



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 AM UTC

PDB ID : 9CRW / pdb_00009crw
Title : Crystal structure of the Candida albicans kinesin-8 proximal tail domain
Authors : Trofimova, D.; Doubleday, C.; Hunter, B.; Serrano Arevalo, J.; Davison, E.;
Wen, E.; Munro, K.; Allingham, J.S.
Deposited on : 2024-07-22
Resolution : 2.49 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

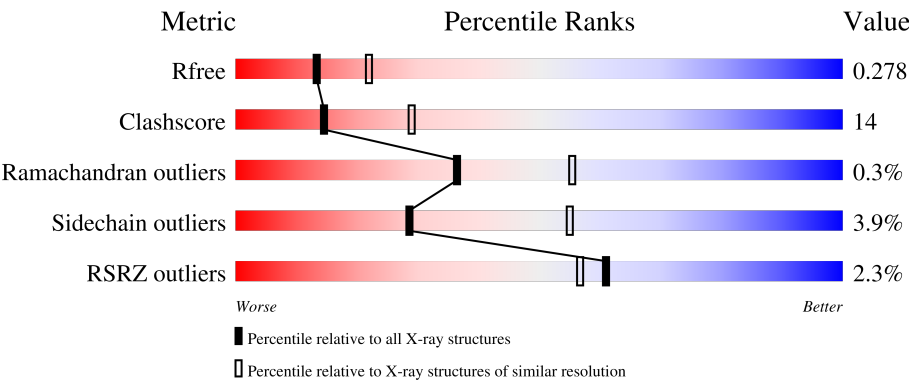
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	232	2% 60% 36% • •
1	B	232	3% 66% 25% • 9%
1	C	232	% 67% 25% • 6%
1	D	232	% 76% 19% • •
1	E	232	3% 64% 29% • 6%

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Mol	Chain	Length	Quality of chain
1	F	232	2% 71% 24% • •
1	G	232	2% 50% 40% • 8%
1	H	232	3% 58% 35% • 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14593 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.

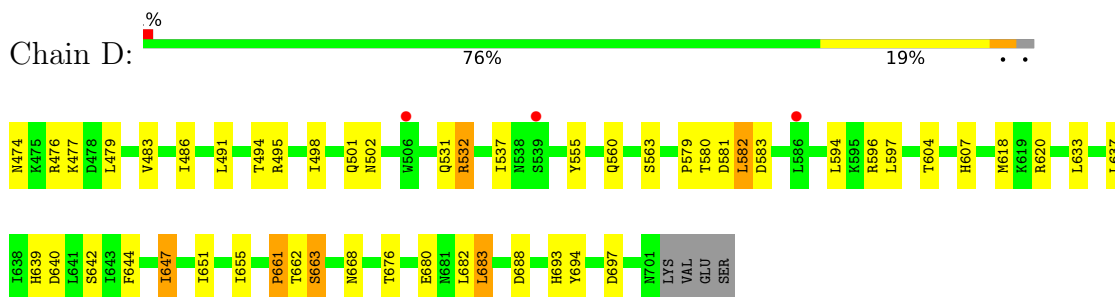
- Molecule 1 is a protein called Kinesin-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	228	Total	C	N	O	S	0	0	0
			1887	1197	310	373	7			
1	C	217	Total	C	N	O	S	0	0	0
			1811	1154	296	354	7			
1	A	226	Total	C	N	O	S	0	0	0
			1870	1187	306	370	7			
1	B	212	Total	C	N	O	S	0	0	0
			1768	1128	286	347	7			
1	E	219	Total	C	N	O	S	0	0	0
			1822	1160	295	360	7			
1	F	222	Total	C	N	O	S	0	0	0
			1841	1171	299	364	7			
1	G	214	Total	C	N	O	S	0	0	0
			1786	1140	292	347	7			
1	H	217	Total	C	N	O	S	0	0	0
			1808	1153	294	354	7			

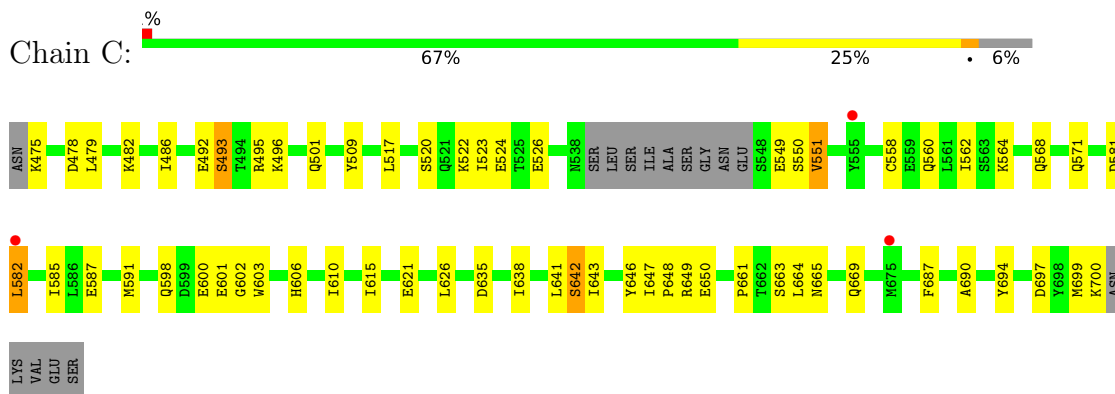
3 Residue-property plots [i](#)

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.

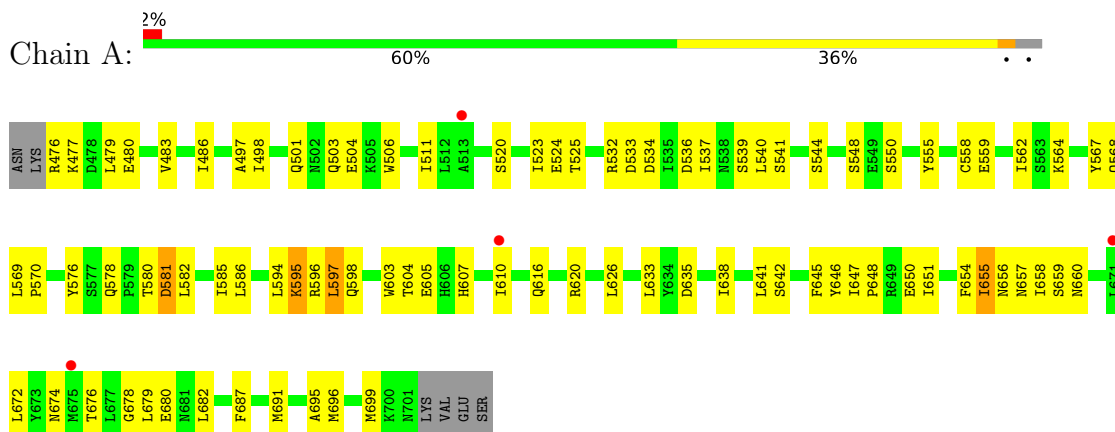
• Molecule 1: Kinesin-like protein



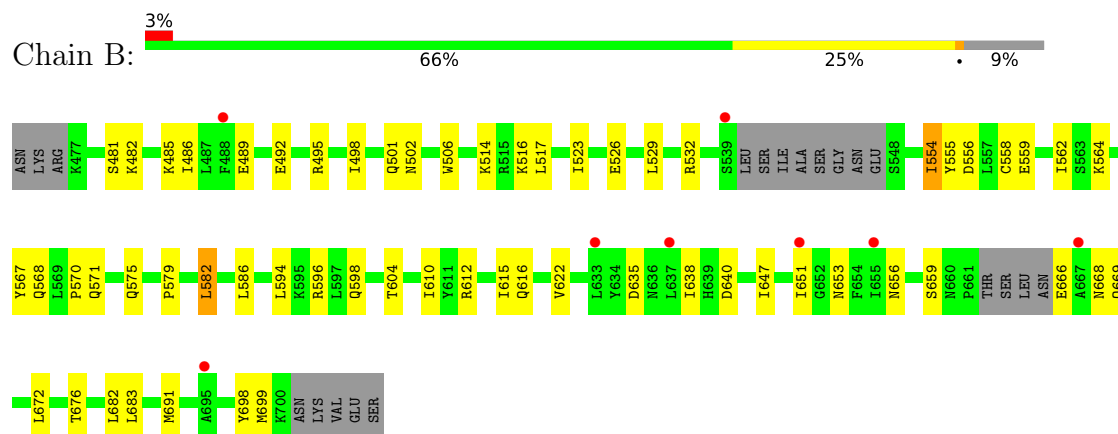
• Molecule 1: Kinesin-like protein



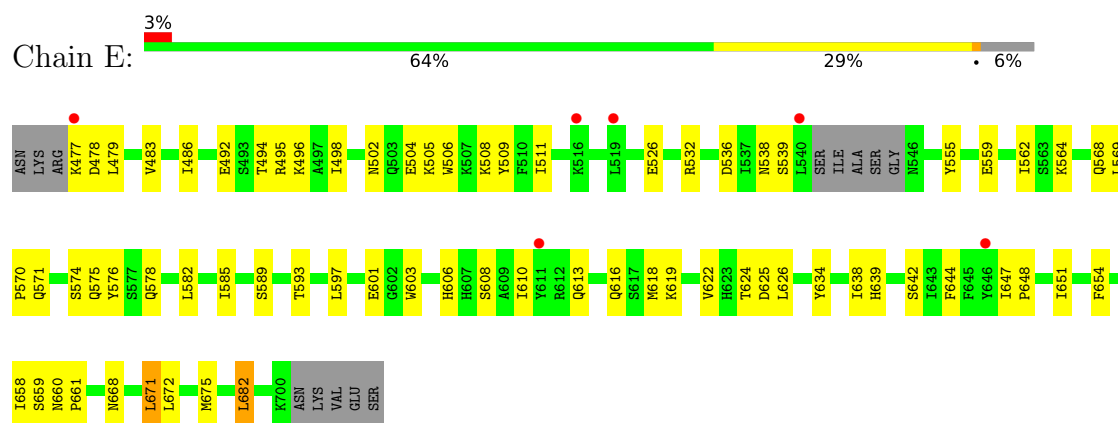
• Molecule 1: Kinesin-like protein



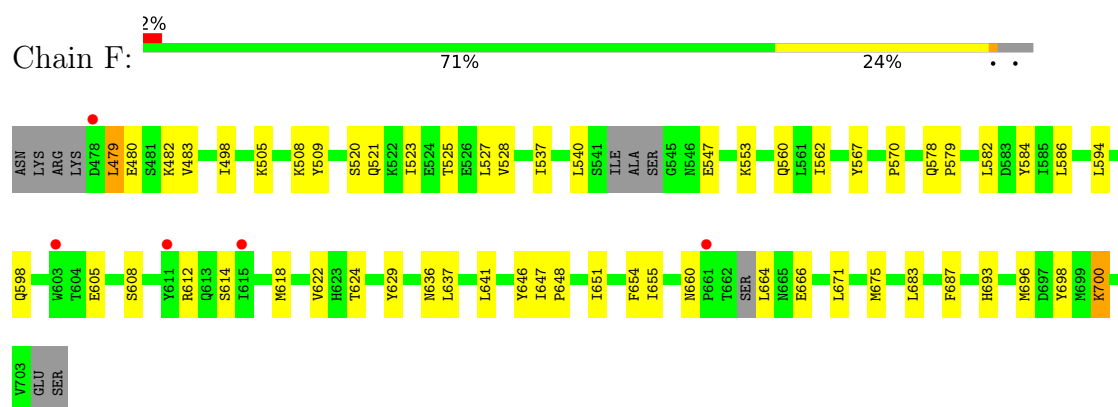
- Molecule 1: Kinesin-like protein



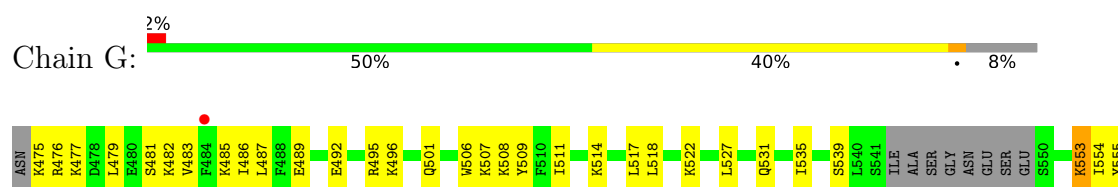
- Molecule 1: Kinesin-like protein

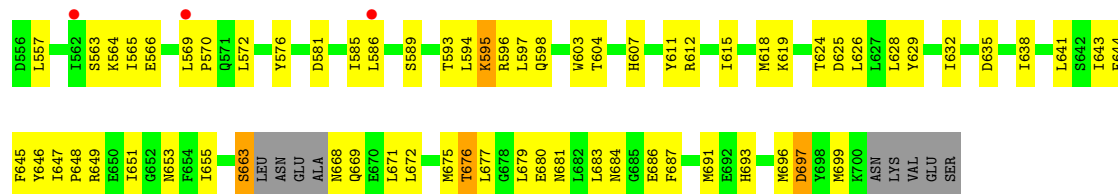


- Molecule 1: Kinesin-like protein

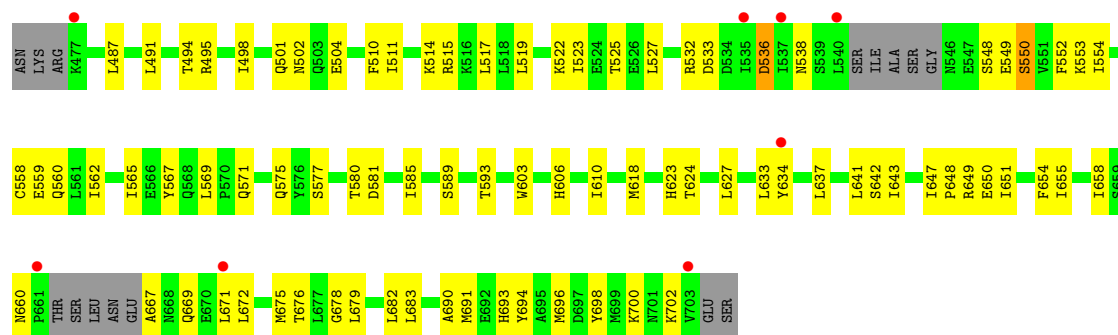


- Molecule 1: Kinesin-like protein





● Molecule 1: Kinesin-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.96Å 104.57Å 118.78Å 90.00° 93.37° 90.00°	Depositor
Resolution (Å)	47.84 – 2.49 47.84 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.84-2.49) 86.3 (47.84-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.234 , 0.278 0.234 , 0.278	Depositor DCC
R_{free} test set	1993 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14593	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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	0.48	0/1902	0.65	0/2563
1	B	0.52	0/1798	0.71	0/2419
1	C	0.50	0/1842	0.68	0/2479
1	D	0.49	0/1919	0.64	1/2585 (0.0%)
1	E	0.45	0/1853	0.64	0/2496
1	F	0.50	0/1871	0.61	0/2519
1	G	0.41	0/1816	0.65	0/2442
1	H	0.47	0/1838	0.65	2/2473 (0.1%)
All	All	0.48	0/14839	0.66	3/19976 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	550	SER	CA-C-N	-7.53	114.86	122.77
1	H	550	SER	C-N-CA	-7.53	114.86	122.77
1	D	647	ILE	CB-CG1-CD1	-5.02	103.25	113.80

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	1870	0	1846	53	0
1	B	1768	0	1744	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1811	0	1795	50	0
1	D	1887	0	1865	36	0
1	E	1822	0	1797	60	0
1	F	1841	0	1814	46	0
1	G	1786	0	1776	89	0
1	H	1808	0	1789	78	0
All	All	14593	0	14426	405	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 14.

All (405) 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:H:554:ILE:HD11	1:H:676:THR:HG22	1.52	0.90
1:H:647:ILE:HG23	1:H:648:PRO:HD3	1.55	0.86
1:H:643:ILE:HA	1:H:649:ARG:HH22	1.39	0.84
1:E:675:MET:HE1	1:F:651:ILE:HG12	1.58	0.84
1:G:553:LYS:O	1:G:557:LEU:HD22	1.77	0.84
1:B:669:GLN:HA	1:B:672:LEU:HD12	1.60	0.83
1:A:498:ILE:HD11	1:A:586:LEU:HD21	1.61	0.82
1:B:529:LEU:HD11	1:B:558:CYS:HB3	1.62	0.81
1:H:501:GLN:HE22	1:H:581:ASP:HB2	1.45	0.81
1:E:647:ILE:HD11	1:F:648:PRO:HA	1.62	0.80
1:E:624:THR:OG1	1:F:624:THR:OG1	1.98	0.79
1:G:554:ILE:HA	1:G:557:LEU:HD23	1.68	0.75
1:C:571:GLN:HE22	1:B:579:PRO:HD2	1.50	0.75
1:C:479:LEU:HD11	1:C:602:GLY:HA3	1.69	0.74
1:A:610:ILE:HD13	1:B:610:ILE:HD13	1.69	0.72
1:E:639:HIS:O	1:E:642:SER:OG	2.08	0.72
1:G:647:ILE:HD11	1:H:648:PRO:HA	1.72	0.72
1:H:643:ILE:HA	1:H:649:ARG:NH2	2.04	0.72
1:E:619:LYS:O	1:E:622:VAL:HG12	1.90	0.71
1:G:672:LEU:O	1:G:676:THR:OG1	2.08	0.71
1:C:598:GLN:HA	1:C:603:TRP:CD1	2.26	0.70
1:H:643:ILE:HG13	1:H:649:ARG:HH12	1.55	0.69
1:H:517:LEU:HD13	1:H:691:MET:HE2	1.76	0.68
1:G:527:LEU:HD11	1:H:642:SER:HB3	1.76	0.68
1:A:646:TYR:CE1	1:A:647:ILE:HG13	2.30	0.67
1:D:494:THR:O	1:D:498:ILE:HG12	1.95	0.67
1:G:514:LYS:HG3	1:G:691:MET:SD	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:611:TYR:O	1:G:615:ILE:HG12	1.95	0.66
1:H:698:TYR:HD1	1:H:702:LYS:HD3	1.59	0.66
1:G:514:LYS:HA	1:G:517:LEU:HD12	1.77	0.66
1:H:495:ARG:NH1	1:H:495:ARG:O	2.30	0.65
1:G:625:ASP:O	1:G:629:TYR:HD2	1.79	0.65
1:E:483:VAL:O	1:E:486:ILE:HG13	1.97	0.65
1:G:485:LYS:O	1:G:489:GLU:HG2	1.95	0.65
1:G:648:PRO:HA	1:H:647:ILE:HD11	1.81	0.63
1:G:647:ILE:HG13	1:H:651:ILE:HD12	1.79	0.63
1:A:534:ASP:OD2	1:G:477:LYS:HD3	1.99	0.63
1:G:506:TRP:HB3	1:G:699:MET:HE1	1.80	0.63
1:H:560:GLN:HB2	1:H:683:LEU:HD11	1.81	0.63
1:E:634:TYR:CZ	1:E:638:ILE:HD11	2.33	0.63
1:G:624:THR:OG1	1:H:624:THR:OG1	2.15	0.63
1:B:669:GLN:H	1:B:669:GLN:CD	2.06	0.63
1:F:560:GLN:HB3	1:F:683:LEU:HD21	1.79	0.62
1:C:524:GLU:CG	1:C:647:ILE:HD12	2.28	0.62
1:E:651:ILE:HG13	1:F:647:ILE:HG23	1.82	0.62
1:C:526:GLU:HG2	1:C:562:ILE:HD13	1.82	0.61
1:A:486:ILE:CG2	1:A:597:LEU:HD11	2.31	0.61
1:C:524:GLU:HG2	1:C:647:ILE:HD12	1.83	0.61
1:B:556:ASP:HA	1:B:559:GLU:OE1	2.00	0.61
1:B:640:ASP:OD2	1:B:698:TYR:OH	2.11	0.60
1:F:498:ILE:HD12	1:F:618:MET:HE2	1.81	0.60
1:G:604:THR:H	1:G:607:HIS:CE1	2.19	0.60
1:A:476:ARG:HD2	1:A:477:LYS:N	2.17	0.60
1:A:486:ILE:HG22	1:A:597:LEU:HD11	1.83	0.60
1:G:492:GLU:HA	1:G:495:ARG:HG3	1.82	0.60
1:H:698:TYR:CD1	1:H:702:LYS:HD3	2.36	0.60
1:E:638:ILE:HG22	1:F:523:ILE:HD12	1.84	0.60
1:F:654:PHE:HB2	1:F:671:LEU:HD13	1.84	0.59
1:G:669:GLN:OE1	1:G:669:GLN:N	2.34	0.59
1:G:508:LYS:HE2	1:G:576:TYR:O	2.02	0.59
1:E:492:GLU:HG3	1:E:496:LYS:HE2	1.84	0.59
1:D:501:GLN:HG3	1:D:582:LEU:HD13	1.84	0.59
1:G:535:ILE:HB	1:H:660:ASN:OD1	2.02	0.59
1:H:501:GLN:NE2	1:H:581:ASP:HB2	2.17	0.59
1:A:657:ASN:HA	1:A:660:ASN:OD1	2.03	0.58
1:D:537:ILE:HD12	1:C:661:PRO:HG3	1.85	0.58
1:G:684:ASN:HB2	1:G:686:GLU:OE1	2.03	0.58
1:G:481:SER:HA	1:H:606:HIS:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:487:LEU:HD23	1:H:603:TRP:HH2	1.68	0.58
1:G:646:TYR:HA	1:G:649:ARG:HD3	1.86	0.58
1:C:571:GLN:NE2	1:B:579:PRO:HD2	2.18	0.58
1:G:514:LYS:HG2	1:G:518:LEU:HD21	1.86	0.58
1:G:651:ILE:HD11	1:H:675:MET:SD	2.44	0.58
1:A:558:CYS:SG	1:A:679:LEU:HD11	2.43	0.58
1:H:532:ARG:NH1	1:H:559:GLU:OE2	2.37	0.58
1:H:655:ILE:HA	1:H:658:ILE:HG22	1.84	0.58
1:E:479:LEU:O	1:E:483:VAL:HG23	2.04	0.57
1:B:529:LEU:CD1	1:B:558:CYS:HB3	2.33	0.57
1:E:532:ARG:HB2	1:E:555:TYR:CZ	2.40	0.57
1:C:665:ASN:O	1:C:669:GLN:HG2	2.05	0.57
1:G:514:LYS:HG2	1:G:518:LEU:CD2	2.35	0.57
1:H:650:GLU:HB3	1:H:671:LEU:HD12	1.87	0.57
1:D:594:LEU:HA	1:D:597:LEU:HD12	1.85	0.56
1:A:506:TRP:CE3	1:A:699:MET:HB3	2.39	0.56
1:A:638:ILE:HD12	1:B:523:ILE:HD12	1.86	0.56
1:B:506:TRP:HE3	1:B:699:MET:HE2	1.70	0.56
1:G:507:LYS:O	1:G:511:ILE:HG12	2.05	0.56
1:G:514:LYS:HD3	1:G:572:LEU:HD11	1.88	0.56
1:D:651:ILE:HD12	1:C:647:ILE:HG23	1.87	0.56
1:D:476:ARG:HA	1:D:479:LEU:HB3	1.87	0.55
1:D:476:ARG:H	1:D:476:ARG:NE	2.05	0.55
1:G:495:ARG:HG2	1:G:618:MET:CE	2.36	0.55
1:C:581:ASP:O	1:C:585:ILE:HG13	2.05	0.55
1:C:475:LYS:N	1:C:478:ASP:OD1	2.40	0.55
1:G:554:ILE:HA	1:G:557:LEU:CD2	2.37	0.55
1:G:647:ILE:HG23	1:G:648:PRO:CD	2.37	0.55
1:H:672:LEU:O	1:H:676:THR:HG23	2.07	0.55
1:C:697:ASP:C	1:C:697:ASP:OD1	2.49	0.55
1:A:532:ARG:HD3	1:A:555:TYR:CE2	2.42	0.55
1:E:532:ARG:NH2	1:E:559:GLU:OE1	2.39	0.54
1:B:492:GLU:OE1	1:B:495:ARG:NH1	2.40	0.54
1:C:492:GLU:OE1	1:C:495:ARG:NH2	2.40	0.54
1:H:487:LEU:HD23	1:H:603:TRP:CH2	2.42	0.54
1:G:663:SER:HB2	1:G:669:GLN:HE22	1.72	0.54
1:H:606:HIS:O	1:H:610:ILE:HG12	2.08	0.54
1:B:635:ASP:O	1:B:638:ILE:HG22	2.08	0.53
1:A:650:GLU:OE2	1:A:674:ASN:HB2	2.08	0.53
1:H:522:LYS:HB2	1:H:565:ILE:HG21	1.90	0.53
1:A:695:ALA:O	1:A:699:MET:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:644:PHE:CE1	1:G:681:ASN:HB3	2.43	0.53
1:C:600:GLU:HG3	1:C:601:GLU:H	1.74	0.53
1:A:594:LEU:O	1:A:598:GLN:HG2	2.08	0.53
1:D:647:ILE:HD11	1:C:648:PRO:HA	1.91	0.53
1:E:569:LEU:HB2	1:E:570:PRO:HD3	1.89	0.53
1:E:495:ARG:HE	1:E:618:MET:HE2	1.74	0.53
1:D:693:HIS:O	1:D:697:ASP:OD1	2.26	0.53
1:G:597:LEU:HD23	1:G:603:TRP:CZ2	2.44	0.53
1:H:511:ILE:CD1	1:H:575:GLN:HB3	2.39	0.53
1:A:676:THR:O	1:A:680:GLU:HG2	2.07	0.53
1:G:595:LYS:HZ2	1:G:598:GLN:HB2	1.74	0.53
1:A:476:ARG:HA	1:A:479:LEU:HB3	1.91	0.52
1:B:582:LEU:HD21	1:B:622:VAL:HG21	1.91	0.52
1:F:664:LEU:HB3	1:F:666:GLU:OE1	2.09	0.52
1:B:482:LYS:O	1:B:486:ILE:HG12	2.09	0.52
1:G:647:ILE:HG23	1:G:648:PRO:HD3	1.90	0.52
1:C:493:SER:HA	1:C:496:LYS:HE3	1.91	0.52
1:A:597:LEU:HD12	1:A:603:TRP:CZ3	2.45	0.52
1:H:623:HIS:O	1:H:627:LEU:HD22	2.09	0.52
1:B:532:ARG:HD3	1:B:555:TYR:CE2	2.45	0.52
1:E:536:ASP:O	1:E:539:SER:OG	2.20	0.52
1:E:668:ASN:O	1:E:672:LEU:HD23	2.08	0.52
1:H:549:GLU:OE1	1:H:549:GLU:N	2.28	0.52
1:A:616:GLN:OE1	1:A:620:ARG:NH2	2.43	0.51
1:D:495:ARG:CZ	1:D:618:MET:HE2	2.40	0.51
1:E:647:ILE:HG23	1:E:648:PRO:HD3	1.91	0.51
1:G:638:ILE:HD11	1:H:523:ILE:HG21	1.92	0.51
1:F:608:SER:O	1:F:612:ARG:HG3	2.11	0.51
1:A:567:TYR:O	1:A:570:PRO:HD2	2.10	0.51
1:G:643:ILE:HA	1:G:649:ARG:NH1	2.26	0.51
1:E:638:ILE:CG2	1:F:523:ILE:HD12	2.40	0.51
1:G:553:LYS:HD3	1:G:557:LEU:HD22	1.92	0.51
1:G:482:LYS:O	1:G:486:ILE:HG23	2.11	0.51
1:A:476:ARG:HD3	1:A:477:LYS:HE2	1.93	0.51
1:G:531:GLN:HA	1:G:531:GLN:OE1	2.11	0.50
1:G:594:LEU:HD21	1:G:598:GLN:NE2	2.25	0.50
1:G:628:LEU:O	1:G:632:ILE:HD12	2.11	0.50
1:E:571:GLN:O	1:E:575:GLN:HG3	2.11	0.50
1:A:476:ARG:HD2	1:A:477:LYS:H	1.75	0.50
1:A:595:LYS:HG3	1:A:596:ARG:N	2.26	0.50
1:G:647:ILE:HG13	1:H:651:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:554:ILE:HG21	1:H:675:MET:HE1	1.93	0.50
1:D:655:ILE:HG23	1:C:551:VAL:HG23	1.93	0.50
1:B:506:TRP:CE3	1:B:699:MET:HE2	2.46	0.50
1:G:668:ASN:OD1	1:G:669:GLN:N	2.43	0.50
1:H:698:TYR:O	1:H:702:LYS:HG2	2.11	0.50
1:H:696:MET:HG3	1:H:700:LYS:HE3	1.92	0.50
1:B:554:ILE:HG13	1:B:676:THR:CG2	2.41	0.50
1:B:554:ILE:HG13	1:B:676:THR:HG23	1.92	0.50
1:B:594:LEU:O	1:B:598:GLN:HG3	2.12	0.50
1:F:636:ASN:HB3	1:F:698:TYR:OH	2.12	0.50
1:D:476:ARG:H	1:D:476:ARG:HE	1.59	0.50
1:E:495:ARG:HH21	1:E:618:MET:HE3	1.77	0.50
1:A:569:LEU:HB2	1:A:570:PRO:HD3	1.94	0.49
1:E:509:TYR:OH	1:E:625:ASP:OD1	2.24	0.49
1:E:593:THR:O	1:E:597:LEU:HD12	2.13	0.49
1:H:549:GLU:HA	1:H:553:LYS:HG2	1.93	0.49
1:H:675:MET:O	1:H:679:LEU:HD12	2.13	0.49
1:A:506:TRP:CZ3	1:A:699:MET:HB3	2.47	0.49
1:E:601:GLU:OE1	1:E:601:GLU:HA	2.11	0.49
1:F:498:ILE:HG12	1:F:582:LEU:HD11	1.95	0.49
1:F:637:LEU:HB3	1:F:641:LEU:HD23	1.94	0.49
1:A:504:GLU:HG3	1:A:580:THR:HB	1.94	0.49
1:B:567:TYR:O	1:B:570:PRO:HD2	2.12	0.49
1:G:635:ASP:OD2	1:H:515:ARG:NH2	2.46	0.49
1:G:643:ILE:HA	1:G:649:ARG:CZ	2.42	0.49
1:H:667:ALA:N	1:H:669:GLN:HE22	2.10	0.49
1:C:642:SER:O	1:C:649:ARG:NH2	2.45	0.49
1:E:644:PHE:HB3	1:E:682:LEU:HD11	1.94	0.49
1:F:582:LEU:HD21	1:F:622:VAL:HG21	1.95	0.49
1:H:504:GLU:HG2	1:H:580:THR:CG2	2.43	0.49
1:H:525:THR:HB	1:H:562:ILE:HD11	1.95	0.49
1:F:521:GLN:NE2	1:F:687:PHE:CE2	2.80	0.48
1:A:533:ASP:HB2	1:B:656:ASN:HD21	1.77	0.48
1:G:509:TYR:OH	1:G:625:ASP:OD1	2.28	0.48
1:G:569:LEU:HB2	1:G:570:PRO:HD3	1.96	0.48
1:C:699:MET:O	1:C:700:LYS:HG3	2.13	0.48
1:A:497:ALA:HB1	1:A:585:ILE:HD13	1.94	0.48
1:E:647:ILE:HD11	1:F:648:PRO:CA	2.40	0.48
1:F:480:GLU:O	1:F:483:VAL:HG12	2.14	0.48
1:H:678:GLY:O	1:H:682:LEU:HG	2.14	0.48
1:G:651:ILE:HB	1:H:651:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:639:HIS:CE1	1:F:523:ILE:HD11	2.49	0.48
1:E:671:LEU:HD21	1:F:654:PHE:CE1	2.49	0.48
1:G:651:ILE:O	1:G:655:ILE:HG12	2.12	0.48
1:G:676:THR:HG22	1:G:680:GLU:OE2	2.13	0.48
1:C:587:GLU:O	1:C:591:MET:HG2	2.14	0.48
1:A:655:ILE:HD11	1:B:555:TYR:CZ	2.49	0.48
1:B:669:GLN:CD	1:B:669:GLN:N	2.72	0.48
1:C:697:ASP:OD1	1:C:697:ASP:O	2.32	0.47
1:B:501:GLN:O	1:B:502:ASN:ND2	2.47	0.47
1:H:690:ALA:O	1:H:694:TYR:HD1	1.97	0.47
1:D:532:ARG:HG3	1:D:555:TYR:CE2	2.49	0.47
1:G:677:LEU:HD13	1:G:681:ASN:OD1	2.14	0.47
1:E:492:GLU:O	1:E:496:LYS:HG3	2.15	0.47
1:G:563:SER:OG	1:G:564:LYS:N	2.47	0.47
1:H:589:SER:O	1:H:593:THR:HG23	2.14	0.47
1:D:620:ARG:HD2	1:C:621:GLU:HG3	1.96	0.47
1:D:604:THR:HG22	1:D:607:HIS:ND1	2.29	0.47
1:D:661:PRO:C	1:D:663:SER:H	2.23	0.47
1:E:532:ARG:HD3	1:E:555:TYR:CD2	2.49	0.47
1:E:606:HIS:O	1:E:610:ILE:HD13	2.14	0.47
1:G:693:HIS:O	1:G:697:ASP:HB3	2.14	0.47
1:H:511:ILE:HD11	1:H:575:GLN:HB3	1.97	0.47
1:D:580:THR:OG1	1:D:581:ASP:N	2.47	0.47
1:E:502:ASN:HB3	1:E:506:TRP:CH2	2.48	0.47
1:F:584:TYR:HB2	1:H:567:TYR:CE2	2.50	0.47
1:H:554:ILE:HG21	1:H:675:MET:CE	2.45	0.47
1:D:479:LEU:O	1:D:483:VAL:HG12	2.14	0.47
1:D:639:HIS:CE1	1:C:523:ILE:HD11	2.50	0.47
1:C:560:GLN:HE22	1:B:596:ARG:HH22	1.62	0.47
1:E:675:MET:HE1	1:F:651:ILE:CG1	2.39	0.47
1:F:594:LEU:O	1:F:598:GLN:HG3	2.15	0.47
1:G:563:SER:HA	1:G:566:GLU:HG3	1.97	0.47
1:G:644:PHE:CE2	1:G:687:PHE:HA	2.50	0.47
1:D:668:ASN:OD1	1:C:664:LEU:HD11	2.14	0.47
1:C:560:GLN:OE1	1:B:596:ARG:NH1	2.46	0.47
1:B:612:ARG:O	1:B:616:GLN:HG2	2.14	0.47
1:C:641:LEU:HD13	1:C:687:PHE:CE1	2.49	0.46
1:A:645:PHE:O	1:A:648:PRO:HD2	2.15	0.46
1:E:593:THR:HG22	1:E:597:LEU:HD11	1.96	0.46
1:A:550:SER:HB2	1:A:672:LEU:HD22	1.97	0.46
1:H:550:SER:HB3	1:H:672:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:GLU:HB3	1:B:669:GLN:OE1	2.16	0.46
1:G:517:LEU:HD13	1:G:691:MET:CE	2.44	0.46
1:D:661:PRO:O	1:D:663:SER:N	2.48	0.46
1:C:509:TYR:CE1	1:C:626:LEU:HD23	2.51	0.46
1:C:522:LYS:O	1:C:526:GLU:HG3	2.16	0.46
1:C:643:ILE:O	1:C:643:ILE:HG13	2.16	0.46
1:G:476:ARG:HA	1:G:479:LEU:HB3	1.97	0.46
1:A:511:ILE:HG21	1:A:576:TYR:HB2	1.97	0.46
1:G:501:GLN:HB3	1:G:581:ASP:OD2	2.16	0.46
1:H:519:LEU:HD23	1:H:519:LEU:HA	1.78	0.46
1:H:548:SER:O	1:H:552:PHE:HB3	2.16	0.46
1:H:580:THR:HG22	1:H:581:ASP:N	2.31	0.46
1:A:635:ASP:OD1	1:B:516:LYS:HE2	2.15	0.46
1:G:553:LYS:HD3	1:G:557:LEU:CD2	2.46	0.46
1:G:645:PHE:O	1:G:649:ARG:HG3	2.16	0.46
1:G:517:LEU:HD13	1:G:691:MET:HE2	1.97	0.45
1:H:675:MET:O	1:H:676:THR:C	2.59	0.45
1:B:651:ILE:HD13	1:B:651:ILE:HA	1.70	0.45
1:G:589:SER:O	1:G:593:THR:OG1	2.30	0.45
1:H:581:ASP:O	1:H:585:ILE:HG12	2.17	0.45
1:A:479:LEU:O	1:A:483:VAL:HG23	2.15	0.45
1:A:604:THR:HG22	1:A:607:HIS:ND1	2.30	0.45
1:E:593:THR:HG22	1:E:597:LEU:CD1	2.46	0.45
1:H:558:CYS:O	1:H:562:ILE:HD13	2.16	0.45
1:A:480:GLU:OE2	1:B:604:THR:HG21	2.17	0.45
1:B:571:GLN:O	1:B:575:GLN:HG3	2.17	0.45
1:E:634:TYR:CZ	1:E:638:ILE:CD1	3.00	0.45
1:F:567:TYR:O	1:F:570:PRO:HD2	2.16	0.45
1:H:536:ASP:H	1:H:538:ASN:ND2	2.15	0.45
1:H:549:GLU:HA	1:H:553:LYS:CG	2.46	0.45
1:A:525:THR:HG22	1:A:562:ILE:HD11	1.98	0.45
1:B:485:LYS:O	1:B:489:GLU:HG3	2.15	0.45
1:A:687:PHE:CE2	1:A:691:MET:HE2	2.51	0.45
1:B:498:ILE:HD11	1:B:586:LEU:HD21	1.97	0.45
1:B:668:ASN:N	1:B:668:ASN:HD22	2.15	0.45
1:H:637:LEU:O	1:H:641:LEU:HB2	2.17	0.45
1:C:646:TYR:O	1:C:650:GLU:HG2	2.16	0.45
1:C:647:ILE:HB	1:C:648:PRO:HD3	1.98	0.45
1:E:505:LYS:N	1:E:505:LYS:HD2	2.31	0.45
1:G:586:LEU:HB3	1:G:619:LYS:NZ	2.32	0.45
1:G:655:ILE:HG22	1:H:672:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:ARG:HH21	1:E:618:MET:CE	2.30	0.45
1:G:563:SER:O	1:G:564:LYS:C	2.60	0.45
1:G:668:ASN:O	1:G:671:LEU:HB3	2.17	0.45
1:C:635:ASP:O	1:C:638:ILE:HG22	2.17	0.44
1:C:501:GLN:HG2	1:C:582:LEU:HB3	1.99	0.44
1:H:649:ARG:HE	1:H:649:ARG:HB2	1.48	0.44
1:A:533:ASP:O	1:A:534:ASP:HB2	2.16	0.44
1:B:514:LYS:HG3	1:B:691:MET:HE1	1.99	0.44
1:F:482:LYS:HB2	1:F:482:LYS:HE2	1.74	0.44
1:F:700:LYS:HE3	1:F:700:LYS:HB2	1.70	0.44
1:G:671:LEU:HD21	1:G:675:MET:HE3	1.99	0.44
1:E:634:TYR:CE2	1:E:638:ILE:HD12	2.52	0.44
1:C:606:HIS:O	1:C:610:ILE:HG13	2.17	0.44
1:F:498:ILE:HD11	1:F:586:LEU:HD11	1.99	0.44
1:B:564:LYS:HE3	1:B:568:GLN:OE1	2.18	0.44
1:H:510:PHE:HE2	1:H:691:MET:HG2	1.82	0.44
1:B:481:SER:O	1:B:485:LYS:HD3	2.18	0.44
1:E:564:LYS:O	1:E:568:GLN:HB2	2.16	0.44
1:F:675:MET:HB2	1:F:675:MET:HE3	1.69	0.44
1:F:479:LEU:O	1:F:482:LYS:N	2.50	0.44
1:F:696:MET:HG2	1:F:700:LYS:HE2	1.98	0.44
1:G:679:LEU:O	1:G:683:LEU:HD13	2.17	0.44
1:G:514:LYS:O	1:G:518:LEU:HD22	2.17	0.44
1:H:514:LYS:HG3	1:H:691:MET:SD	2.58	0.44
1:H:491:LEU:O	1:H:618:MET:HE1	2.18	0.43
1:C:522:LYS:HE2	1:C:526:GLU:OE2	2.18	0.43
1:C:549:GLU:CD	1:C:550:SER:H	2.26	0.43
1:A:501:GLN:HG2	1:A:581:ASP:HB3	1.99	0.43
1:E:508:LYS:HD2	1:E:626:LEU:HD21	1.99	0.43
1:F:553:LYS:O	1:F:553:LYS:HD3	2.18	0.43
1:F:693:HIS:O	1:F:696:MET:HB3	2.17	0.43
1:G:482:LYS:HA	1:G:485:LYS:HE2	1.99	0.43
1:G:628:LEU:HD23	1:G:632:ILE:CD1	2.48	0.43
1:H:675:MET:O	1:H:678:GLY:N	2.51	0.43
1:D:579:PRO:HA	1:D:583:ASP:OD2	2.18	0.43
1:G:649:ARG:HG2	1:H:527:LEU:HD22	1.99	0.43
1:B:482:LYS:O	1:B:482:LYS:HD3	2.19	0.43
1:E:574:SER:O	1:E:578:GLN:HG2	2.18	0.43
1:G:496:LYS:O	1:G:496:LYS:HD3	2.18	0.43
1:G:696:MET:HE2	1:G:696:MET:HB2	1.85	0.43
1:H:515:ARG:NH1	1:H:519:LEU:HD11	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:ASN:OD1	1:D:502:ASN:N	2.51	0.43
1:D:647:ILE:HG21	1:D:647:ILE:HD13	1.87	0.43
1:H:633:LEU:HG	1:H:637:LEU:HD11	2.01	0.43
1:D:474:ASN:HB3	1:D:477:LYS:HB3	1.99	0.43
1:E:511:ILE:HG21	1:E:576:TYR:HB2	2.01	0.43
1:F:578:GLN:HA	1:F:579:PRO:HD3	1.92	0.43
1:G:479:LEU:O	1:G:483:VAL:HG12	2.19	0.43
1:A:604:THR:OG1	1:A:605:GLU:N	2.51	0.43
1:E:647:ILE:HG12	1:F:647:ILE:HG22	2.01	0.43
1:F:579:PRO:HB2	1:H:571:GLN:OE1	2.19	0.43
1:G:475:LYS:HD2	1:G:476:ARG:HB3	2.01	0.43
1:G:581:ASP:OD1	1:G:581:ASP:N	2.51	0.43
1:D:483:VAL:O	1:D:486:ILE:HG13	2.19	0.43
1:A:537:ILE:H	1:A:537:ILE:HD12	1.84	0.43
1:A:654:PHE:CE1	1:A:658:ILE:HD11	2.54	0.43
1:E:647:ILE:HG23	1:E:648:PRO:CD	2.48	0.43
1:G:522:LYS:HB2	1:G:565:ILE:HG21	2.01	0.43
1:C:482:LYS:O	1:C:486:ILE:HG12	2.18	0.42
1:E:671:LEU:HD13	1:F:651:ILE:HD11	2.00	0.42
1:F:505:LYS:HG2	1:F:509:TYR:CZ	2.54	0.42
1:A:656:ASN:O	1:A:659:SER:OG	2.35	0.42
1:F:509:TYR:CE1	1:F:629:TYR:HB2	2.53	0.42
1:E:555:TYR:CE1	1:F:655:ILE:HD11	2.54	0.42
1:E:634:TYR:OH	1:E:638:ILE:HD11	2.19	0.42
1:F:614:SER:O	1:F:618:MET:HG3	2.19	0.42
1:E:675:MET:HB2	1:E:675:MET:HE3	1.55	0.42
1:H:519:LEU:HD21	1:H:569:LEU:HD21	2.01	0.42
1:H:691:MET:HE3	1:H:691:MET:HB2	1.96	0.42
1:G:481:SER:HA	1:H:606:HIS:CE1	2.52	0.42
1:A:678:GLY:O	1:A:682:LEU:HG	2.18	0.42
1:E:526:GLU:HG3	1:E:562:ILE:HD13	2.01	0.42
1:G:477:LYS:HB3	1:G:477:LYS:HE3	1.66	0.42
1:C:643:ILE:HA	1:C:649:ARG:NH2	2.35	0.42
1:G:663:SER:O	1:G:663:SER:OG	2.35	0.42
1:E:495:ARG:HE	1:E:495:ARG:HB2	1.36	0.42
1:F:636:ASN:HB3	1:F:698:TYR:CZ	2.54	0.42
1:C:560:GLN:NE2	1:B:596:ARG:HH22	2.18	0.42
1:E:582:LEU:O	1:E:585:ILE:HG22	2.19	0.42
1:D:688:ASP:OD1	1:D:688:ASP:N	2.53	0.41
1:C:564:LYS:HE2	1:C:568:GLN:OE1	2.20	0.41
1:A:595:LYS:HA	1:A:598:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ILE:HG13	1:B:647:ILE:HG23	2.02	0.41
1:E:603:TRP:HE1	1:E:608:SER:HG	1.67	0.41
1:D:477:LYS:HD3	1:D:477:LYS:C	2.45	0.41
1:E:494:THR:O	1:E:498:ILE:HD13	2.20	0.41
1:H:510:PHE:CE2	1:H:691:MET:HG2	2.54	0.41
1:D:531:GLN:OE1	1:C:649:ARG:HG3	2.21	0.41
1:C:663:SER:OG	1:C:664:LEU:N	2.53	0.41
1:E:597:LEU:HB3	1:E:603:TRP:CZ3	2.56	0.41
1:E:613:GLN:HA	1:E:616:GLN:HG2	2.02	0.41
1:B:683:LEU:O	1:B:683:LEU:HD23	2.20	0.41
1:G:531:GLN:O	1:G:555:TYR:OH	2.38	0.41
1:G:647:ILE:O	1:G:651:ILE:HG22	2.21	0.41
1:A:597:LEU:HD13	1:A:597:LEU:HA	1.86	0.41
1:E:654:PHE:O	1:E:658:ILE:HG23	2.20	0.41
1:E:659:SER:HA	1:F:547:GLU:OE1	2.21	0.41
1:D:633:LEU:O	1:D:637:LEU:HG	2.21	0.41
1:A:540:LEU:H	1:A:540:LEU:HD22	1.86	0.41
1:E:659:SER:O	1:E:660:ASN:ND2	2.54	0.41
1:F:660:ASN:OD1	1:F:660:ASN:N	2.53	0.41
1:H:504:GLU:HG2	1:H:580:THR:HG21	2.02	0.41
1:H:654:PHE:HB2	1:H:671:LEU:HD13	2.03	0.41
1:A:506:TRP:HE3	1:A:699:MET:SD	2.44	0.41
1:E:536:ASP:OD2	1:E:538:ASN:ND2	2.39	0.41
1:H:633:LEU:O	1:H:634:TYR:C	2.64	0.41
1:D:676:THR:HG22	1:D:680:GLU:OE1	2.21	0.41
1:C:700:LYS:HD2	1:C:700:LYS:C	2.46	0.41
1:D:581:ASP:N	1:D:581:ASP:OD2	2.53	0.41
1:C:626:LEU:HD23	1:C:626:LEU:HA	1.87	0.41
1:F:525:THR:O	1:F:528:VAL:HG22	2.21	0.41
1:G:648:PRO:HA	1:G:651:ILE:HG22	2.03	0.41
1:D:640:ASP:HB3	1:D:694:TYR:CD1	2.56	0.40
1:F:648:PRO:O	1:F:651:ILE:HG22	2.21	0.40
1:D:644:PHE:HB3	1:D:682:LEU:HD21	2.03	0.40
1:C:496:LYS:HE3	1:C:496:LYS:HB2	1.94	0.40
1:C:615:ILE:HA	1:C:615:ILE:HD13	1.77	0.40
1:B:492:GLU:HA	1:B:495:ARG:HG3	2.03	0.40
1:B:526:GLU:HG3	1:B:562:ILE:HD12	2.03	0.40
1:F:646:TYR:CE1	1:F:647:ILE:HG13	2.56	0.40
1:G:595:LYS:HA	1:G:595:LYS:HD2	1.80	0.40
1:H:606:HIS:N	1:H:606:HIS:CD2	2.89	0.40
1:C:690:ALA:O	1:C:694:TYR:HD2	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ASP:O	1:A:539:SER:OG	2.35	0.40
1:A:564:LYS:HZ1	1:A:568:GLN:HE22	1.69	0.40
1:G:486:ILE:HG13	1:G:487:LEU:N	2.36	0.40
1:D:491:LEU:HD23	1:D:491:LEU:HA	1.79	0.40
1:D:560:GLN:HB3	1:D:683:LEU:HD11	2.03	0.40
1:C:558:CYS:O	1:C:562:ILE:HG13	2.22	0.40
1:A:541:SER:O	1:A:544:SER:OG	2.26	0.40
1:G:585:ILE:HA	1:G:585:ILE:HD13	1.81	0.40
1:H:494:THR:HG22	1:H:498:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/232 (97%)	215 (96%)	9 (4%)	0	100	100
1	B	206/232 (89%)	196 (95%)	10 (5%)	0	100	100
1	C	213/232 (92%)	202 (95%)	11 (5%)	0	100	100
1	D	226/232 (97%)	217 (96%)	7 (3%)	2 (1%)	14	27
1	E	215/232 (93%)	209 (97%)	4 (2%)	2 (1%)	14	27
1	F	216/232 (93%)	208 (96%)	8 (4%)	0	100	100
1	G	208/232 (90%)	193 (93%)	15 (7%)	0	100	100
1	H	211/232 (91%)	196 (93%)	13 (6%)	2 (1%)	14	27
All	All	1719/1856 (93%)	1636 (95%)	77 (4%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	662	THR

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Mol	Chain	Res	Type
1	E	478	ASP
1	H	533	ASP
1	D	661	PRO
1	H	536	ASP
1	E	661	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	212/218 (97%)	195 (92%)	17 (8%)	11	24
1	B	200/218 (92%)	193 (96%)	7 (4%)	32	58
1	C	205/218 (94%)	199 (97%)	6 (3%)	37	65
1	D	214/218 (98%)	207 (97%)	7 (3%)	33	61
1	E	207/218 (95%)	202 (98%)	5 (2%)	43	70
1	F	209/218 (96%)	200 (96%)	9 (4%)	26	51
1	G	203/218 (93%)	192 (95%)	11 (5%)	20	41
1	H	205/218 (94%)	202 (98%)	3 (2%)	57	80
All	All	1655/1744 (95%)	1590 (96%)	65 (4%)	28	55

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	532	ARG
1	D	563	SER
1	D	582	LEU
1	D	596	ARG
1	D	642	SER
1	D	663	SER
1	D	683	LEU
1	C	493	SER
1	C	517	LEU
1	C	520	SER

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Mol	Chain	Res	Type
1	C	551	VAL
1	C	582	LEU
1	C	642	SER
1	A	503	GLN
1	A	520	SER
1	A	523	ILE
1	A	524	GLU
1	A	548	SER
1	A	559	GLU
1	A	578	GLN
1	A	581	ASP
1	A	582	LEU
1	A	595	LYS
1	A	597	LEU
1	A	626	LEU
1	A	633	LEU
1	A	641	LEU
1	A	642	SER
1	A	655	ILE
1	A	696	MET
1	B	517	LEU
1	B	554	ILE
1	B	582	LEU
1	B	615	ILE
1	B	653	ASN
1	B	659	SER
1	B	682	LEU
1	E	477	LYS
1	E	504	GLU
1	E	589	SER
1	E	671	LEU
1	E	682	LEU
1	F	479	LEU
1	F	508	LYS
1	F	520	SER
1	F	527	LEU
1	F	537	ILE
1	F	540	LEU
1	F	562	ILE
1	F	605	GLU
1	F	700	LYS
1	G	539	SER

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Mol	Chain	Res	Type
1	G	553	LYS
1	G	595	LYS
1	G	596	ARG
1	G	612	ARG
1	G	626	LEU
1	G	641	LEU
1	G	653	ASN
1	G	663	SER
1	G	676	THR
1	G	697	ASP
1	H	502	ASN
1	H	577	SER
1	H	693	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	501	GLN
1	D	568	GLN
1	D	592	GLN
1	D	616	GLN
1	D	668	ASN
1	C	571	GLN
1	C	578	GLN
1	C	592	GLN
1	C	613	GLN
1	A	538	ASN
1	A	598	GLN
1	A	636	ASN
1	A	668	ASN
1	B	501	GLN
1	B	598	GLN
1	B	668	ASN
1	E	560	GLN
1	E	598	GLN
1	E	639	HIS
1	E	660	ASN
1	E	674	ASN
1	E	684	ASN
1	F	521	GLN
1	F	531	GLN
1	F	575	GLN

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Mol	Chain	Res	Type
1	F	578	GLN
1	F	636	ASN
1	F	653	ASN
1	G	636	ASN
1	G	674	ASN
1	H	501	GLN
1	H	503	GLN
1	H	538	ASN
1	H	657	ASN

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	226/232 (97%)	0.11	4 (1%) 67 64	52, 89, 132, 161	0
1	B	212/232 (91%)	0.15	8 (3%) 44 39	53, 83, 126, 152	0
1	C	217/232 (93%)	-0.05	3 (1%) 73 70	60, 86, 127, 165	0
1	D	228/232 (98%)	-0.05	3 (1%) 75 71	63, 87, 122, 172	0
1	E	219/232 (94%)	0.10	6 (2%) 56 51	60, 96, 133, 177	0
1	F	222/232 (95%)	0.12	5 (2%) 61 57	57, 91, 148, 177	0
1	G	214/232 (92%)	0.38	4 (1%) 66 62	74, 136, 165, 184	0
1	H	217/232 (93%)	0.22	8 (3%) 45 40	79, 109, 160, 184	0
All	All	1755/1856 (94%)	0.12	41 (2%) 61 57	52, 96, 154, 184	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	661	PRO	3.7
1	H	537	ILE	3.4
1	E	540	LEU	3.3
1	B	667	ALA	3.3
1	B	539	SER	3.2
1	E	519	LEU	3.1
1	F	603	TRP	3.0
1	A	610	ILE	2.8
1	E	516	LYS	2.7
1	G	484	PHE	2.7
1	D	586	LEU	2.7
1	A	671	LEU	2.7
1	G	569	LEU	2.7
1	F	615	ILE	2.6
1	B	655	ILE	2.6
1	H	703	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	477	LYS	2.6
1	G	586	LEU	2.5
1	H	634	TYR	2.5
1	B	633	LEU	2.5
1	A	513	ALA	2.5
1	F	478	ASP	2.4
1	C	582	LEU	2.4
1	F	661	PRO	2.3
1	H	535	ILE	2.3
1	H	671	LEU	2.3
1	F	611	TYR	2.3
1	A	675	MET	2.3
1	B	488	PHE	2.3
1	E	646	TYR	2.2
1	C	675	MET	2.2
1	C	555	TYR	2.2
1	D	506	TRP	2.2
1	E	611	TYR	2.1
1	H	540	LEU	2.1
1	G	562	ILE	2.1
1	D	539	SER	2.1
1	H	477	LYS	2.1
1	B	695	ALA	2.0
1	B	637	LEU	2.0
1	B	651	ILE	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.