYS:HB3	1:A:754:LYS:HE3	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:LEU:O	1:A:801:ILE:C	2.61	0.43
1:B:771:ASN:HD22	1:B:771:ASN:HA	1.60	0.43
1:A:605:LEU:N	1:A:605:LEU:HD22	2.32	0.43
1:A:683:LEU:HD13	1:A:742:ILE:HD11	2.00	0.43
1:B:1080:ARG:NH1	1:B:1080:ARG:HG3	2.33	0.43
1:A:1020:ASP:C	1:A:1022:GLU:H	2.26	0.43
1:A:1116:ASN:HD22	1:A:1116:ASN:HA	1.56	0.43
1:A:747:TRP:HA	1:A:748:PRO:HA	1.89	0.43
1:A:606:ASN:OD1	1:A:608:ILE:CG2	2.54	0.43
1:B:1159:ASP:CA	1:B:724:VAL:HG23	2.45	0.43
1:A:825:PHE:HB3	1:A:826:PRO:CD	2.42	0.43
1:B:1161:TYR:O	1:B:724:VAL:C	2.60	0.43
1:B:1004:PHE:HA	1:B:1067:PHE:HE2	1.80	0.43
1:A:1111:VAL:C	1:A:1113:GLY:N	2.77	0.43
1:A:797:SER:O	1:A:798:PRO:C	2.61	0.43
1:B:628:LYS:HE3	1:B:815:GLN:C	2.44	0.43
1:B:628:LYS:O	1:B:628:LYS:HG3	2.19	0.43
1:B:766:LEU:HD21	1:B:805:TYR:CE2	2.54	0.43
1:B:813:LYS:HD3	1:B:813:LYS:HA	1.71	0.43
1:B:802:THR:CG2	1:B:847:ILE:HD13	2.49	0.42
1:A:782:CYS:SG	1:A:788:ALA:HA	2.59	0.42
1:B:616:TYR:CD1	1:B:616:TYR:C	2.96	0.42
1:B:1134:ALA:HA	1:B:1139:TYR:CD1	2.53	0.42
1:B:802:THR:HG21	1:B:847:ILE:CD1	2.49	0.42
1:A:663:ARG:NH2	1:A:870:GLU:OE2	2.52	0.42
1:A:1034:THR:OG1	1:A:1036:SER:HB3	2.18	0.42
1:A:822:VAL:HG11	1:A:855:LEU:HD21	2.00	0.42
1:B:732:TRP:O	1:B:736:VAL:HB	2.19	0.42
1:A:1039:LEU:O	1:A:1043:LYS:HG2	2.18	0.42
1:A:1148:ARG:HD2	1:A:1161:TYR:CE1	2.54	0.42
1:A:807:ASP:OD2	1:A:811:ARG:NH1	2.53	0.42
1:B:1067:PHE:O	1:B:1071:VAL:HG23	2.19	0.42
1:A:852:TYR:CE2	1:A:856:ARG:NH1	2.74	0.42
1:B:621:TRP:CD1	1:B:622:PRO:HD3	2.54	0.42
1:B:681:ARG:CZ	1:B:681:ARG:HB3	2.49	0.42
1:B:814:ASN:O	1:B:816:GLY:N	2.52	0.42
1:A:714:SER:OG	1:A:871:GLY:O	2.26	0.42
1:A:1116:ASN:ND2	1:A:1119:ARG:HH12	2.18	0.42
1:B:653:LEU:C	1:B:653:LEU:HD23	2.45	0.42
1:B:1036:SER:HA	1:B:1037:PRO:HD3	1.86	0.42
1:A:790:LEU:N	1:A:790:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:GLU:CD	1:B:633:GLU:H	2.27	0.42
1:B:651:HIS:O	1:B:652:ALA:C	2.63	0.42
1:B:820:LEU:HD12	1:B:820:LEU:HA	1.89	0.42
1:A:787:ILE:O	1:A:787:ILE:HG22	2.20	0.42
1:B:693:ASN:ND2	1:B:694:ASN:O	2.53	0.42
1:B:825:PHE:N	1:B:826:PRO:CD	2.82	0.42
1:A:618:THR:CG2	1:A:619:LYS:HG3	2.39	0.42
1:A:1111:VAL:C	1:A:1113:GLY:H	2.28	0.42
1:B:1003:ILE:HG12	1:B:1097:ALA:HB1	2.02	0.42
1:B:825:PHE:HB3	1:B:826:PRO:HD3	2.02	0.42
1:B:662:SER:C	1:B:664:THR:H	2.27	0.41
1:B:1020:ASP:C	1:B:1022:GLU:H	2.28	0.41
1:B:847:ILE:HD11	1:B:848:MSE:HE3	2.02	0.41
1:A:1161:TYR:HB2	1:A:727:MSE:HE3	2.02	0.41
1:A:759:ILE:HG13	1:A:760:SER:N	2.36	0.41
1:A:797:SER:CB	1:A:798:PRO:HD2	2.42	0.41
1:B:1017:ILE:HD11	1:B:1056:GLY:CA	2.50	0.41
1:B:1098:ALA:HB3	1:B:1153:PHE:CE1	2.55	0.41
1:A:674:SER:O	1:A:677:LEU:HB2	2.19	0.41
1:A:1097:ALA:HA	1:A:1100:ILE:HG13	2.01	0.41
1:A:662:SER:HA	1:A:665:GLU:O	2.21	0.41
1:A:676:ARG:NH1	1:A:708:ASP:OD2	2.47	0.41
1:A:716:ASP:OD2	1:A:716:ASP:N	2.51	0.41
1:A:724:VAL:HA	1:A:727:MSE:HB2	2.03	0.41
1:A:854:LEU:HD12	1:A:854:LEU:HA	1.90	0.41
1:A:654:LEU:HD12	1:A:675:HIS:CD2	2.55	0.41
1:A:1078:ILE:CD1	1:A:1103:VAL:HG21	2.51	0.41
1:A:793:VAL:O	1:A:795:LEU:N	2.53	0.41
1:B:608:ILE:HG23	1:B:609:ASP:H	1.85	0.41
1:B:682:LEU:N	1:B:682:LEU:CD2	2.82	0.41
1:A:605:LEU:CD2	1:A:605:LEU:H	2.27	0.41
1:A:687:VAL:HG13	1:A:690:ILE:HD11	2.03	0.41
1:B:604:ASN:CG	1:B:605:LEU:H	2.28	0.41
1:B:1025:TYR:HE2	1:B:1039:LEU:HD12	1.86	0.41
1:B:1054:THR:O	1:B:1055:ASN:HB3	2.20	0.41
1:B:747:TRP:CD1	1:B:759:ILE:HD13	2.39	0.41
1:B:866:VAL:C	1:B:867:TRP:O	2.63	0.41
1:A:639:ILE:HB	1:A:640:PRO:HD3	2.02	0.41
1:A:1064:GLU:O	1:A:1065:LYS:C	2.64	0.41
1:A:1064:GLU:HA	1:A:1067:PHE:HB3	2.01	0.41
1:B:628:LYS:HG2	1:B:816:GLY:CA	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:ARG:HA	1:B:684:ARG:NE	2.32	0.41
1:B:778:THR:HG21	1:B:800:LEU:CD1	2.51	0.41
1:B:829:LEU:HB3	1:B:834:LEU:HD13	2.02	0.41
1:A:618:THR:HG22	1:A:619:LYS:N	2.36	0.41
1:A:670:GLN:O	1:A:670:GLN:NE2	2.53	0.41
1:A:1071:VAL:O	1:A:1075:VAL:HG23	2.20	0.41
1:A:828:LEU:HD23	1:A:828:LEU:HA	1.90	0.41
1:A:877:PRO:CG	1:A:878:GLN:H	2.33	0.41
1:B:702:ALA:CB	1:B:743:LEU:HD13	2.51	0.41
1:B:855:LEU:HD23	1:B:855:LEU:N	2.35	0.41
1:A:648:PHE:HB3	1:A:682:LEU:CB	2.48	0.41
1:A:781:VAL:HG22	1:A:782:CYS:N	2.35	0.41
1:B:1050:ILE:HD13	1:B:1052:ARG:O	2.21	0.41
1:B:795:LEU:O	1:B:796:ASP:C	2.64	0.41
1:B:814:ASN:C	1:B:814:ASN:ND2	2.79	0.41
1:A:1024:TYR:CD1	1:A:1035:LYS:HA	2.56	0.40
1:A:865:LYS:NZ	1:A:878:GLN:HA	2.36	0.40
1:B:660:HIS:HB2	1:B:867:TRP:CH2	2.57	0.40
1:A:680:LEU:O	1:A:684:ARG:HB2	2.21	0.40
1:A:706:ILE:HD12	1:A:736:VAL:HG13	2.02	0.40
1:A:1039:LEU:HG	1:A:1043:LYS:HE3	2.03	0.40
1:B:643:ALA:HB1	1:B:650:MSE:HE2	2.03	0.40
1:B:1019:LYS:HG3	1:B:1024:TYR:O	2.21	0.40
1:A:787:ILE:C	1:A:789:ASP:N	2.79	0.40
1:B:620:VAL:O	1:B:623:THR:HG23	2.20	0.40
1:B:706:ILE:HD11	1:B:740:ALA:CB	2.51	0.40
1:A:1054:THR:C	1:A:1056:GLY:N	2.79	0.40
1:A:1161:TYR:O	1:A:724:VAL:C	2.63	0.40
1:A:795:LEU:HG	1:A:797:SER:HB3	2.04	0.40
1:B:1029:ILE:H	1:B:1029:ILE:CD1	2.28	0.40
1:B:1034:THR:HG22	1:B:1042:ALA:HB2	2.02	0.40
1:B:1048:LYS:HE3	1:B:1048:LYS:HB2	1.87	0.40
1:B:814:ASN:C	1:B:816:GLY:N	2.78	0.40
1:B:874:GLN:NE2	1:B:874:GLN:CA	2.84	0.40
1:A:634:ILE:HD11	1:A:755:PHE:CZ	2.56	0.40
1:B:1025:TYR:CB	1:B:1034:THR:HG22	2.45	0.40
1:B:1050:ILE:HD12	1:B:1050:ILE:H	1.87	0.40
1:B:782:CYS:HB2	1:B:791:TYR:CD2	2.57	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	426/438 (97%)	355 (83%)	48 (11%)	23 (5%)	1	5
1	B	426/438 (97%)	338 (79%)	59 (14%)	29 (7%)	1	2
All	All	852/876 (97%)	693 (81%)	107 (13%)	52 (6%)	1	4

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	LEU
1	A	669	GLU
1	A	724	VAL
1	A	761	VAL
1	A	785	GLU
1	A	787	ILE
1	A	798	PRO
1	A	815	GLN
1	A	868	PHE
1	B	628	LYS
1	B	630	SER
1	B	691	SER
1	B	1044	SER
1	B	1115	THR
1	B	1126	TRP
1	B	730	SER
1	B	731	ALA
1	B	739	ALA
1	B	785	GLU
1	B	797	SER
1	B	868	PHE
1	B	874	GLN
1	A	800	LEU
1	A	841	ASP
1	A	867	TRP

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Mol	Chain	Res	Type
1	B	693	ASN
1	B	1029	ILE
1	B	724	VAL
1	B	815	GLN
1	B	867	TRP
1	A	770	ILE
1	A	863	LYS
1	B	1046	LEU
1	B	1056	GLY
1	B	831	LYS
1	B	873	THR
1	A	1021	THR
1	A	772	PRO
1	B	726	SER
1	B	760	SER
1	A	874	GLN
1	A	875	VAL
1	B	627	ALA
1	B	740	ALA
1	B	875	VAL
1	A	794	GLY
1	A	801	ILE
1	B	793	VAL
1	A	877	PRO
1	A	1050	ILE
1	A	748	PRO
1	B	877	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	367/363 (101%)	322 (88%)	45 (12%)	4	15
1	B	367/363 (101%)	325 (89%)	42 (11%)	5	18
All	All	734/726 (101%)	647 (88%)	87 (12%)	5	16

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	605	LEU
1	A	608	ILE
1	A	618	THR
1	A	620	VAL
1	A	682	LEU
1	A	693	ASN
1	A	695	THR
1	A	716	ASP
1	A	1002	ASN
1	A	1003	ILE
1	A	1007	LEU
1	A	1009	ILE
1	A	1013	LEU
1	A	1014	ARG
1	A	1026	THR
1	A	1078	ILE
1	A	1083	LYS
1	A	1100	ILE
1	A	1106	MSE
1	A	1109	THR
1	A	1116	ASN
1	A	1120	MSE
1	A	1159	ASP
1	A	725	ASP
1	A	741	THR
1	A	743	LEU
1	A	749	LEU
1	A	754	LYS
1	A	763	LEU
1	A	770	ILE
1	A	773	ASP
1	A	778	THR
1	A	779	GLU
1	A	787	ILE
1	A	798	PRO
1	A	811	ARG
1	A	813	LYS
1	A	815	GLN
1	A	824	THR
1	A	839	THR
1	A	846	ARG
1	A	847	ILE

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Mol	Chain	Res	Type
1	A	854	LEU
1	A	868	PHE
1	A	876	LEU
1	B	608	ILE
1	B	618	THR
1	B	629	VAL
1	B	640	PRO
1	B	647	PRO
1	B	663	ARG
1	B	664	THR
1	B	665	GLU
1	B	673	SER
1	B	685	GLU
1	B	688	LEU
1	B	716	ASP
1	B	1017	ILE
1	B	1018	TYR
1	B	1024	TYR
1	B	1026	THR
1	B	1027	ILE
1	B	1047	ASP
1	B	1050	ILE
1	B	1083	LYS
1	B	1094	VAL
1	B	725	ASP
1	B	736	VAL
1	B	742	ILE
1	B	743	LEU
1	B	769	VAL
1	B	777	ILE
1	B	781	VAL
1	B	789	ASP
1	B	790	LEU
1	B	803	LEU
1	B	814	ASN
1	B	824	THR
1	B	829	LEU
1	B	832	THR
1	B	834	LEU
1	B	839	THR
1	B	842	LEU
1	B	864	ASP

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Mol	Chain	Res	Type
1	B	866	VAL
1	B	874	GLN
1	B	876	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	HIS
1	A	1002	ASN
1	A	1053	ASN
1	A	1069	GLN
1	A	1116	ASN
1	A	1132	ASN
1	A	1144	ASN
1	A	814	ASN
1	B	615	HIS
1	B	651	HIS
1	B	675	HIS
1	B	694	ASN
1	B	1068	ASN
1	B	1101	ASN
1	B	1144	ASN
1	B	757	ASN
1	B	771	ASN
1	B	814	ASN
1	B	874	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	417/438 (95%)	0.24	19 (4%) 37 29	28, 55, 91, 112	0
1	B	417/438 (95%)	0.54	31 (7%) 20 17	36, 70, 124, 131	0
All	All	834/876 (95%)	0.39	50 (5%) 27 21	28, 61, 114, 131	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	690	ILE	4.8
1	B	1042	ALA	4.5
1	A	795	LEU	4.4
1	A	877	PRO	4.3
1	B	1041	ALA	3.9
1	B	671	TYR	3.9
1	B	873	THR	3.9
1	A	794	GLY	3.7
1	B	1036	SER	3.5
1	B	1029	ILE	3.2
1	B	1035	LYS	3.2
1	B	1032	LEU	3.2
1	B	1050	ILE	3.0
1	B	729	PRO	3.0
1	A	878	GLN	2.9
1	A	759	ILE	2.8
1	B	1039	LEU	2.7
1	B	1038	SER	2.7
1	B	1015	LEU	2.6
1	B	1031	HIS	2.6
1	B	691	SER	2.6
1	A	784	ASP	2.6
1	A	774	VAL	2.5
1	B	1046	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	777	ILE	2.4
1	B	689	GLU	2.4
1	B	688	LEU	2.4
1	A	776	THR	2.3
1	A	747	TRP	2.3
1	B	1033	LEU	2.3
1	B	1025	TYR	2.3
1	A	758	ILE	2.2
1	B	1141	GLN	2.2
1	A	775	GLY	2.2
1	A	850	SER	2.2
1	B	630	SER	2.2
1	A	771	ASN	2.2
1	A	761	VAL	2.2
1	B	1103	VAL	2.2
1	B	668	LEU	2.1
1	A	787	ILE	2.1
1	B	815	GLN	2.1
1	A	773	ASP	2.1
1	B	728	SER	2.1
1	A	670	GLN	2.1
1	A	876	LEU	2.1
1	B	1057	VAL	2.0
1	B	1051	GLY	2.0
1	B	874	GLN	2.0
1	B	759	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.