Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:43 PM GMT

PDB ID	:	1GXL
Title	:	SMC HINGE DOMAIN FROM T. MARITIMA WITH COILED COIL
Authors	:	Lowe, J.; Haering, C.; Nasmyth, K.
Deposited on	:	2002-04-07
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

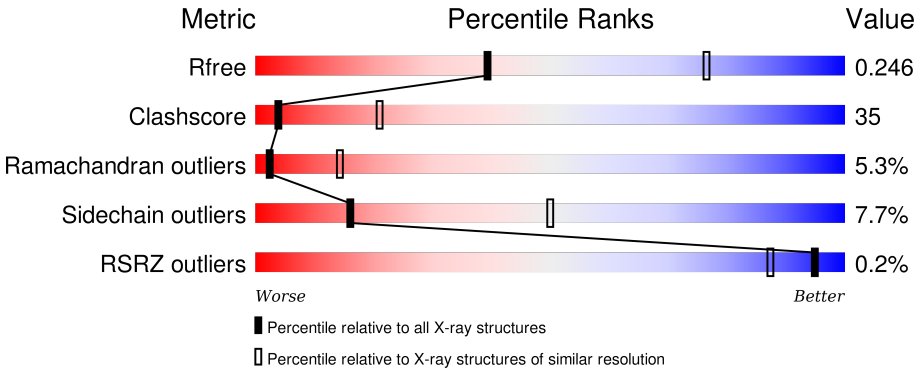
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	51% 39% 6% ·
1	B	213	44% 43% 9% ·
1	C	213	50% 37% 8% ·
1	D	213	51% 35% 7% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6490 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 CHROMOSOME SEGREGATION SMC PROTEIN.

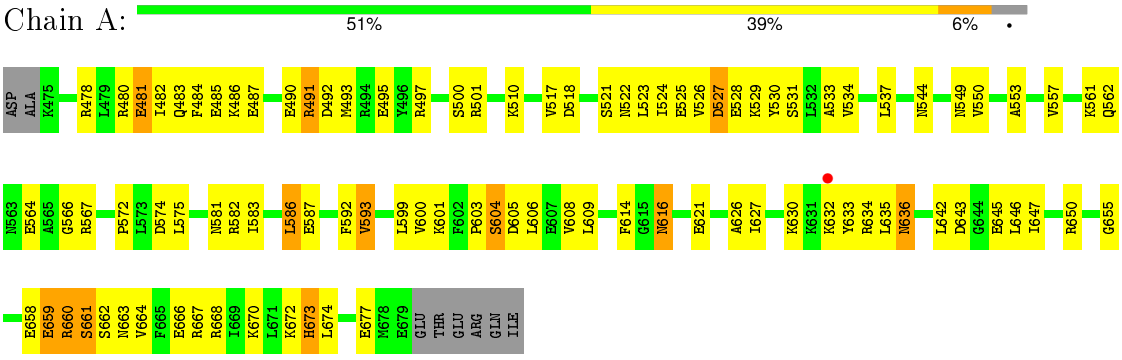
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1639	1031	293	311	4			
1	B	205	Total	C	N	O	S	0	0	0
			1639	1031	293	311	4			
1	C	205	Total	C	N	O	S	0	0	0
			1639	1031	293	311	4			
1	D	198	Total	C	N	O	S	0	0	0
			1573	991	278	300	4			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

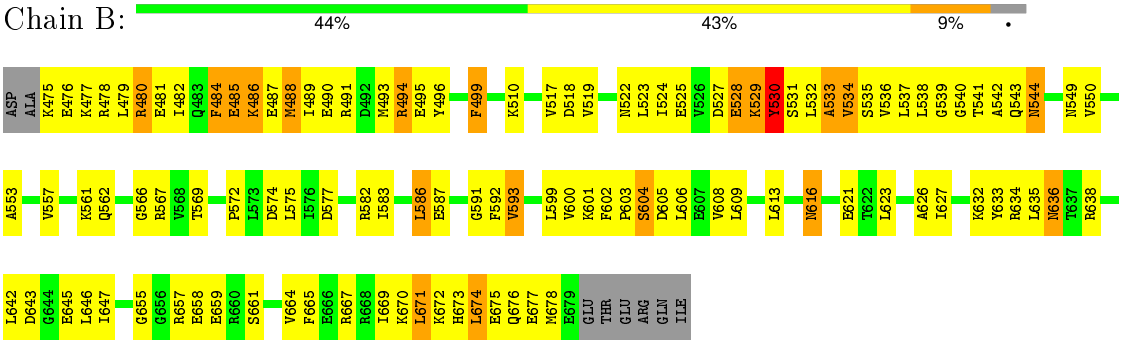
- Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

Chain A:



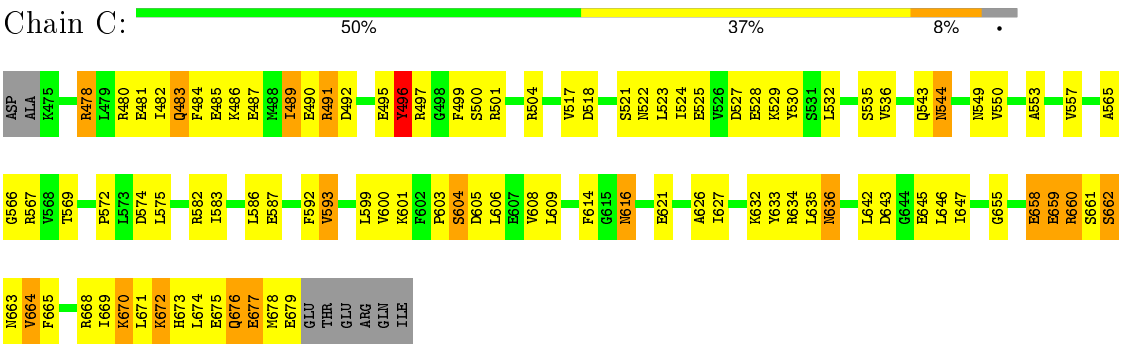
- Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

Chain B:



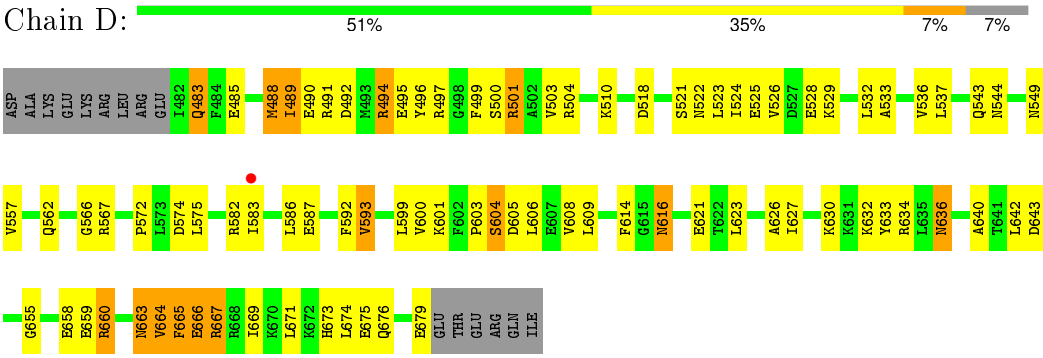
- Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

Chain C:



- Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

Chain D:


51%
35%
7%
7%
ASP ALA LYS GLU LYS ARG LEU ARG GLU I482 Q483 F484 E485 M488 I489 E490 R491 D492 M493 R494 E495 Y496 R497 G498 F499 S500 R501 A502 V503 R504 K510 D518 S521 N522 L523 I524 E525 V526 D527 E528 K529 L532 A533 V536 L537 Q543 N544 N549 V550 A553
V557 Q562 G566 R567 P572 L573 D574 L575 R582 I583 L586 E587 F592 V593 L599 V600 K601 F602 P603 S604 D605 L606 E607 V608 L609 F614 G615 N616 E621 T622 L623 A626 I627 K630 K631 K632 Y633 R634 L635 N636 A640 T641 L642 D643 G644 E645 L646 I647
G655 E658 E659 R660 N663 V664 F665 E666 R667 R668 I669 K670 L671 K672 H673 L674 E675 Q676 E679 GLU THR GLU ARG GLN ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.40Å 115.50Å 68.96Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 88.07 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-3.00) 94.8 (88.07-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.252 , 0.301 0.252 , 0.246	Depositor DCC
R_{free} test set	1052 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	93.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 21432 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6490	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/1657	0.69	0/2219
1	B	0.45	0/1657	0.70	0/2219
1	C	0.43	0/1657	0.67	0/2219
1	D	0.44	0/1591	0.66	0/2134
All	All	0.44	0/6562	0.68	0/8791

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	496	TYR	Sidechain

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	1639	0	1674	100	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1639	0	1674	155	0
1	C	1639	0	1674	111	0
1	D	1573	0	1599	109	0
All	All	6490	0	6621	453	1

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 35.

All (453) 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:D:518:ASP:HB3	1:D:523:LEU:HD11	1.26	1.16
1:B:518:ASP:HB3	1:B:523:LEU:HD11	1.17	1.14
1:C:518:ASP:HB3	1:C:523:LEU:HD11	1.22	1.11
1:A:518:ASP:HB3	1:A:523:LEU:HD11	1.22	1.08
1:B:494:ARG:HE	1:B:494:ARG:HA	1.20	1.05
1:A:655:GLY:HA2	1:B:567:ARG:HH21	1.31	0.95
1:C:566:GLY:HA2	1:D:658:GLU:HB3	1.50	0.94
1:A:482:ILE:HG13	1:A:674:LEU:HD22	1.54	0.88
1:B:667:ARG:O	1:B:671:LEU:HD12	1.73	0.88
1:B:482:ILE:HG21	1:B:678:MET:HB3	1.56	0.88
1:D:528:GLU:HG3	1:D:669:ILE:HG21	1.57	0.86
1:A:521:SER:HB2	1:A:664:VAL:HG13	1.58	0.86
1:C:672:LYS:HE2	1:C:675:GLU:HG2	1.56	0.86
1:B:533:ALA:O	1:B:536:VAL:HG22	1.76	0.85
1:A:550:VAL:HG11	1:B:627:ILE:HG21	1.58	0.85
1:C:482:ILE:HG21	1:C:678:MET:HG3	1.58	0.84
1:A:534:VAL:HA	1:A:537:LEU:HD12	1.58	0.83
1:B:494:ARG:NE	1:B:494:ARG:HA	1.93	0.83
1:A:482:ILE:HD11	1:A:674:LEU:O	1.78	0.83
1:D:525:GLU:HB3	1:D:601:LYS:HB2	1.58	0.83
1:D:500:SER:HB3	1:D:503:VAL:HG23	1.60	0.82
1:D:665:PHE:O	1:D:669:ILE:HG12	1.79	0.81
1:D:500:SER:H	1:D:543:GLN:HE22	1.30	0.79
1:D:491:ARG:HG2	1:D:494:ARG:HH22	1.46	0.79
1:D:533:ALA:O	1:D:536:VAL:HG22	1.83	0.79
1:B:478:ARG:O	1:B:482:ILE:HG12	1.82	0.79
1:D:488:MET:HA	1:D:488:MET:CE	2.13	0.79
1:B:673:HIS:HA	1:B:676:GLN:HE21	1.47	0.78
1:B:621:GLU:HA	1:B:642:LEU:HD12	1.66	0.78
1:A:567:ARG:HH21	1:B:655:GLY:HA2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:LEU:HA	1:D:663:ASN:HD22	1.50	0.77
1:D:664:VAL:O	1:D:666:GLU:N	2.18	0.76
1:D:572:PRO:HG2	1:D:575:LEU:HB3	1.66	0.76
1:B:673:HIS:HA	1:B:676:GLN:NE2	2.01	0.75
1:C:627:ILE:HD13	1:D:550:VAL:HG11	1.68	0.75
1:A:481:GLU:HG2	1:A:482:ILE:N	2.00	0.75
1:A:636:ASN:HD22	1:A:636:ASN:H	1.33	0.75
1:C:572:PRO:HG2	1:C:575:LEU:HB3	1.69	0.75
1:C:549:ASN:HA	1:C:574:ASP:OD1	1.86	0.74
1:B:518:ASP:HB3	1:B:523:LEU:CD1	2.09	0.74
1:C:550:VAL:HG11	1:D:627:ILE:HD13	1.69	0.74
1:D:636:ASN:HD22	1:D:636:ASN:H	1.35	0.74
1:D:664:VAL:C	1:D:666:GLU:H	1.90	0.74
1:C:535:SER:OG	1:C:663:ASN:HB3	1.88	0.74
1:B:636:ASN:HD22	1:B:636:ASN:H	1.34	0.74
1:A:518:ASP:HB3	1:A:523:LEU:CD1	2.12	0.73
1:B:572:PRO:HG2	1:B:575:LEU:HB3	1.68	0.73
1:A:549:ASN:HA	1:A:574:ASP:OD1	1.89	0.73
1:D:491:ARG:HG2	1:D:494:ARG:NH2	2.04	0.73
1:C:678:MET:O	1:C:679:GLU:HG3	1.89	0.73
1:C:636:ASN:HD22	1:C:636:ASN:H	1.34	0.73
1:D:524:ILE:HG23	1:D:600:VAL:HG13	1.69	0.73
1:A:572:PRO:HG2	1:A:575:LEU:HB3	1.71	0.72
1:D:528:GLU:HG3	1:D:669:ILE:CG2	2.18	0.72
1:A:524:ILE:HG23	1:A:600:VAL:HG13	1.70	0.71
1:C:567:ARG:HH21	1:D:655:GLY:HA2	1.54	0.71
1:B:536:VAL:O	1:B:646:LEU:HD21	1.91	0.71
1:D:488:MET:HA	1:D:488:MET:HE3	1.72	0.70
1:B:499:PHE:CD2	1:B:543:GLN:HB3	2.26	0.70
1:D:632:LYS:HD3	1:D:633:TYR:CE1	2.27	0.70
1:B:528:GLU:HG2	1:B:669:ILE:CG2	2.21	0.70
1:D:549:ASN:HA	1:D:574:ASP:OD1	1.91	0.70
1:B:603:PRO:O	1:B:605:ASP:N	2.24	0.70
1:C:632:LYS:HD3	1:C:633:TYR:CE1	2.27	0.70
1:B:528:GLU:HG2	1:B:669:ILE:HG23	1.72	0.70
1:C:491:ARG:O	1:C:495:GLU:HG2	1.92	0.70
1:A:593:VAL:HG12	1:A:593:VAL:O	1.92	0.70
1:B:593:VAL:HG12	1:B:593:VAL:O	1.92	0.69
1:A:550:VAL:CG1	1:B:627:ILE:HD13	2.21	0.69
1:C:655:GLY:HA2	1:D:567:ARG:HH21	1.57	0.69
1:D:521:SER:HB2	1:D:664:VAL:HG11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ASN:HA	1:B:574:ASP:OD1	1.92	0.69
1:C:621:GLU:HA	1:C:642:LEU:HD12	1.76	0.68
1:A:528:GLU:HA	1:A:531:SER:HB2	1.74	0.68
1:D:485:GLU:O	1:D:489:ILE:HG22	1.94	0.68
1:A:621:GLU:HA	1:A:642:LEU:HD12	1.75	0.68
1:A:632:LYS:HD3	1:A:633:TYR:CE1	2.29	0.68
1:B:645:GLU:O	1:B:646:LEU:HD12	1.94	0.68
1:C:482:ILE:CG2	1:C:678:MET:HG3	2.24	0.68
1:C:501:ARG:NH2	1:C:565:ALA:HA	2.09	0.68
1:B:485:GLU:HA	1:B:488:MET:CG	2.24	0.67
1:A:603:PRO:O	1:A:605:ASP:N	2.26	0.67
1:B:524:ILE:HG23	1:B:600:VAL:HG13	1.75	0.67
1:D:532:LEU:O	1:D:532:LEU:HD23	1.94	0.67
1:C:659:GLU:HG3	1:C:660:ARG:N	2.10	0.67
1:C:583:ILE:HD12	1:C:583:ILE:N	2.10	0.66
1:B:527:ASP:O	1:B:529:LYS:N	2.29	0.66
1:D:621:GLU:HA	1:D:642:LEU:HD12	1.77	0.66
1:C:518:ASP:HB3	1:C:523:LEU:CD1	2.13	0.66
1:B:534:VAL:HA	1:B:537:LEU:HD13	1.77	0.66
1:A:550:VAL:HG23	1:A:574:ASP:OD2	1.96	0.66
1:C:603:PRO:O	1:C:605:ASP:N	2.30	0.65
1:C:523:LEU:HD12	1:C:523:LEU:N	2.11	0.65
1:B:485:GLU:HA	1:B:488:MET:HG3	1.78	0.65
1:B:632:LYS:HD3	1:B:633:TYR:CE1	2.31	0.65
1:A:486:LYS:O	1:A:490:GLU:HG3	1.96	0.65
1:A:529:LYS:HD2	1:A:530:TYR:HE1	1.59	0.65
1:B:487:GLU:HA	1:B:490:GLU:HG3	1.78	0.65
1:B:657:ARG:HG3	1:B:658:GLU:H	1.62	0.65
1:D:593:VAL:HG12	1:D:593:VAL:O	1.97	0.65
1:D:603:PRO:O	1:D:605:ASP:N	2.29	0.64
1:C:627:ILE:HD13	1:D:550:VAL:CG1	2.27	0.64
1:D:489:ILE:O	1:D:489:ILE:HG23	1.97	0.64
1:D:664:VAL:HG12	1:D:665:PHE:H	1.61	0.64
1:B:536:VAL:CG2	1:B:537:LEU:HD12	2.28	0.64
1:B:536:VAL:HG23	1:B:646:LEU:HD11	1.80	0.64
1:D:518:ASP:HB3	1:D:523:LEU:CD1	2.17	0.64
1:C:677:GLU:HG2	1:C:677:GLU:O	1.97	0.63
1:B:671:LEU:O	1:B:675:GLU:HB2	1.98	0.63
1:B:499:PHE:HD2	1:B:543:GLN:HE21	1.46	0.63
1:B:583:ILE:HD12	1:B:583:ILE:N	2.14	0.62
1:D:550:VAL:HG23	1:D:574:ASP:OD2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:SER:HB2	1:C:664:VAL:HG11	1.81	0.62
1:C:486:LYS:HG2	1:C:490:GLU:OE2	1.98	0.62
1:C:521:SER:HB2	1:C:664:VAL:CG1	2.30	0.62
1:D:489:ILE:HD11	1:D:667:ARG:HD2	1.82	0.62
1:B:678:MET:O	1:B:678:MET:HG3	2.00	0.62
1:B:477:LYS:O	1:B:481:GLU:HG3	2.00	0.61
1:B:529:LYS:C	1:B:531:SER:H	2.04	0.61
1:A:529:LYS:HD2	1:A:530:TYR:CE1	2.35	0.61
1:C:524:ILE:HG23	1:C:600:VAL:HG13	1.82	0.61
1:B:659:GLU:N	1:B:659:GLU:OE1	2.34	0.61
1:B:529:LYS:O	1:B:531:SER:N	2.35	0.60
1:A:627:ILE:HG21	1:B:550:VAL:HG11	1.81	0.60
1:B:550:VAL:HG23	1:B:574:ASP:OD2	2.01	0.60
1:C:550:VAL:HG23	1:C:574:ASP:OD2	2.00	0.60
1:D:492:ASP:HB2	1:D:497:ARG:HB2	1.83	0.60
1:D:645:GLU:O	1:D:646:LEU:HD12	2.02	0.59
1:C:566:GLY:CA	1:D:658:GLU:HB3	2.29	0.59
1:C:550:VAL:CG1	1:D:627:ILE:HD13	2.31	0.59
1:B:499:PHE:CD1	1:B:499:PHE:N	2.71	0.59
1:B:537:LEU:O	1:B:638:ARG:NH1	2.36	0.59
1:B:475:LYS:O	1:B:478:ARG:HB3	2.02	0.59
1:C:660:ARG:NH2	1:C:660:ARG:HB2	2.18	0.59
1:A:659:GLU:O	1:A:660:ARG:O	2.21	0.59
1:B:536:VAL:HG23	1:B:537:LEU:HD12	1.84	0.58
1:D:664:VAL:C	1:D:666:GLU:N	2.57	0.58
1:D:500:SER:HB3	1:D:503:VAL:CG2	2.33	0.58
1:B:524:ILE:HG23	1:B:600:VAL:CG1	2.34	0.58
1:B:523:LEU:HD12	1:B:523:LEU:N	2.18	0.58
1:A:523:LEU:N	1:A:523:LEU:HD12	2.18	0.58
1:B:499:PHE:CE2	1:B:543:GLN:HB3	2.38	0.58
1:A:564:GLU:HG2	1:B:657:ARG:HG2	1.86	0.58
1:D:521:SER:CB	1:D:664:VAL:HG11	2.34	0.57
1:C:658:GLU:HA	1:D:566:GLY:HA2	1.87	0.57
1:D:523:LEU:HD12	1:D:523:LEU:N	2.18	0.57
1:D:658:GLU:HB2	1:D:659:GLU:OE1	2.03	0.57
1:C:593:VAL:HG12	1:C:593:VAL:O	2.04	0.57
1:A:482:ILE:HG23	1:A:483:GLN:N	2.19	0.56
1:B:530:TYR:CG	1:B:599:LEU:HD23	2.40	0.56
1:D:485:GLU:OE1	1:D:674:LEU:HD21	2.05	0.56
1:C:660:ARG:CZ	1:C:660:ARG:HB2	2.34	0.56
1:C:604:SER:C	1:C:606:LEU:H	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ILE:N	1:A:583:ILE:HD12	2.21	0.56
1:D:497:ARG:HB3	1:D:667:ARG:HH12	1.71	0.56
1:B:530:TYR:HB3	1:B:533:ALA:CB	2.36	0.55
1:C:672:LYS:O	1:C:676:GLN:HB3	2.04	0.55
1:D:489:ILE:HG23	1:D:671:LEU:HD21	1.87	0.55
1:D:604:SER:C	1:D:606:LEU:H	2.08	0.55
1:A:645:GLU:O	1:A:646:LEU:HD12	2.06	0.55
1:B:665:PHE:O	1:B:669:ILE:HG12	2.07	0.55
1:A:530:TYR:CD1	1:A:530:TYR:N	2.75	0.55
1:A:604:SER:C	1:A:606:LEU:H	2.09	0.55
1:C:676:GLN:HG2	1:C:677:GLU:N	2.22	0.55
1:D:488:MET:HE1	1:D:491:ARG:HE	1.71	0.55
1:C:645:GLU:O	1:C:646:LEU:HD12	2.07	0.54
1:B:671:LEU:C	1:B:673:HIS:N	2.61	0.54
1:A:550:VAL:HG11	1:B:627:ILE:HD13	1.90	0.54
1:B:536:VAL:CG2	1:B:646:LEU:HD11	2.38	0.54
1:C:487:GLU:O	1:C:491:ARG:HB3	2.08	0.54
1:A:647:ILE:N	1:A:647:ILE:HD12	2.23	0.54
1:A:518:ASP:CB	1:A:523:LEU:HD11	2.16	0.53
1:A:521:SER:HB2	1:A:664:VAL:CG1	2.35	0.53
1:D:491:ARG:HG2	1:D:494:ARG:HH12	1.73	0.53
1:A:636:ASN:N	1:A:636:ASN:HD22	1.98	0.53
1:A:485:GLU:HB3	1:A:674:LEU:HD11	1.90	0.53
1:D:537:LEU:HD21	1:D:640:ALA:CB	2.39	0.53
1:D:500:SER:N	1:D:543:GLN:HE22	2.03	0.53
1:B:527:ASP:C	1:B:529:LYS:N	2.61	0.53
1:D:491:ARG:HA	1:D:494:ARG:NH1	2.24	0.53
1:C:499:PHE:O	1:C:504:ARG:NH2	2.41	0.53
1:C:553:ALA:O	1:C:557:VAL:HG23	2.08	0.53
1:D:587:GLU:CD	1:D:587:GLU:H	2.12	0.53
1:A:529:LYS:HB2	1:A:530:TYR:CD1	2.44	0.53
1:D:647:ILE:HD12	1:D:647:ILE:N	2.24	0.53
1:D:483:GLN:H	1:D:483:GLN:CD	2.12	0.53
1:A:482:ILE:HD12	1:A:677:GLU:HB3	1.91	0.53
1:B:657:ARG:HG3	1:B:658:GLU:N	2.24	0.52
1:C:489:ILE:HG23	1:C:489:ILE:O	2.08	0.52
1:B:670:LYS:HE3	1:B:674:LEU:HD11	1.90	0.52
1:B:476:GLU:OE2	1:B:477:LYS:HD3	2.09	0.52
1:C:489:ILE:HA	1:C:492:ASP:OD2	2.08	0.52
1:A:566:GLY:N	1:B:657:ARG:O	2.37	0.52
1:A:500:SER:O	1:A:501:ARG:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLU:OE2	1:B:674:LEU:HD21	2.09	0.52
1:D:626:ALA:HB1	1:D:647:ILE:HD13	1.91	0.52
1:B:592:PHE:C	1:B:593:VAL:HG23	2.30	0.52
1:B:626:ALA:HB1	1:B:647:ILE:HD13	1.90	0.52
1:C:478:ARG:C	1:C:480:ARG:H	2.12	0.52
1:C:532:LEU:O	1:C:536:VAL:HG13	2.08	0.52
1:B:537:LEU:H	1:B:537:LEU:HD12	1.75	0.52
1:D:491:ARG:HG2	1:D:494:ARG:NH1	2.24	0.52
1:B:499:PHE:HB3	1:B:543:GLN:NE2	2.25	0.52
1:D:495:GLU:O	1:D:495:GLU:HG2	2.10	0.52
1:B:534:VAL:CA	1:B:537:LEU:HD13	2.40	0.51
1:D:528:GLU:CG	1:D:669:ILE:HG21	2.36	0.51
1:D:525:GLU:OE2	1:D:525:GLU:HA	2.11	0.51
1:B:524:ILE:HG12	1:B:602:PHE:CE2	2.45	0.51
1:A:482:ILE:CD1	1:A:677:GLU:HB3	2.41	0.51
1:B:524:ILE:HD11	1:B:613:LEU:HD13	1.92	0.51
1:A:530:TYR:H	1:A:530:TYR:HD1	1.58	0.51
1:C:525:GLU:HB3	1:C:601:LYS:HB2	1.91	0.51
1:A:478:ARG:C	1:A:480:ARG:H	2.13	0.51
1:C:662:SER:O	1:C:663:ASN:ND2	2.36	0.51
1:B:486:LYS:HD3	1:B:486:LYS:O	2.11	0.51
1:C:664:VAL:O	1:C:665:PHE:HB2	2.11	0.51
1:D:500:SER:H	1:D:543:GLN:NE2	2.05	0.51
1:D:532:LEU:CA	1:D:663:ASN:HD22	2.21	0.51
1:C:484:PHE:C	1:C:486:LYS:N	2.62	0.51
1:A:626:ALA:HB1	1:A:647:ILE:HD13	1.93	0.51
1:B:604:SER:C	1:B:606:LEU:H	2.13	0.51
1:C:600:VAL:HG12	1:C:601:LYS:N	2.25	0.51
1:A:526:VAL:HG22	1:A:527:ASP:O	2.11	0.51
1:C:647:ILE:N	1:C:647:ILE:HD12	2.25	0.51
1:B:476:GLU:OE2	1:B:477:LYS:N	2.43	0.51
1:B:525:GLU:HB3	1:B:601:LYS:HB2	1.92	0.51
1:D:532:LEU:HD23	1:D:532:LEU:C	2.31	0.50
1:C:587:GLU:CD	1:C:587:GLU:H	2.15	0.50
1:D:583:ILE:HD12	1:D:583:ILE:N	2.25	0.50
1:B:671:LEU:C	1:B:673:HIS:H	2.12	0.50
1:C:481:GLU:HA	1:C:484:PHE:HB3	1.93	0.50
1:C:496:TYR:CD1	1:C:496:TYR:N	2.79	0.50
1:D:636:ASN:HD22	1:D:636:ASN:N	2.01	0.50
1:A:658:GLU:O	1:A:659:GLU:C	2.50	0.50
1:B:599:LEU:N	1:B:599:LEU:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:VAL:O	1:C:553:ALA:HB3	2.12	0.50
1:A:492:ASP:OD1	1:A:497:ARG:HD2	2.11	0.50
1:B:479:LEU:HA	1:B:482:ILE:HG12	1.93	0.50
1:C:626:ALA:HB1	1:C:647:ILE:HD13	1.93	0.50
1:A:493:MET:CE	1:A:668:ARG:HG2	2.42	0.50
1:B:673:HIS:O	1:B:677:GLU:N	2.38	0.49
1:C:661:SER:O	1:C:662:SER:C	2.50	0.49
1:C:491:ARG:HH21	1:C:491:ARG:HG2	1.77	0.49
1:D:674:LEU:C	1:D:676:GLN:H	2.14	0.49
1:C:659:GLU:CG	1:C:660:ARG:N	2.75	0.49
1:D:600:VAL:HG12	1:D:601:LYS:N	2.26	0.49
1:C:522:ASN:C	1:C:523:LEU:HD12	2.32	0.49
1:B:480:ARG:NE	1:B:480:ARG:HA	2.26	0.49
1:D:491:ARG:HG2	1:D:494:ARG:CZ	2.42	0.49
1:A:587:GLU:CD	1:A:587:GLU:H	2.15	0.49
1:B:647:ILE:HD12	1:B:647:ILE:N	2.27	0.49
1:A:492:ASP:CB	1:A:667:ARG:NH2	2.76	0.49
1:D:673:HIS:O	1:D:676:GLN:HB3	2.12	0.49
1:B:623:LEU:O	1:B:623:LEU:HD12	2.11	0.49
1:C:499:PHE:N	1:C:499:PHE:CD1	2.80	0.49
1:A:492:ASP:HB3	1:A:667:ARG:NH2	2.28	0.49
1:B:621:GLU:HA	1:B:642:LEU:CD1	2.40	0.48
1:A:593:VAL:O	1:A:593:VAL:CG1	2.61	0.48
1:A:600:VAL:HG12	1:A:601:LYS:N	2.28	0.48
1:B:600:VAL:HG12	1:B:601:LYS:N	2.26	0.48
1:B:485:GLU:C	1:B:487:GLU:N	2.67	0.48
1:B:530:TYR:CB	1:B:599:LEU:HD23	2.43	0.48
1:B:499:PHE:CD2	1:B:543:GLN:NE2	2.81	0.48
1:A:666:GLU:HG3	1:A:667:ARG:N	2.28	0.48
1:B:486:LYS:C	1:B:486:LYS:HD3	2.34	0.48
1:C:482:ILE:HG22	1:C:483:GLN:N	2.29	0.48
1:A:567:ARG:HA	1:B:655:GLY:O	2.14	0.48
1:C:501:ARG:HH21	1:C:565:ALA:HA	1.78	0.47
1:A:658:GLU:HB2	1:B:566:GLY:HA2	1.94	0.47
1:C:484:PHE:C	1:C:486:LYS:H	2.17	0.47
1:B:485:GLU:C	1:B:487:GLU:H	2.17	0.47
1:C:636:ASN:HD22	1:C:636:ASN:N	1.99	0.47
1:B:482:ILE:HG22	1:B:678:MET:HE2	1.94	0.47
1:B:532:LEU:HD23	1:B:532:LEU:O	2.13	0.47
1:B:534:VAL:O	1:B:537:LEU:N	2.47	0.47
1:D:636:ASN:H	1:D:636:ASN:ND2	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:SER:C	1:C:606:LEU:N	2.67	0.47
1:A:599:LEU:N	1:A:599:LEU:HD12	2.29	0.47
1:D:537:LEU:HD21	1:D:640:ALA:HB2	1.96	0.47
1:D:599:LEU:HD12	1:D:599:LEU:N	2.29	0.47
1:A:483:GLN:O	1:A:487:GLU:HG3	2.15	0.47
1:B:592:PHE:O	1:B:593:VAL:CG2	2.63	0.47
1:B:593:VAL:CG1	1:B:593:VAL:O	2.62	0.47
1:D:499:PHE:HD2	1:D:543:GLN:HE21	1.62	0.47
1:C:495:GLU:O	1:C:496:TYR:C	2.53	0.47
1:C:499:PHE:HD1	1:C:499:PHE:H	1.61	0.47
1:A:616:ASN:HD22	1:A:616:ASN:HA	1.51	0.47
1:A:636:ASN:H	1:A:636:ASN:ND2	2.08	0.47
1:B:489:ILE:CG2	1:B:671:LEU:HD21	2.46	0.46
1:C:616:ASN:HD22	1:C:616:ASN:HA	1.51	0.46
1:A:481:GLU:O	1:A:484:PHE:HB3	2.15	0.46
1:B:669:ILE:C	1:B:671:LEU:H	2.18	0.46
1:D:604:SER:C	1:D:606:LEU:N	2.68	0.46
1:A:491:ARG:O	1:A:495:GLU:HB2	2.16	0.46
1:D:616:ASN:HD22	1:D:616:ASN:HA	1.52	0.46
1:D:485:GLU:HG3	1:D:674:LEU:HD11	1.97	0.46
1:D:608:VAL:HG23	1:D:609:LEU:N	2.30	0.46
1:A:524:ILE:HG23	1:A:600:VAL:CG1	2.42	0.46
1:B:587:GLU:H	1:B:587:GLU:CD	2.18	0.46
1:C:678:MET:C	1:C:679:GLU:HG3	2.36	0.46
1:A:604:SER:C	1:A:606:LEU:N	2.69	0.46
1:C:636:ASN:H	1:C:636:ASN:ND2	2.08	0.46
1:C:484:PHE:CD1	1:C:485:GLU:N	2.84	0.46
1:B:636:ASN:HD22	1:B:636:ASN:N	1.99	0.46
1:A:525:GLU:HB3	1:A:601:LYS:HB2	1.98	0.46
1:A:530:TYR:HD2	1:A:599:LEU:HD23	1.81	0.46
1:A:608:VAL:HG23	1:A:609:LEU:H	1.81	0.46
1:C:529:LYS:HD2	1:C:530:TYR:CE1	2.50	0.46
1:C:664:VAL:HG12	1:C:665:PHE:N	2.31	0.45
1:B:486:LYS:HE3	1:B:675:GLU:OE2	2.16	0.45
1:D:608:VAL:HG23	1:D:609:LEU:H	1.80	0.45
1:D:623:LEU:O	1:D:623:LEU:HD12	2.16	0.45
1:B:542:ALA:HB1	1:B:664:VAL:HG11	1.98	0.45
1:D:526:VAL:HG23	1:D:599:LEU:O	2.16	0.45
1:C:484:PHE:O	1:C:486:LYS:N	2.49	0.45
1:B:484:PHE:O	1:B:488:MET:HG2	2.17	0.45
1:B:530:TYR:O	1:B:531:SER:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:GLU:HG3	1:C:660:ARG:H	1.81	0.45
1:D:664:VAL:HG12	1:D:665:PHE:N	2.31	0.45
1:D:488:MET:HA	1:D:488:MET:HE2	1.95	0.45
1:B:553:ALA:O	1:B:557:VAL:HG23	2.17	0.45
1:A:491:ARG:NH2	1:A:492:ASP:OD1	2.50	0.45
1:A:493:MET:HE3	1:A:668:ARG:HG2	1.98	0.45
1:C:599:LEU:N	1:C:599:LEU:HD12	2.32	0.45
1:D:553:ALA:O	1:D:557:VAL:HG23	2.17	0.45
1:B:608:VAL:HG23	1:B:609:LEU:H	1.81	0.45
1:C:480:ARG:C	1:C:482:ILE:H	2.19	0.45
1:A:621:GLU:HA	1:A:642:LEU:CD1	2.45	0.45
1:C:600:VAL:CG1	1:C:601:LYS:N	2.79	0.45
1:C:518:ASP:CB	1:C:523:LEU:HD11	2.16	0.45
1:B:478:ARG:O	1:B:478:ARG:HD3	2.17	0.45
1:B:538:LEU:O	1:B:541:THR:OG1	2.29	0.45
1:B:536:VAL:HG22	1:B:537:LEU:HD12	1.98	0.45
1:B:482:ILE:HB	1:B:678:MET:HE1	1.98	0.45
1:C:677:GLU:CG	1:C:677:GLU:O	2.65	0.45
1:B:636:ASN:H	1:B:636:ASN:ND2	2.07	0.44
1:B:524:ILE:HG12	1:B:602:PHE:CZ	2.52	0.44
1:B:539:GLY:C	1:B:541:THR:H	2.20	0.44
1:B:491:ARG:O	1:B:495:GLU:HB3	2.17	0.44
1:B:485:GLU:HG3	1:B:674:LEU:CD1	2.48	0.44
1:A:608:VAL:HG23	1:A:609:LEU:N	2.32	0.44
1:A:553:ALA:O	1:A:557:VAL:HG23	2.17	0.44
1:C:523:LEU:CD1	1:C:523:LEU:N	2.79	0.44
1:B:531:SER:OG	1:B:669:ILE:HG13	2.17	0.44
1:A:521:SER:CB	1:A:664:VAL:HG13	2.40	0.44
1:C:659:GLU:C	1:C:659:GLU:OE1	2.56	0.44
1:C:614:PHE:C	1:C:616:ASN:H	2.21	0.44
1:C:665:PHE:O	1:C:669:ILE:HG12	2.18	0.44
1:A:670:LYS:HA	1:A:673:HIS:HB2	2.00	0.44
1:C:483:GLN:HE21	1:C:483:GLN:HA	1.82	0.44
1:D:504:ARG:HH21	1:D:504:ARG:HG3	1.83	0.44
1:D:485:GLU:HG3	1:D:674:LEU:CD1	2.47	0.44
1:C:661:SER:O	1:C:663:ASN:ND2	2.51	0.44
1:D:659:GLU:N	1:D:659:GLU:OE1	2.46	0.44
1:B:530:TYR:HB3	1:B:533:ALA:HB2	1.99	0.44
1:A:530:TYR:O	1:A:533:ALA:HB3	2.17	0.44
1:D:489:ILE:CD1	1:D:667:ARG:HD2	2.45	0.43
1:D:621:GLU:HA	1:D:642:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:614:PHE:C	1:D:616:ASN:H	2.20	0.43
1:D:500:SER:O	1:D:501:ARG:C	2.57	0.43
1:D:537:LEU:CD2	1:D:640:ALA:HB2	2.48	0.43
1:B:537:LEU:N	1:B:537:LEU:HD12	2.32	0.43
1:D:600:VAL:CG1	1:D:601:LYS:N	2.81	0.43
1:D:501:ARG:O	1:D:504:ARG:HB2	2.18	0.43
1:C:663:ASN:O	1:C:664:VAL:O	2.37	0.43
1:A:633:TYR:O	1:A:634:ARG:C	2.57	0.43
1:C:525:GLU:OE2	1:C:525:GLU:HA	2.18	0.43
1:A:478:ARG:C	1:A:480:ARG:N	2.71	0.43
1:B:669:ILE:C	1:B:671:LEU:N	2.72	0.43
1:C:478:ARG:O	1:C:482:ILE:HD13	2.18	0.43
1:D:489:ILE:HD11	1:D:667:ARG:CD	2.48	0.43
1:A:663:ASN:O	1:A:666:GLU:HG2	2.19	0.43
1:B:484:PHE:N	1:B:484:PHE:CD1	2.86	0.43
1:B:536:VAL:HG23	1:B:537:LEU:N	2.33	0.43
1:A:633:TYR:O	1:A:635:LEU:HG	2.19	0.43
1:B:527:ASP:C	1:B:529:LYS:H	2.22	0.43
1:A:600:VAL:CG1	1:A:601:LYS:N	2.82	0.43
1:D:562:GLN:HA	1:D:562:GLN:NE2	2.34	0.43
1:B:530:TYR:O	1:B:533:ALA:N	2.51	0.43
1:B:586:LEU:HD23	1:B:586:LEU:HA	1.82	0.43
1:B:537:LEU:H	1:B:537:LEU:CD1	2.32	0.42
1:B:539:GLY:O	1:B:541:THR:N	2.52	0.42
1:A:650:ARG:NH1	1:B:577:ASP:O	2.52	0.42
1:B:636:ASN:ND2	1:B:636:ASN:N	2.67	0.42
1:A:592:PHE:C	1:A:593:VAL:HG23	2.40	0.42
1:B:587:GLU:HA	1:B:592:PHE:CD2	2.55	0.42
1:D:489:ILE:HG23	1:D:671:LEU:CD2	2.49	0.42
1:A:634:ARG:HH21	1:A:634:ARG:HG2	1.84	0.42
1:C:592:PHE:C	1:C:593:VAL:HG23	2.40	0.42
1:B:522:ASN:C	1:B:523:LEU:HD12	2.40	0.42
1:B:493:MET:HG2	1:B:667:ARG:HD2	2.02	0.42
1:C:633:TYR:O	1:C:635:LEU:HG	2.19	0.42
1:D:592:PHE:C	1:D:593:VAL:HG23	2.39	0.42
1:A:661:SER:O	1:A:662:SER:C	2.57	0.42
1:C:544:ASN:ND2	1:C:569:THR:HB	2.35	0.42
1:D:522:ASN:C	1:D:523:LEU:HD12	2.40	0.42
1:B:600:VAL:CG1	1:B:601:LYS:N	2.81	0.42
1:B:499:PHE:CD2	1:B:543:GLN:CB	3.00	0.42
1:C:633:TYR:O	1:C:634:ARG:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.89	0.42
1:B:530:TYR:O	1:B:533:ALA:HB3	2.19	0.42
1:B:557:VAL:O	1:B:561:LYS:HB2	2.19	0.42
1:C:481:GLU:HG2	1:C:481:GLU:O	2.19	0.42
1:B:604:SER:C	1:B:606:LEU:N	2.72	0.42
1:D:634:ARG:HH21	1:D:634:ARG:HG2	1.84	0.42
1:A:655:GLY:O	1:B:567:ARG:HA	2.20	0.42
1:A:482:ILE:CG2	1:A:483:GLN:N	2.83	0.42
1:B:487:GLU:C	1:B:489:ILE:N	2.73	0.42
1:B:530:TYR:HB3	1:B:533:ALA:HB3	2.02	0.42
1:C:634:ARG:HH21	1:C:634:ARG:HG2	1.84	0.42
1:B:480:ARG:O	1:B:484:PHE:CD1	2.73	0.41
1:C:480:ARG:C	1:C:482:ILE:N	2.72	0.41
1:C:636:ASN:ND2	1:C:636:ASN:N	2.67	0.41
1:B:608:VAL:O	1:B:609:LEU:C	2.59	0.41
1:B:484:PHE:HD1	1:B:484:PHE:N	2.17	0.41
1:C:664:VAL:O	1:C:665:PHE:CB	2.68	0.41
1:B:550:VAL:O	1:B:553:ALA:HB3	2.19	0.41
1:C:671:LEU:HA	1:C:671:LEU:HD23	1.86	0.41
1:B:616:ASN:HD22	1:B:616:ASN:HA	1.50	0.41
1:B:634:ARG:HH21	1:B:634:ARG:HG2	1.84	0.41
1:A:522:ASN:C	1:A:523:LEU:HD12	2.41	0.41
1:D:636:ASN:N	1:D:636:ASN:ND2	2.68	0.41
1:B:591:GLY:O	1:B:593:VAL:HG23	2.20	0.41
1:C:587:GLU:HA	1:C:592:PHE:CD2	2.55	0.41
1:D:679:GLU:HG2	1:D:679:GLU:OXT	2.20	0.41
1:A:587:GLU:HA	1:A:592:PHE:CD2	2.55	0.41
1:C:524:ILE:HG23	1:C:600:VAL:CG1	2.50	0.41
1:C:608:VAL:HG23	1:C:609:LEU:N	2.36	0.41
1:B:534:VAL:O	1:B:535:SER:C	2.58	0.41
1:D:491:ARG:HA	1:D:494:ARG:CZ	2.51	0.41
1:C:603:PRO:HG2	1:C:606:LEU:HD12	2.02	0.41
1:A:562:GLN:HA	1:A:562:GLN:NE2	2.36	0.41
1:B:499:PHE:CB	1:B:543:GLN:NE2	2.84	0.41
1:A:630:LYS:O	1:A:630:LYS:HG3	2.21	0.41
1:C:672:LYS:HA	1:C:672:LYS:HD3	1.65	0.41
1:A:636:ASN:N	1:A:636:ASN:ND2	2.67	0.41
1:C:658:GLU:OE2	1:D:567:ARG:HD2	2.21	0.41
1:D:630:LYS:O	1:D:630:LYS:HG3	2.21	0.41
1:B:519:VAL:O	1:B:523:LEU:HD13	2.21	0.41
1:B:672:LYS:O	1:B:676:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:VAL:O	1:A:561:LYS:HB2	2.21	0.41
1:A:592:PHE:O	1:A:593:VAL:CG2	2.69	0.40
1:A:614:PHE:C	1:A:616:ASN:H	2.25	0.40
1:C:527:ASP:HB3	1:C:530:TYR:HD1	1.85	0.40
1:C:500:SER:H	1:C:543:GLN:HE22	1.69	0.40
1:B:562:GLN:HA	1:B:562:GLN:NE2	2.36	0.40
1:A:586:LEU:HA	1:A:586:LEU:HD23	1.86	0.40
1:C:670:LYS:HZ1	1:C:674:LEU:HD21	1.87	0.40
1:D:659:GLU:O	1:D:660:ARG:CB	2.70	0.40
1:A:525:GLU:OE2	1:A:525:GLU:HA	2.21	0.40
1:B:592:PHE:C	1:B:593:VAL:CG2	2.89	0.40
1:B:633:TYR:O	1:B:635:LEU:HG	2.20	0.40
1:B:544:ASN:ND2	1:B:569:THR:HB	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ASN:ND2	1:A:581:ASN:ND2[2_555]	1.85	0.35

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	203/213 (95%)	169 (83%)	27 (13%)	7 (3%)	5 25
1	B	203/213 (95%)	160 (79%)	29 (14%)	14 (7%)	1 7
1	C	203/213 (95%)	162 (80%)	31 (15%)	10 (5%)	3 16
1	D	196/213 (92%)	155 (79%)	29 (15%)	12 (6%)	2 11
All	All	805/852 (94%)	646 (80%)	116 (14%)	43 (5%)	2 14

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	SER
1	A	660	ARG
1	B	528	GLU
1	B	529	LYS
1	B	530	TYR
1	B	604	SER
1	C	489	ILE
1	C	604	SER
1	C	664	VAL
1	D	604	SER
1	D	663	ASN
1	D	664	VAL
1	D	665	PHE
1	A	593	VAL
1	B	484	PHE
1	B	593	VAL
1	C	478	ARG
1	C	662	SER
1	A	659	GLU
1	B	485	GLU
1	B	533	ALA
1	C	496	TYR
1	C	677	GLU
1	D	593	VAL
1	D	666	GLU
1	D	675	GLU
1	A	510	LYS
1	B	496	TYR
1	B	510	LYS
1	B	540	GLY
1	B	674	LEU
1	C	593	VAL
1	D	490	GLU
1	D	510	LYS
1	D	529	LYS
1	A	661	SER
1	C	676	GLN
1	D	660	ARG
1	D	489	ILE
1	B	534	VAL
1	A	517	VAL
1	B	517	VAL
1	C	517	VAL

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	177/184 (96%)	166 (94%)	11 (6%)	23 60
1	B	177/184 (96%)	163 (92%)	14 (8%)	15 48
1	C	177/184 (96%)	159 (90%)	18 (10%)	9 33
1	D	170/184 (92%)	159 (94%)	11 (6%)	21 58
All	All	701/736 (95%)	647 (92%)	54 (8%)	16 50

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	481	GLU
1	A	491	ARG
1	A	527	ASP
1	A	544	ASN
1	A	582	ARG
1	A	586	LEU
1	A	616	ASN
1	A	636	ASN
1	A	643	ASP
1	A	672	LYS
1	A	673	HIS
1	B	480	ARG
1	B	486	LYS
1	B	488	MET
1	B	494	ARG
1	B	499	PHE
1	B	530	TYR
1	B	544	ASN
1	B	582	ARG
1	B	586	LEU
1	B	616	ASN
1	B	636	ASN
1	B	643	ASP
1	B	661	SER

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Mol	Chain	Res	Type
1	B	671	LEU
1	C	483	GLN
1	C	491	ARG
1	C	496	TYR
1	C	497	ARG
1	C	528	GLU
1	C	544	ASN
1	C	582	ARG
1	C	586	LEU
1	C	616	ASN
1	C	636	ASN
1	C	643	ASP
1	C	658	GLU
1	C	659	GLU
1	C	660	ARG
1	C	668	ARG
1	C	670	LYS
1	C	672	LYS
1	C	673	HIS
1	D	483	GLN
1	D	488	MET
1	D	494	ARG
1	D	501	ARG
1	D	544	ASN
1	D	582	ARG
1	D	586	LEU
1	D	616	ASN
1	D	636	ASN
1	D	643	ASP
1	D	667	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	GLN
1	A	543	GLN
1	A	544	ASN
1	A	562	GLN
1	A	616	ASN
1	A	636	ASN
1	A	676	GLN
1	B	543	GLN

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Mol	Chain	Res	Type
1	B	544	ASN
1	B	562	GLN
1	B	616	ASN
1	B	636	ASN
1	B	676	GLN
1	C	483	GLN
1	C	543	GLN
1	C	544	ASN
1	C	562	GLN
1	C	636	ASN
1	C	663	ASN
1	C	673	HIS
1	D	483	GLN
1	D	543	GLN
1	D	544	ASN
1	D	562	GLN
1	D	636	ASN
1	D	663	ASN
1	D	673	HIS
1	D	676	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 carbohydrates 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, 95^{th} 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	205/213 (96%)	-0.07	1 (0%) 91 76	50, 77, 120, 137	0
1	B	205/213 (96%)	-0.08	0 100 100	53, 81, 116, 133	0
1	C	205/213 (96%)	-0.11	0 100 100	50, 81, 117, 137	0
1	D	198/213 (92%)	-0.09	1 (0%) 91 76	49, 81, 114, 134	0
All	All	813/852 (95%)	-0.09	2 (0%) 95 87	49, 80, 117, 137	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	583	ILE	2.2
1	A	632	LYS	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.