



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:00 AM UTC

PDB ID : 1GXL / pdb_00001gxl
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

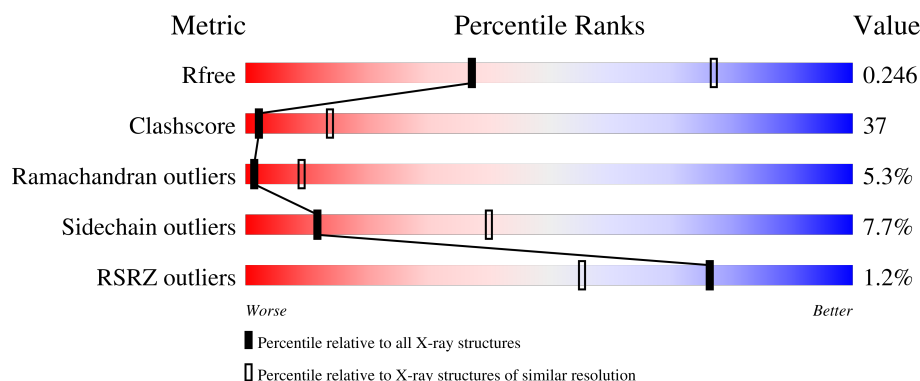
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	213	2% 47% 40% 8% .
1	B	213	2% 39% 46% 10% . .
1	C	213	48% 38% 9% . .
1	D	213	2% 48% 35% 10% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6486 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.

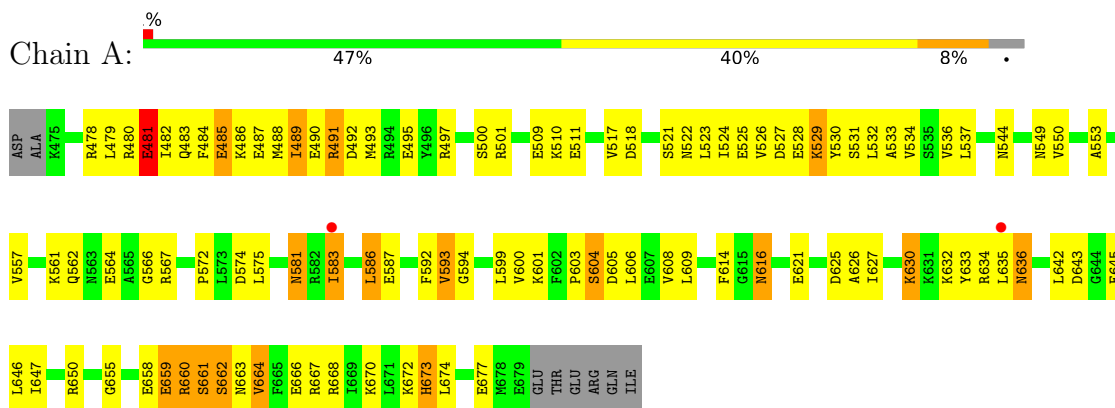
- Molecule 1 is a protein called CHROMOSOME SEGREGATION SMC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1638	1031	293	310	4			
1	B	205	Total	C	N	O	S	0	0	0
			1638	1031	293	310	4			
1	C	205	Total	C	N	O	S	0	0	0
			1638	1031	293	310	4			
1	D	198	Total	C	N	O	S	0	0	0
			1572	991	278	299	4			

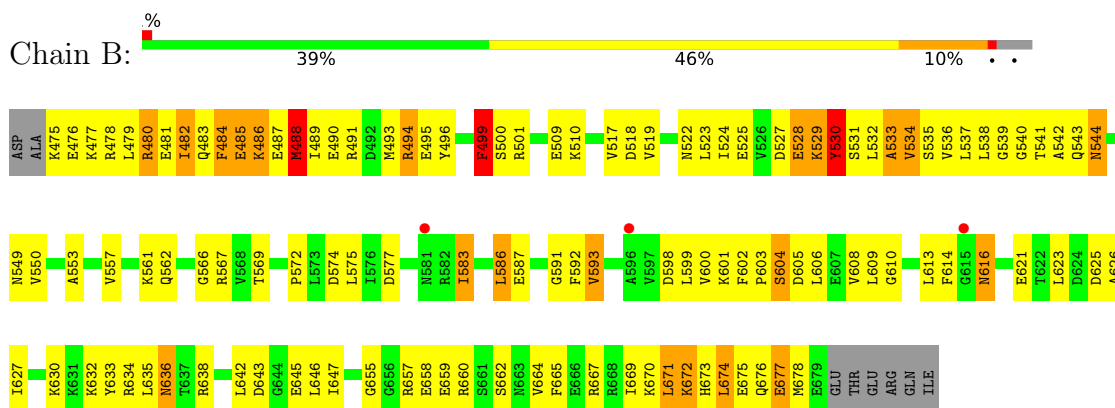
3 Residue-property plots

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.

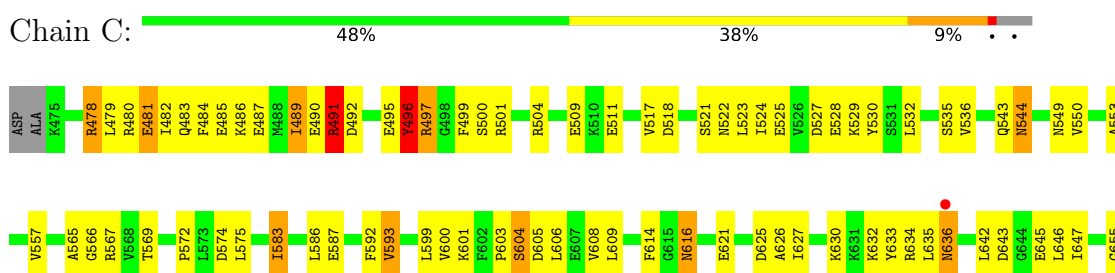
• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN



• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN

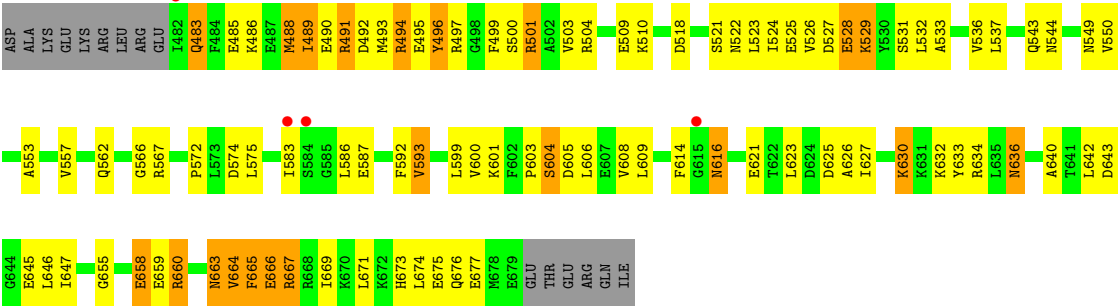


• Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN





● Molecule 1: CHROMOSOME SEGREGATION SMC PROTEIN



4 Data and refinement statistics

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 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-3.00) 94.7 (30.00-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	1098 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.6	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	0.93	EDS
Total number of atoms	6486	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.*

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	0.55	0/1656	1.03	10/2219 (0.5%)
1	B	0.53	0/1656	1.03	9/2219 (0.4%)
1	C	0.51	0/1656	1.02	7/2219 (0.3%)
1	D	0.52	0/1590	0.99	8/2134 (0.4%)
All	All	0.52	0/6558	1.02	34/8791 (0.4%)

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.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	672	LYS	N-CA-C	-8.61	102.68	113.01
1	B	677	GLU	N-CA-C	-7.95	102.31	110.97
1	D	493	MET	N-CA-C	-7.81	102.77	111.28
1	A	662	SER	N-CA-C	-7.46	100.95	111.24
1	A	544	ASN	N-CA-C	-7.13	98.93	110.20
1	A	481	GLU	N-CA-C	-6.92	103.67	111.14
1	D	658	GLU	N-CA-C	6.67	117.44	108.23
1	C	544	ASN	N-CA-C	-6.63	99.72	110.20
1	B	486	LYS	N-CA-C	-6.44	105.28	113.01
1	A	529	LYS	N-CA-C	-6.38	104.02	110.97
1	D	544	ASN	N-CA-C	-6.32	100.21	110.20
1	D	625	ASP	N-CA-C	-6.32	104.31	111.07
1	B	488	MET	N-CA-C	-6.22	105.54	113.01
1	B	544	ASN	N-CA-C	-6.12	100.53	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	491	ARG	N-CA-C	-6.02	104.06	111.40
1	A	485	GLU	N-CA-C	-6.00	104.82	111.36
1	C	625	ASP	N-CA-C	-5.98	104.67	111.07
1	A	509	GLU	N-CA-C	-5.71	104.53	112.30
1	A	594	GLY	N-CA-C	5.56	117.23	111.95
1	A	625	ASP	N-CA-C	-5.53	105.16	111.07
1	C	491	ARG	N-CA-C	-5.50	106.41	113.01
1	D	486	LYS	N-CA-C	-5.48	105.41	111.71
1	C	509	GLU	N-CA-C	-5.45	105.33	112.41
1	D	509	GLU	N-CA-C	-5.39	105.40	112.41
1	C	481	GLU	N-CA-C	-5.31	106.87	113.19
1	B	499	PHE	N-CA-C	5.31	118.38	110.52
1	B	482	ILE	CB-CA-C	-5.21	105.15	111.87
1	C	675	GLU	N-CA-C	-5.19	105.05	111.33
1	B	625	ASP	N-CA-C	-5.11	105.60	111.07
1	D	677	GLU	N-CA-C	-5.11	106.14	112.38
1	A	489	ILE	N-CA-C	-5.10	105.57	110.72
1	C	497	ARG	N-CA-C	5.09	116.68	111.03
1	A	581	ASN	N-CA-C	5.05	117.80	109.72
1	B	509	GLU	N-CA-C	-5.01	105.88	112.94

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	1638	0	1674	105	1
1	B	1638	0	1674	171	0
1	C	1638	0	1674	116	0
1	D	1572	0	1599	112	0
All	All	6486	0	6621	482	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 37.

All (482) 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:D:488:MET:HE3	1:D:488:MET:HA	1.42	1.01
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:A:482:ILE:HD11	1:A:674:LEU:O	1.78	0.83
1:B:494:ARG:HA	1:B:494:ARG:NE	1.93	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:664:VAL:C	1:D:666:GLU:H	1.90	0.79
1:B:673:HIS:HA	1:B:676:GLN:HE21	1.47	0.78
1:D:488:MET:HA	1:D:488:MET:CE	2.13	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
1:D:532:LEU:HA	1:D:663:ASN:HD22	1.50	0.77
1:D:572:PRO:HG2	1:D:575:LEU:HB3	1.66	0.76
1:D:664:VAL:O	1:D:666:GLU:N	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:HG2	1:A:482:ILE:N	2.00	0.75
1:A:636:ASN:H	1:A:636:ASN:HD22	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:H	1:D:636:ASN:HD22	1.35	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:636:ASN:HD22	1:C:636:ASN:H	1.34	0.73
1:C:678:MET:O	1:C:679:GLU:HG3	1.89	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: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:B:603:PRO:O	1:B:605:ASP:N	2.24	0.70
1:D:549:ASN:HA	1:D:574:ASP:OD1	1.91	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:B:549:ASN:HA	1:B:574:ASP:OD1	1.92	0.69
1:D:521:SER:HB2	1:D:664:VAL:HG11	1.75	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:A:621:GLU:HA	1:A:642:LEU:HD12	1.75	0.68
1:D:485:GLU:O	1:D:489:ILE:HG22	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:D:532:LEU:O	1.94	0.67
1:C:659:GLU:HG3	1:C:660:ARG:N	2.10	0.67
1:C:583:ILE:N	1:C:583:ILE:HD12	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:B:534:VAL:HA	1:B:537:LEU:HD13	1.77	0.66
1:C:518:ASP:HB3	1:C:523:LEU:CD1	2.13	0.66
1:B:529:LYS:C	1:B:531:SER:H	2.04	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:A:486:LYS:O	1:A:490:GLU:HG3	1.96	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: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: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:HG23	1:D:489:ILE:O	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:O	1:C:677:GLU:HG2	1.97	0.63
1:D:593:VAL:HG12	1:D:593:VAL:O	1.97	0.63
1:B:482:ILE:CG2	1:B:678:MET:HE2	2.28	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:N	1:B:583:ILE:HD12	2.14	0.62
1:D:550:VAL:HG23	1:D:574:ASP:OD2	1.98	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:HG11	1.81	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:477:LYS:O	1:B:481:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:627:ILE:HG21	1:B:550:VAL:HG11	1.81	0.60
1:B:529:LYS:O	1:B:531:SER:N	2.35	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:B:678:MET:O	1:B:678:MET:HG3	2.00	0.60
1:A:604:SER:C	1:A:606:LEU:H	2.09	0.60
1:D:492:ASP:HB2	1:D:497:ARG:HB2	1.83	0.60
1:D:604:SER:C	1:D:606:LEU:H	2.08	0.60
1:C:604:SER:C	1:C:606:LEU:H	2.07	0.60
1:D:645:GLU:O	1:D:646:LEU:HD12	2.02	0.59
1:C:550:VAL:CG1	1:D:627:ILE:HD13	2.31	0.59
1:C:566:GLY:CA	1:D:658:GLU:HB3	2.29	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:A:659:GLU:O	1:A:660:ARG:O	2.21	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:B:536:VAL:HG23	1:B:537:LEU:HD12	1.84	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:N	1:B:523:LEU:HD12	2.18	0.58
1:A:523:LEU:HD12	1:A:523:LEU:N	2.18	0.58
1:A:564:GLU:HG2	1:B:657:ARG:HG2	1.86	0.58
1:B:499:PHE:CE2	1:B:543:GLN:HB3	2.38	0.58
1:B:527:ASP:C	1:B:529:LYS:N	2.61	0.58
1:D:483:GLN:CD	1:D:483:GLN:H	2.12	0.57
1:D:521:SER:CB	1:D:664:VAL:HG11	2.34	0.57
1:D:587:GLU:CD	1:D:587:GLU:H	2.12	0.57
1:C:658:GLU:HA	1:D:566:GLY:HA2	1.87	0.57
1:D:523:LEU:N	1:D:523:LEU:HD12	2.18	0.57
1:A:500:SER:O	1:A:501:ARG:C	2.47	0.57
1:D:658:GLU:HB2	1:D:659:GLU:OE1	2.03	0.57
1:B:671:LEU:C	1:B:673:HIS:H	2.12	0.57
1:C:593:VAL:O	1:C:593:VAL:HG12	2.04	0.57
1:B:592:PHE:C	1:B:593:VAL:HG23	2.30	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:C:478:ARG:C	1:C:480:ARG:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ILE:HD12	1:A:583:ILE:N	2.21	0.56
1:C:660:ARG:HB2	1:C:660:ARG:CZ	2.34	0.56
1:D:485:GLU:OE1	1:D:674:LEU:HD21	2.05	0.56
1:B:604:SER:C	1:B:606:LEU:H	2.13	0.56
1:B:488:MET:HE3	1:B:488:MET:O	2.06	0.56
1:D:497:ARG:HB3	1:D:667:ARG:HH12	1.71	0.56
1:A:478:ARG:C	1:A:480:ARG:H	2.13	0.56
1:A:493:MET:HE3	1:A:668:ARG:HG2	1.87	0.56
1:D:674:LEU:C	1:D:676:GLN:H	2.14	0.56
1:B:530:TYR:HB3	1:B:533:ALA:CB	2.36	0.55
1:C:484:PHE:C	1:C:486:LYS:N	2.62	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: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:C:587:GLU:H	1:C:587:GLU:CD	2.15	0.55
1:D:532:LEU:HD23	1:D:532:LEU:C	2.31	0.55
1:A:530:TYR:CD1	1:A:530:TYR:N	2.75	0.55
1:C:676:GLN:HG2	1:C:677:GLU:N	2.22	0.55
1:A:658:GLU:O	1:A:659:GLU:C	2.50	0.55
1:B:671:LEU:C	1:B:673:HIS:N	2.61	0.54
1:C:645:GLU:O	1:C:646:LEU:HD12	2.07	0.54
1:C:661:SER:O	1:C:662:SER:C	2.50	0.54
1:C:522:ASN:C	1:C:523:LEU:HD12	2.32	0.54
1:A:550:VAL:HG11	1:B:627:ILE:HD13	1.90	0.54
1:A:587:GLU:H	1:A:587:GLU:CD	2.15	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:A:636:ASN:HD22	1:A:636:ASN:N	1.98	0.53
1:D:491:ARG:HG2	1:D:494:ARG:HH12	1.73	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:C:499:PHE:O	1:C:504:ARG:NH2	2.41	0.53
1:D:491:ARG:HA	1:D:494:ARG:NH1	2.24	0.53
1:C:553:ALA:O	1:C:557:VAL:HG23	2.08	0.53
1:B:485:GLU:C	1:B:487:GLU:N	2.67	0.53
1:A:529:LYS:HB2	1:A:530:TYR:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:647:ILE:N	1:D:647:ILE:HD12	2.24	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:O	1:C:489:ILE:HG23	2.08	0.52
1:B:476:GLU:OE2	1:B:477:LYS:HD3	2.09	0.52
1:B:486:LYS:C	1:B:486:LYS:HD3	2.34	0.52
1:B:670:LYS:HE3	1:B:674:LEU:HD11	1.90	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: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:626:ALA:HB1	1:B:647:ILE:HD13	1.90	0.52
1:C:484:PHE:C	1:C:486:LYS:H	2.17	0.52
1:C:532:LEU:O	1:C:536:VAL:HG13	2.08	0.52
1:B:499:PHE:HB3	1:B:543:GLN:NE2	2.25	0.52
1:B:537:LEU:HD12	1:B:537:LEU:H	1.75	0.52
1:D:491:ARG:HG2	1:D:494:ARG:NH1	2.24	0.52
1:B:482:ILE:HB	1:B:678:MET:HE2	1.92	0.52
1:B:485:GLU:C	1:B:487:GLU:H	2.17	0.52
1:D:495:GLU:HG2	1:D:495:GLU:O	2.10	0.52
1:B:534:VAL:CA	1:B:537:LEU:HD13	2.40	0.51
1:D:525:GLU:OE2	1:D:525:GLU:HA	2.11	0.51
1:D:528:GLU:CG	1:D:669:ILE:HG21	2.36	0.51
1:B:524:ILE:HG12	1:B:602:PHE:CE2	2.45	0.51
1:C:495:GLU:O	1:C:496:TYR:C	2.53	0.51
1:A:482:ILE:CD1	1:A:677:GLU:HB3	2.41	0.51
1:A:530:TYR:HD1	1:A:530:TYR:H	1.58	0.51
1:B:524:ILE:HD11	1:B:613:LEU:HD13	1.92	0.51
1:C:525:GLU:HB3	1:C:601:LYS:HB2	1.91	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:A:626:ALA:HB1	1:A:647:ILE:HD13	1.93	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:A:526:VAL:HG22	1:A:527:ASP:O	2.11	0.51
1:B:587:GLU:CD	1:B:587:GLU:H	2.18	0.51
1:B:669:ILE:C	1:B:671:LEU:H	2.18	0.51
1:C:600:VAL:HG12	1:C:601:LYS:N	2.25	0.51
1:C:647:ILE:HD12	1:C:647:ILE:N	2.25	0.51
1:B:476:GLU:OE2	1:B:477:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:MET:C	1:C:679:GLU:HG3	2.36	0.51
1:D:604:SER:C	1:D:606:LEU:N	2.68	0.51
1:B:525:GLU:HB3	1:B:601:LYS:HB2	1.92	0.51
1:D:583:ILE:HD12	1:D:583:ILE:N	2.25	0.50
1:C:481:GLU:HA	1:C:484:PHE:HB3	1.93	0.50
1:C:496:TYR:N	1:C:496:TYR:CD1	2.79	0.50
1:D:636:ASN:HD22	1:D:636:ASN:N	2.01	0.50
1:B:482:ILE:HG22	1:B:678:MET:HE2	1.92	0.50
1:A:492:ASP:OD1	1:A:497:ARG:HD2	2.11	0.50
1:B:530:TYR:O	1:B:531:SER:C	2.55	0.50
1:B:599:LEU:N	1:B:599:LEU:HD12	2.27	0.50
1:C:550:VAL:O	1:C:553:ALA:HB3	2.12	0.50
1:A:493:MET:CE	1:A:668:ARG:HG2	2.42	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:B:673:HIS:O	1:B:677:GLU:N	2.38	0.49
1:C:491:ARG:HG2	1:C:491:ARG:HH21	1.77	0.49
1:C:480:ARG:C	1:C:482:ILE:H	2.19	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:B:480:ARG:HA	1:B:480:ARG:NE	2.26	0.49
1:B:647:ILE:N	1:B:647:ILE:HD12	2.27	0.49
1:D:491:ARG:HG2	1:D:494:ARG:CZ	2.42	0.49
1:A:492:ASP:CB	1:A:667:ARG:NH2	2.76	0.49
1:B:539:GLY:C	1:B:541:THR:H	2.20	0.49
1:B:623:LEU:HD12	1:B:623:LEU:O	2.11	0.49
1:C:659:GLU:C	1:C:659:GLU:OE1	2.56	0.49
1:D:673:HIS:O	1:D:676:GLN:HB3	2.12	0.49
1:A:492:ASP:HB3	1:A:667:ARG:NH2	2.28	0.49
1:C:499:PHE:CD1	1:C:499:PHE:N	2.80	0.49
1:C:614:PHE:C	1:C:616:ASN:H	2.21	0.49
1:A:604:SER:C	1:A:606:LEU:N	2.69	0.49
1:B:486:LYS:CB	1:B:678:MET:HE3	2.41	0.49
1:C:604:SER:C	1:C:606:LEU:N	2.67	0.49
1:D:664:VAL:C	1:D:666:GLU:N	2.57	0.49
1:A:593:VAL:O	1:A:593:VAL:CG1	2.61	0.48
1:B:621:GLU:HA	1:B:642:LEU:CD1	2.40	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:530:TYR:CB	1:B:599:LEU:HD23	2.43	0.48
1:D:500:SER:O	1:D:501:ARG:C	2.57	0.48

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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	0.48
1:A:666:GLU:HG3	1:A:667:ARG:N	2.28	0.48
1:B:499:PHE:CD2	1:B:543:GLN:NE2	2.81	0.48
1:A:633:TYR:O	1:A:634:ARG:C	2.57	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:B:669:ILE:C	1:B:671:LEU:N	2.72	0.48
1:A:478:ARG:C	1:A:480:ARG:N	2.71	0.47
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:636:ASN:HD22	1:C:636:ASN:N	1.99	0.47
1:B:532:LEU:O	1:B:532:LEU:HD23	2.13	0.47
1:B:604:SER:C	1:B:606:LEU:N	2.72	0.47
1:A:592:PHE:C	1:A:593:VAL:HG23	2.40	0.47
1:A:599:LEU:N	1:A:599:LEU:HD12	2.29	0.47
1:A:661:SER:O	1:A:662:SER:C	2.57	0.47
1:B:522:ASN:C	1:B:523:LEU:HD12	2.40	0.47
1:B:534:VAL:O	1:B:537:LEU:N	2.47	0.47
1:D:537:LEU:HD21	1:D:640:ALA:HB2	1.96	0.47
1:D:592:PHE:C	1:D:593:VAL:HG23	2.39	0.47
1:D:599:LEU:N	1:D:599:LEU:HD12	2.29	0.47
1:D:636:ASN:H	1:D:636:ASN:ND2	2.09	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:O	1:B:593:VAL:CG1	2.62	0.47
1:D:522:ASN:C	1:D:523:LEU:HD12	2.40	0.47
1:A:616:ASN:HD22	1:A:616:ASN:HA	1.51	0.47
1:C:499:PHE:HD1	1:C:499:PHE:H	1.61	0.47
1:C:633:TYR:O	1:C:634:ARG:C	2.57	0.47
1:D:499:PHE:HD2	1:D:543:GLN:HE21	1.62	0.47
1:A:636:ASN:H	1:A:636:ASN:ND2	2.08	0.47
1:C:592:PHE:C	1:C:593:VAL:HG23	2.40	0.47
1:B:489:ILE:CG2	1:B:671:LEU:HD21	2.46	0.46
1:B:527:ASP:C	1:B:529:LYS:H	2.22	0.46
1:B:608:VAL:O	1:B:609:LEU:C	2.59	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:A:491:ARG:O	1:A:495:GLU:HB2	2.16	0.46
1:C:480:ARG:C	1:C:482:ILE:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:608:VAL:HG23	1:D:609:LEU:N	2.30	0.46
1:A:522:ASN:C	1:A:523:LEU:HD12	2.41	0.46
1:A:524:ILE:HG23	1:A:600:VAL:CG1	2.42	0.46
1:B:534:VAL:O	1:B:535:SER:C	2.58	0.46
1:C:484:PHE:CD1	1:C:485:GLU:N	2.84	0.46
1:C:636:ASN:H	1:C:636:ASN:ND2	2.08	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:B:636:ASN:HD22	1:B:636:ASN:N	1.99	0.46
1:C:529:LYS:HD2	1:C:530:TYR:CE1	2.50	0.46
1:B:482:ILE:CB	1:B:678:MET:HE2	2.46	0.45
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:B:542:ALA:HB1	1:B:664:VAL:HG11	1.98	0.45
1:D:608:VAL:HG23	1:D:609:LEU:H	1.80	0.45
1:D:623:LEU:HD12	1:D:623:LEU:O	2.16	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:C:659:GLU:HG3	1:C:660:ARG:H	1.81	0.45
1:A:491:ARG:NH2	1:A:492:ASP:OD1	2.50	0.45
1:B:553:ALA:O	1:B:557:VAL:HG23	2.17	0.45
1:B:608:VAL:HG23	1:B:609:LEU:H	1.81	0.45
1:C:599:LEU:HD12	1:C:599:LEU:N	2.32	0.45
1:D:553:ALA:O	1:D:557:VAL:HG23	2.17	0.45
1:D:664:VAL:HG12	1:D:665:PHE:N	2.31	0.45
1:A:621:GLU:HA	1:A:642:LEU:CD1	2.45	0.45
1:B:592:PHE:C	1:B:593:VAL:CG2	2.89	0.45
1:C:600:VAL:CG1	1:C:601:LYS:N	2.79	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:C:518:ASP:CB	1:C:523:LEU:HD11	2.16	0.45
1:B:536:VAL:HG22	1:B:537:LEU:HD12	1.98	0.45
1:B:539:GLY:C	1:B:541:THR:N	2.75	0.45
1:C:677:GLU:O	1:C:677:GLU:CG	2.65	0.45
1:A:614:PHE:C	1:A:616:ASN:H	2.25	0.44
1:B:491:ARG:O	1:B:495:GLU:HB3	2.17	0.44
1:B:524:ILE:HG12	1:B:602:PHE:CZ	2.52	0.44
1:B:636:ASN:H	1:B:636:ASN:ND2	2.07	0.44
1:B:485:GLU:HG3	1:B:674:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:ASP:C	1:B:599:LEU:HD12	2.43	0.44
1:A:553:ALA:O	1:A:557:VAL:HG23	2.17	0.44
1:A:608:VAL:HG23	1:A:609:LEU:N	2.32	0.44
1:A:521:SER:CB	1:A:664:VAL:HG13	2.40	0.44
1:B:531:SER:OG	1:B:669:ILE:HG13	2.17	0.44
1:C:523:LEU:CD1	1:C:523:LEU:N	2.79	0.44
1:A:670:LYS:HA	1:A:673:HIS:HB2	2.00	0.44
1:C:665:PHE:O	1:C:669:ILE:HG12	2.18	0.44
1:B:486:LYS:HB3	1:B:678:MET:HE3	2.00	0.44
1:C:483:GLN:HE21	1:C:483:GLN:HA	1.82	0.44
1:C:669:ILE:O	1:C:670:LYS:C	2.60	0.44
1:A:532:LEU:HD23	1:A:532:LEU:C	2.42	0.44
1:B:614:PHE:C	1:B:616:ASN:H	2.26	0.44
1:D:485:GLU:HG3	1:D:674:LEU:CD1	2.47	0.44
1:D:504:ARG:HH21	1:D:504:ARG:HG3	1.83	0.44
1:D:608:VAL:O	1:D:609:LEU:C	2.61	0.44
1:B:487:GLU:C	1:B:489:ILE:N	2.73	0.44
1:B:660:ARG:C	1:B:662:SER:H	2.25	0.44
1:C:661:SER:O	1:C:663:ASN:ND2	2.51	0.44
1:A:530:TYR:O	1:A:533:ALA:HB3	2.17	0.44
1:B:530:TYR:HB3	1:B:533:ALA:HB2	1.99	0.44
1:D:659:GLU:OE1	1:D:659:GLU:N	2.46	0.44
1:D:489:ILE:CD1	1:D:667:ARG:HD2	2.45	0.43
1:B:633:TYR:O	1:B:634:ARG:C	2.60	0.43
1:D:621:GLU:HA	1:D:642:LEU:CD1	2.48	0.43
1:D:537:LEU:CD2	1:D:640:ALA:HB2	2.48	0.43
1:B:537:LEU:HD12	1:B:537:LEU:N	2.32	0.43
1:D:633:TYR:O	1:D:634:ARG:C	2.61	0.43
1:B:608:VAL:C	1:B:610:GLY:N	2.76	0.43
1:C:525:GLU:OE2	1:C:525:GLU:HA	2.18	0.43
1:C:663:ASN:O	1:C:664:VAL:O	2.37	0.43
1:D:501:ARG:O	1:D:504:ARG:HB2	2.18	0.43
1:D:600:VAL:CG1	1:D:601:LYS:N	2.81	0.43
1:A:511:GLU:H	1:A:511:GLU:CD	2.27	0.43
1:A:663:ASN:O	1:A:666:GLU:HG2	2.19	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:633:TYR:O	1:A:635:LEU:HG	2.19	0.43
1:B:484:PHE:N	1:B:484:PHE:CD1	2.86	0.43
1:B:493:MET:C	1:B:495:GLU:H	2.26	0.43
1:B:536:VAL:HG23	1:B:537:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:VAL:CG1	1:A:601:LYS:N	2.82	0.43
1:B:483:GLN:C	1:B:485:GLU:H	2.26	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:658:GLU:OE2	1:B:662:SER:OG	2.31	0.43
1:C:662:SER:C	1:C:663:ASN:HD22	2.26	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:N	1:B:636:ASN:ND2	2.67	0.42
1:A:634:ARG:HG2	1:A:634:ARG:HH21	1.84	0.42
1:B:527:ASP:O	1:B:528:GLU:C	2.62	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:B:493:MET:HG2	1:B:667:ARG:HD2	2.02	0.42
1:C:544:ASN:ND2	1:C:569:THR:HB	2.35	0.42
1:C:633:TYR:O	1:C:635:LEU:HG	2.19	0.42
1:B:600:VAL:CG1	1:B:601:LYS:N	2.81	0.42
1:D:527:ASP:O	1:D:528:GLU:C	2.63	0.42
1:B:499:PHE:CD2	1:B:543:GLN:CB	3.00	0.42
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:C:511:GLU:H	1:C:511:GLU:CD	2.27	0.42
1:D:529:LYS:C	1:D:531:SER:H	2.28	0.42
1:D:634:ARG:HH21	1:D:634:ARG:HG2	1.84	0.42
1:A:482:ILE:CG2	1:A:483:GLN:N	2.83	0.42
1:A:655:GLY:O	1:B:567:ARG:HA	2.20	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:636:ASN:N	1:C:636:ASN:ND2	2.67	0.41
1:B:484:PHE:N	1:B:484:PHE:HD1	2.17	0.41
1:B:550:VAL:O	1:B:553:ALA:HB3	2.19	0.41
1:C:664:VAL:O	1:C:665:PHE:CB	2.68	0.41
1:C:671:LEU:HA	1:C:671:LEU:HD23	1.86	0.41
1:D:494:ARG:C	1:D:496:TYR:H	2.27	0.41
1:B:616:ASN:HD22	1:B:616:ASN:HA	1.50	0.41
1:B:634:ARG:HG2	1:B:634:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:C	1:A:482:ILE:HG22	2.45	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:636:ASN:N	1:D:636:ASN:ND2	2.68	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:D:495:GLU:O	1:D:496:TYR:C	2.62	0.41
1:A:562:GLN:HA	1:A:562:GLN:NE2	2.36	0.41
1:C:478:ARG:C	1:C:480:ARG:N	2.79	0.41
1:C:603:PRO:HG2	1:C:606:LEU:HD12	2.02	0.41
1:D:491:ARG:HA	1:D:494:ARG:CZ	2.51	0.41
1:A:630:LYS:O	1:A:630:LYS:HG3	2.21	0.41
1:B:499:PHE:CB	1:B:543:GLN:NE2	2.84	0.41
1:C:487:GLU:C	1:C:489:ILE:H	2.28	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:C:672:LYS:HA	1:C:672:LYS:HD3	1.65	0.41
1:D:630:LYS:O	1:D:630:LYS:HG3	2.21	0.41
1:A:557:VAL:O	1:A:561:LYS:HB2	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
1:A:484:PHE:CE2	1:A:488:MET:HE3	2.56	0.40
1:A:592:PHE:O	1:A:593:VAL:CG2	2.69	0.40
1:B:500:SER:O	1:B:501:ARG:C	2.64	0.40
1:C:500:SER:H	1:C:543:GLN:HE22	1.69	0.40
1:C:527:ASP:HB3	1:C:530:TYR:HD1	1.85	0.40
1:A:586:LEU:HD23	1:A:586:LEU:HA	1.86	0.40
1:A:608:VAL:O	1:A:609:LEU:C	2.62	0.40
1:B:562:GLN:NE2	1:B:562:GLN:HA	2.36	0.40
1:C:670:LYS:HZ1	1:C:674:LEU:HD21	1.87	0.40
1:A:525:GLU:HA	1:A:525:GLU:OE2	2.21	0.40
1:B:633:TYR:O	1:B:635:LEU:HG	2.20	0.40
1:D:659:GLU:O	1:D:660:ARG:CB	2.70	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 ⓘ

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	203/213 (95%)	169 (83%)	27 (13%)	7 (3%)	3	17
1	B	203/213 (95%)	160 (79%)	29 (14%)	14 (7%)	1	5
1	C	203/213 (95%)	162 (80%)	31 (15%)	10 (5%)	1	10
1	D	196/213 (92%)	155 (79%)	29 (15%)	12 (6%)	1	7
All	All	805/852 (94%)	646 (80%)	116 (14%)	43 (5%)	1	9

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	164 (93%)	13 (7%)	13	42
1	B	177/184 (96%)	165 (93%)	12 (7%)	14	45
1	C	177/184 (96%)	159 (90%)	18 (10%)	7	29
1	D	170/184 (92%)	159 (94%)	11 (6%)	15	47
All	All	701/736 (95%)	647 (92%)	54 (8%)	12	40

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

Mol	Chain	Res	Type
1	A	481	GLU
1	A	489	ILE
1	A	491	ARG
1	A	536	VAL
1	A	583	ILE
1	A	586	LEU
1	A	616	ASN
1	A	630	LYS
1	A	636	ASN
1	A	643	ASP
1	A	664	VAL
1	A	672	LYS
1	A	673	HIS
1	B	480	ARG
1	B	488	MET
1	B	494	ARG
1	B	499	PHE
1	B	530	TYR
1	B	583	ILE
1	B	586	LEU
1	B	616	ASN
1	B	630	LYS
1	B	636	ASN
1	B	643	ASP
1	B	671	LEU
1	C	479	LEU
1	C	491	ARG
1	C	496	TYR
1	C	497	ARG
1	C	528	GLU
1	C	583	ILE
1	C	586	LEU
1	C	616	ASN
1	C	630	LYS
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

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Mol	Chain	Res	Type
1	D	483	GLN
1	D	488	MET
1	D	494	ARG
1	D	501	ARG
1	D	528	GLU
1	D	586	LEU
1	D	616	ASN
1	D	630	LYS
1	D	636	ASN
1	D	643	ASP
1	D	667	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) 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
1	B	544	ASN
1	B	562	GLN
1	B	581	ASN
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	581	ASN
1	D	636	ASN

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Mol	Chain	Res	Type
1	D	663	ASN
1	D	673	HIS
1	D	676	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	205/213 (96%)	-0.05	2 (0%) 79 59	50, 77, 120, 137	0
1	B	205/213 (96%)	0.04	3 (1%) 72 49	53, 81, 116, 133	0
1	C	205/213 (96%)	-0.12	1 (0%) 87 72	50, 81, 117, 137	0
1	D	198/213 (92%)	-0.10	4 (2%) 65 41	49, 81, 114, 135	0
All	All	813/852 (95%)	-0.06	10 (1%) 76 55	49, 80, 117, 137	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	583	ILE	3.3
1	B	581	ASN	3.0
1	B	615	GLY	2.8
1	D	482	ILE	2.6
1	D	584	SER	2.6
1	B	596	ALA	2.5
1	A	583	ILE	2.4
1	D	615	GLY	2.2
1	C	636	ASN	2.2
1	A	635	LEU	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.