



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:57 PM UTC

PDB ID : 4RSJ / pdb_00004rsj
Title : Pyrococcus furiosus Smc hinge domain with an extended coiled coil
Authors : Soh, Y.M.; Shin, H.C.; Oh, B.H.
Deposited on : 2014-11-08
Resolution : 3.50 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

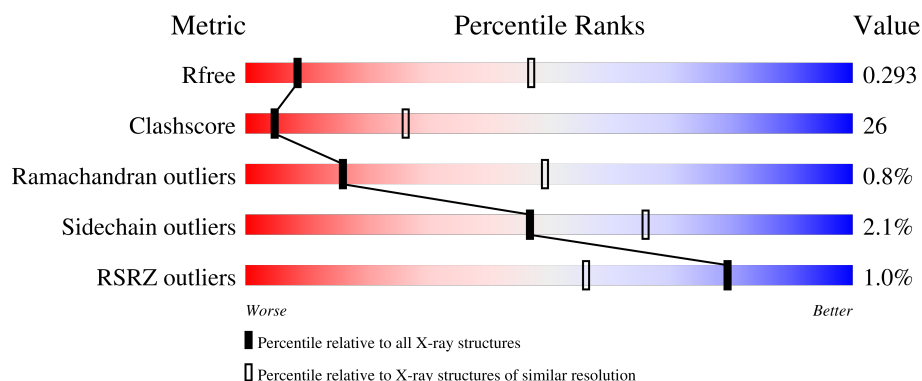
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	276	59%37%..
1	B	276	2% 53%42%..
1	C	276	% 61%34%..
1	D	276	% 57%36%. 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7715 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.

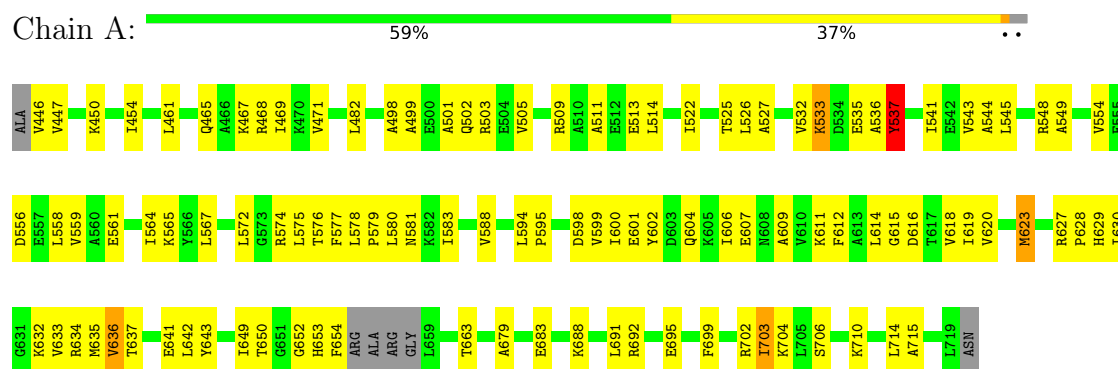
- Molecule 1 is a protein called Chromosome partition protein Smc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	30	0	0
			1954	1217	346	389	2			
1	B	266	Total	C	N	O	S	36	0	0
			1994	1246	360	386	2			
1	C	265	Total	C	N	O	S	32	0	0
			1908	1187	336	383	2			
1	D	263	Total	C	N	O	S	36	0	0
			1859	1155	340	362	2			

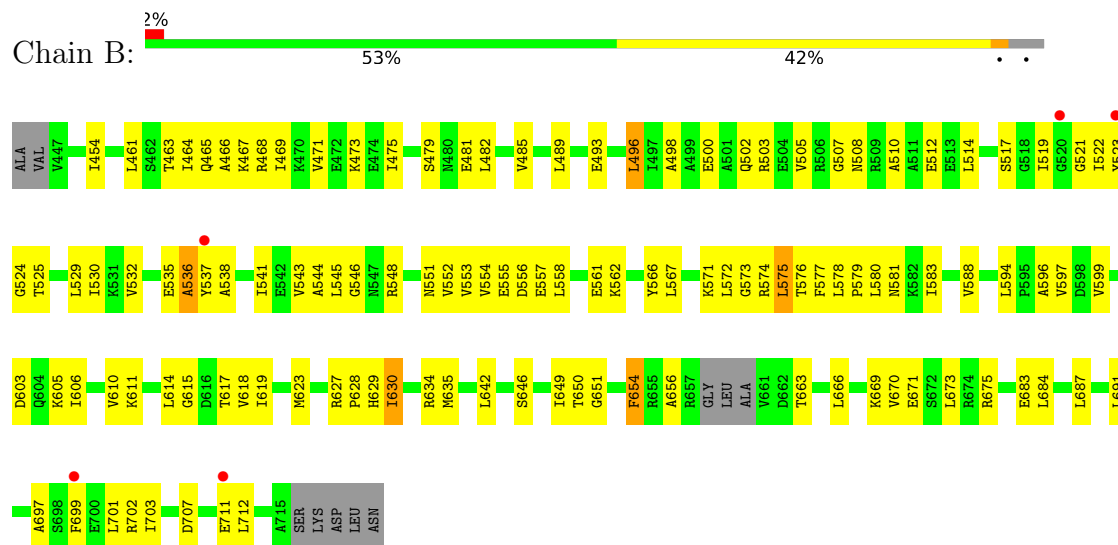
3 Residue-property plots [i](#)

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: Chromosome partition protein Smc

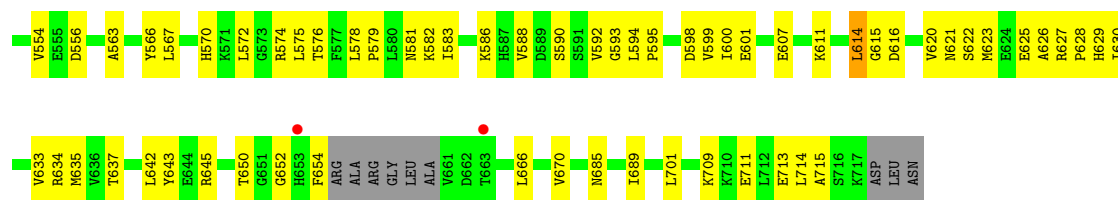


• Molecule 1: Chromosome partition protein Smc

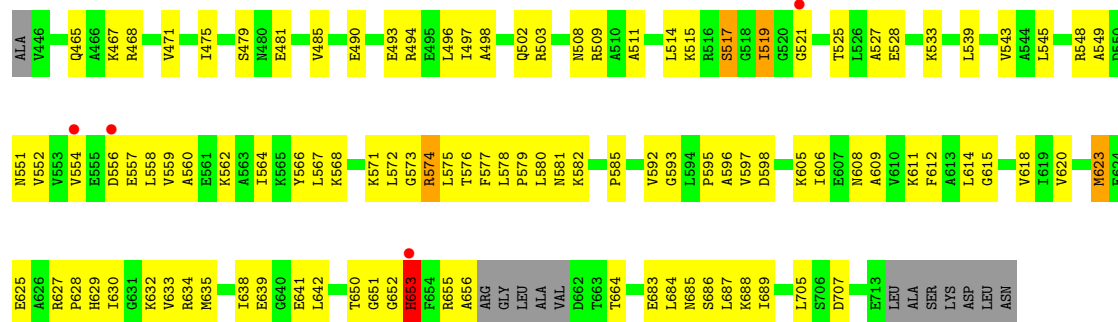


• Molecule 1: Chromosome partition protein Smc





● Molecule 1: Chromosome partition protein Smc



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.92Å 116.88Å 145.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.50) 86.6 (50.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.284 0.251 , 0.293	Depositor DCC
R_{free} test set	1278 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7715	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7565e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.30	0/1969	0.86	3/2661 (0.1%)
1	B	0.30	0/2009	0.83	2/2705 (0.1%)
1	C	0.29	0/1922	0.86	1/2598 (0.0%)
1	D	0.63	2/1873 (0.1%)	0.99	4/2535 (0.2%)
All	All	0.40	2/7773 (0.0%)	0.88	10/10499 (0.1%)

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	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	653	HIS	C-N	19.47	1.59	1.33
1	D	517	SER	C-N	-13.02	1.14	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	653	HIS	O-C-N	-20.50	95.33	122.59
1	D	653	HIS	CA-C-N	10.69	140.28	122.33
1	D	653	HIS	C-N-CA	10.69	140.28	122.33
1	D	517	SER	O-C-N	-9.62	110.96	123.28
1	A	714	LEU	N-CA-C	-6.79	105.03	113.38
1	C	459	GLY	N-CA-C	-5.87	107.05	114.16
1	B	522	ILE	N-CA-C	5.76	116.40	107.99
1	B	630	ILE	N-CA-C	-5.50	102.10	109.30
1	A	559	VAL	N-CA-C	-5.19	104.61	111.09
1	A	537	TYR	N-CA-C	-5.15	105.89	113.61

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	517	SER	Mainchain
1	D	653	HIS	Peptide,Mainchain

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	1954	0	1861	108	0
1	B	1994	0	1990	117	0
1	C	1908	0	1818	87	0
1	D	1859	0	1746	93	0
All	All	7715	0	7415	381	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 26.

All (381) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HG2	1:A:601:GLU:HG3	1.23	1.19
1:C:533:LYS:HE3	1:C:601:GLU:CG	1.78	1.12
1:A:699:PHE:HZ	1:B:702:ARG:HD2	1.19	1.07
1:A:465:GLN:HG2	1:A:468:ARG:HH11	1.19	1.05
1:C:500:GLU:HB3	1:C:509:ARG:HH21	1.22	1.04
1:A:699:PHE:CZ	1:B:702:ARG:HD2	1.96	1.00
1:C:627:ARG:HA	1:C:630:ILE:HG13	1.38	1.00
1:C:533:LYS:HE3	1:C:601:GLU:HG2	1.01	0.99
1:C:533:LYS:CE	1:C:601:GLU:HG2	1.94	0.97
1:C:578:LEU:HB3	1:C:583:ILE:HD11	1.45	0.96
1:A:578:LEU:HB3	1:A:583:ILE:HD11	1.46	0.96
1:A:533:LYS:HG2	1:A:601:GLU:CG	1.96	0.94
1:C:447:VAL:HG22	1:C:715:ALA:HB1	1.49	0.93
1:B:537:TYR:OH	1:B:594:LEU:HD11	1.71	0.91
1:B:537:TYR:CZ	1:B:594:LEU:HD11	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:TYR:HB2	1:B:553:VAL:CG2	2.05	0.86
1:A:446:VAL:HG12	1:A:447:VAL:H	1.41	0.86
1:A:533:LYS:CG	1:A:601:GLU:HG3	2.04	0.85
1:B:464:ILE:HD12	1:B:701:LEU:HD12	1.61	0.82
1:A:653:HIS:O	1:A:654:PHE:HB2	1.79	0.82
1:A:541:ILE:HD11	1:A:599:VAL:HG23	1.64	0.78
1:B:523:TYR:HB2	1:B:553:VAL:HG23	1.64	0.78
1:A:623:MET:HE1	1:A:630:ILE:HD11	1.66	0.76
1:D:655:ARG:O	1:D:656:ALA:HB2	1.86	0.75
1:B:532:VAL:HG13	1:B:541:ILE:HD12	1.67	0.75
1:A:580:LEU:HD11	1:A:606:ILE:HG22	1.69	0.74
1:D:519:ILE:HD12	1:D:562:LYS:NZ	2.01	0.74
1:A:699:PHE:HZ	1:B:702:ARG:CD	2.00	0.74
1:C:627:ARG:CA	1:C:630:ILE:HG13	2.17	0.74
1:B:529:LEU:HD23	1:B:606:ILE:HD13	1.70	0.74
1:C:621:ASN:HB2	1:C:625:GLU:OE1	1.87	0.74
1:C:533:LYS:CE	1:C:601:GLU:CG	2.62	0.73
1:B:523:TYR:HE2	1:B:580:LEU:HD11	1.53	0.72
1:B:521:GLY:O	1:B:554:VAL:HA	1.88	0.72
1:A:447:VAL:HG22	1:A:715:ALA:HB1	1.72	0.70
1:B:523:TYR:O	1:B:529:LEU:HD11	1.91	0.69
1:A:465:GLN:HG2	1:A:468:ARG:NH1	2.02	0.69
1:A:635:MET:O	1:A:642:LEU:HD12	1.92	0.69
1:C:533:LYS:HG2	1:C:601:GLU:HG3	1.75	0.69
1:C:607:GLU:HG2	1:C:611:LYS:HE3	1.75	0.69
1:A:652:GLY:HA3	1:B:574:ARG:HA	1.75	0.69
1:C:578:LEU:HB3	1:C:583:ILE:CD1	2.20	0.69
1:B:579:PRO:O	1:B:583:ILE:HG13	1.92	0.68
1:D:684:LEU:HB3	1:D:688:LYS:HE3	1.75	0.68
1:D:465:GLN:HA	1:D:468:ARG:HG3	1.74	0.68
1:B:537:TYR:OH	1:B:594:LEU:CD1	2.41	0.67
1:C:533:LYS:HD2	1:C:600:ILE:O	1.94	0.67
1:B:629:HIS:HB2	1:B:635:MET:HE1	1.77	0.67
1:B:699:PHE:O	1:B:703:ILE:HG13	1.94	0.67
1:D:519:ILE:HD12	1:D:562:LYS:HZ2	1.58	0.66
1:B:523:TYR:CE2	1:B:580:LEU:HD11	2.31	0.66
1:C:533:LYS:CG	1:C:601:GLU:HG3	2.26	0.66
1:A:532:VAL:HG22	1:A:541:ILE:HD12	1.78	0.65
1:B:544:ALA:HB1	1:B:617:THR:HG21	1.77	0.65
1:C:620:VAL:HG11	1:C:635:MET:HE2	1.77	0.65
1:C:541:ILE:HD11	1:C:599:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ILE:HG22	1:B:473:LYS:HE3	1.78	0.65
1:A:633:VAL:HB	1:A:635:MET:HE3	1.76	0.65
1:A:578:LEU:HB3	1:A:583:ILE:CD1	2.25	0.64
1:A:575:LEU:HD23	1:A:576:THR:N	2.11	0.64
1:C:532:VAL:HG22	1:C:541:ILE:HD12	1.79	0.64
1:C:628:PRO:HB2	1:C:629:HIS:CE1	2.32	0.64
1:C:491:SER:O	1:C:495:GLU:HG3	1.97	0.64
1:A:627:ARG:HA	1:A:630:ILE:HG13	1.80	0.64
1:B:523:TYR:HB2	1:B:553:VAL:HG21	1.80	0.64
1:D:559:VAL:HA	1:D:562:LYS:HD3	1.78	0.64
1:D:627:ARG:CG	1:D:628:PRO:HD3	2.28	0.63
1:C:588:VAL:HG12	1:C:590:SER:H	1.63	0.63
1:C:522:ILE:HA	1:C:554:VAL:HG12	1.80	0.63
1:C:627:ARG:HA	1:C:630:ILE:CG1	2.21	0.63
1:C:626:ALA:O	1:C:630:ILE:HG13	1.98	0.63
1:A:620:VAL:HG23	1:A:637:THR:HG22	1.80	0.62
1:B:475:ILE:CD1	1:B:691:LEU:HD12	2.29	0.62
1:B:514:LEU:HD23	1:B:514:LEU:O	1.98	0.62
1:A:574:ARG:CZ	1:B:543:VAL:HG22	2.30	0.61
1:D:595:PRO:HB2	1:D:598:ASP:OD2	2.00	0.61
1:D:627:ARG:HG3	1:D:628:PRO:HD3	1.82	0.61
1:C:594:LEU:HD12	1:C:595:PRO:HD2	1.83	0.60
1:C:533:LYS:O	1:C:534:ASP:HB2	2.01	0.60
1:D:629:HIS:HB2	1:D:635:MET:HE1	1.82	0.60
1:A:574:ARG:NH1	1:B:543:VAL:HA	2.17	0.60
1:B:523:TYR:HE2	1:B:580:LEU:CD1	2.13	0.60
1:A:600:ILE:HG22	1:A:602:TYR:HD2	1.67	0.60
1:C:626:ALA:O	1:C:630:ILE:CG1	2.50	0.60
1:B:464:ILE:O	1:B:468:ARG:HG3	2.02	0.60
1:C:652:GLY:O	1:D:574:ARG:NH1	2.35	0.59
1:B:594:LEU:HD23	1:B:594:LEU:H	1.67	0.59
1:C:579:PRO:O	1:C:583:ILE:HG13	2.03	0.59
1:D:581:ASN:ND2	1:D:582:LYS:HG3	2.17	0.59
1:D:639:GLU:O	1:D:653:HIS:CE1	2.56	0.59
1:D:503:ARG:HH12	1:D:664:THR:HG22	1.67	0.59
1:A:465:GLN:O	1:A:469:ILE:HG13	2.02	0.58
1:C:467:LYS:O	1:C:471:VAL:HG23	2.03	0.58
1:C:627:ARG:HG3	1:C:628:PRO:HD3	1.85	0.58
1:D:467:LYS:O	1:D:471:VAL:HG23	2.03	0.58
1:D:539:LEU:HD11	1:D:653:HIS:CD2	2.39	0.58
1:B:519:ILE:HD13	1:B:562:LYS:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:ARG:NH2	1:D:642:LEU:HD21	2.18	0.58
1:C:578:LEU:CB	1:C:583:ILE:HD11	2.29	0.58
1:B:654:PHE:HD1	1:B:654:PHE:H	1.50	0.58
1:D:551:ASN:HA	1:D:576:THR:HG23	1.86	0.57
1:D:551:ASN:HD22	1:D:578:LEU:HD21	1.69	0.57
1:C:450:LYS:HE2	1:C:711:GLU:HB2	1.86	0.57
1:C:502:GLN:O	1:C:506:ARG:HD3	2.04	0.57
1:B:500:GLU:HG2	1:B:503:ARG:HH21	1.69	0.57
1:C:623:MET:HG2	1:C:643:TYR:OH	2.04	0.57
1:A:642:LEU:HB3	1:A:650:THR:HG22	1.86	0.57
1:C:533:LYS:HG2	1:C:601:GLU:CG	2.34	0.57
1:D:521:GLY:HA3	1:D:559:VAL:HG11	1.85	0.57
1:B:629:HIS:O	1:B:630:ILE:C	2.45	0.57
1:C:500:GLU:HB3	1:C:509:ARG:NH2	2.06	0.57
1:C:501:ALA:O	1:C:505:VAL:HG23	2.04	0.56
1:D:503:ARG:HH22	1:D:664:THR:HG22	1.69	0.56
1:A:499:ALA:O	1:A:503:ARG:HG3	2.04	0.56
1:A:543:VAL:HG22	1:B:574:ARG:HH11	1.70	0.56
1:A:588:VAL:HG22	1:A:616:ASP:HA	1.87	0.56
1:B:496:LEU:HD12	1:B:670:VAL:HG21	1.86	0.56
1:A:607:GLU:HG2	1:A:611:LYS:HE3	1.87	0.56
1:D:559:VAL:O	1:D:562:LYS:HB2	2.06	0.56
1:A:635:MET:HB2	1:A:643:TYR:HB2	1.86	0.56
1:A:642:LEU:HB3	1:A:650:THR:CG2	2.35	0.56
1:A:653:HIS:HB2	1:B:573:GLY:H	1.70	0.56
1:B:618:VAL:HG12	1:B:619:ILE:N	2.21	0.56
1:C:545:LEU:CD2	1:C:614:LEU:HD21	2.36	0.56
1:D:574:ARG:NH1	1:D:574:ARG:HB3	2.20	0.56
1:A:509:ARG:O	1:A:513:GLU:HG2	2.06	0.56
1:A:618:VAL:O	1:A:636:VAL:HG12	2.06	0.55
1:B:535:GLU:O	1:B:536:ALA:HB2	2.06	0.55
1:C:525:THR:HA	1:C:551:ASN:O	2.07	0.55
1:A:595:PRO:HB2	1:A:598:ASP:OD1	2.06	0.55
1:A:623:MET:HG2	1:A:643:TYR:OH	2.06	0.55
1:A:636:VAL:HG13	1:A:636:VAL:O	2.06	0.55
1:C:595:PRO:HB2	1:C:598:ASP:OD2	2.06	0.55
1:B:517:SER:HB3	1:B:566:TYR:CE2	2.42	0.55
1:A:525:THR:HG22	1:A:527:ALA:H	1.71	0.55
1:A:594:LEU:HD12	1:A:595:PRO:HD2	1.89	0.55
1:A:561:GLU:HB3	1:A:565:LYS:HE3	1.89	0.54
1:B:467:LYS:O	1:B:471:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:GLY:HA2	1:B:555:GLU:HB2	1.90	0.54
1:D:560:ALA:O	1:D:564:ILE:HG13	2.07	0.54
1:B:454:ILE:HD12	1:B:712:LEU:HD11	1.89	0.54
1:B:503:ARG:CZ	1:B:663:THR:HG21	2.37	0.54
1:A:450:LYS:O	1:A:454:ILE:HG13	2.08	0.54
1:A:691:LEU:O	1:A:695:GLU:HG3	2.08	0.53
1:B:578:LEU:HB3	1:B:583:ILE:CD1	2.38	0.53
1:B:654:PHE:CE2	1:B:656:ALA:HB2	2.42	0.53
1:D:511:ALA:O	1:D:515:LYS:HG3	2.07	0.53
1:A:467:LYS:O	1:A:471:VAL:HG23	2.08	0.53
1:A:482:LEU:C	1:A:482:LEU:HD23	2.34	0.53
1:A:545:LEU:HB3	1:A:549:ALA:HB2	1.91	0.53
1:A:653:HIS:CG	1:B:571:LYS:HA	2.42	0.53
1:D:606:ILE:O	1:D:606:ILE:HG13	2.08	0.53
1:D:539:LEU:O	1:D:543:VAL:HG23	2.08	0.53
1:C:579:PRO:HB2	1:C:582:LYS:HB2	1.91	0.53
1:C:627:ARG:CG	1:C:628:PRO:HD3	2.39	0.53
1:B:503:ARG:HB3	1:B:508:ASN:HB2	1.91	0.53
1:B:634:ARG:NH2	1:B:642:LEU:HD21	2.24	0.53
1:D:554:VAL:O	1:D:579:PRO:HA	2.09	0.53
1:B:603:ASP:OD2	1:B:605:LYS:HB2	2.09	0.53
1:B:537:TYR:O	1:B:538:ALA:C	2.52	0.53
1:A:702:ARG:HD3	1:B:703:ILE:CD1	2.38	0.52
1:B:557:GLU:O	1:B:561:GLU:HG3	2.09	0.52
1:A:629:HIS:O	1:A:632:LYS:HB3	2.09	0.52
1:D:564:ILE:O	1:D:568:LYS:HG3	2.08	0.52
1:A:532:VAL:CG2	1:A:541:ILE:HD12	2.40	0.52
1:A:609:ALA:O	1:A:612:PHE:HB3	2.09	0.52
1:B:666:LEU:O	1:B:670:VAL:HG23	2.09	0.52
1:B:556:ASP:HA	1:B:581:ASN:OD1	2.10	0.52
1:C:574:ARG:HA	1:D:652:GLY:HA3	1.91	0.52
1:C:626:ALA:HA	1:C:635:MET:HE1	1.92	0.52
1:D:655:ARG:O	1:D:656:ALA:CB	2.53	0.52
1:C:714:LEU:O	1:C:714:LEU:HD23	2.10	0.52
1:D:503:ARG:HB3	1:D:508:ASN:HB2	1.91	0.52
1:A:653:HIS:O	1:A:654:PHE:CB	2.55	0.52
1:B:525:THR:O	1:B:529:LEU:HD13	2.10	0.51
1:C:556:ASP:HA	1:C:581:ASN:OD1	2.11	0.51
1:D:556:ASP:HA	1:D:581:ASN:OD1	2.11	0.51
1:A:643:TYR:HD1	1:A:649:ILE:HG12	1.76	0.51
1:D:705:LEU:C	1:D:707:ASP:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:VAL:CG1	1:B:541:ILE:HD12	2.39	0.51
1:C:489:LEU:HD23	1:C:489:LEU:O	2.10	0.50
1:A:578:LEU:CB	1:A:583:ILE:HD11	2.31	0.50
1:C:576:THR:HA	1:D:650:THR:HA	1.94	0.50
1:C:626:ALA:C	1:C:630:ILE:HG13	2.36	0.50
1:B:508:ASN:O	1:B:512:GLU:HG3	2.11	0.50
1:B:503:ARG:CB	1:B:508:ASN:HB2	2.41	0.50
1:D:503:ARG:NH1	1:D:664:THR:HG22	2.26	0.50
1:A:637:THR:OG1	1:A:641:GLU:HB2	2.11	0.50
1:A:499:ALA:HB1	1:A:663:THR:HG22	1.93	0.50
1:B:554:VAL:O	1:B:580:LEU:HG	2.12	0.50
1:A:611:LYS:O	1:A:615:GLY:HA3	2.12	0.49
1:B:683:GLU:O	1:B:687:LEU:HD13	2.12	0.49
1:B:481:GLU:O	1:B:485:VAL:HG23	2.13	0.49
1:B:464:ILE:CD1	1:B:701:LEU:HD12	2.39	0.49
1:C:570:HIS:HB2	1:C:572:LEU:HG	1.95	0.49
1:A:636:VAL:HA	1:A:641:GLU:O	2.11	0.49
1:B:461:LEU:C	1:B:461:LEU:HD23	2.37	0.49
1:B:530:ILE:HD11	1:B:610:VAL:HG22	1.95	0.49
1:D:503:ARG:NH2	1:D:664:THR:HG22	2.27	0.49
1:B:465:GLN:O	1:B:469:ILE:HG13	2.13	0.49
1:B:548:ARG:HA	1:B:551:ASN:HD21	1.78	0.49
1:A:525:THR:HG22	1:A:527:ALA:N	2.28	0.48
1:D:519:ILE:HD12	1:D:562:LYS:HZ1	1.77	0.48
1:B:465:GLN:HE22	1:B:468:ARG:HH11	1.60	0.48
1:B:489:LEU:O	1:B:493:GLU:HB2	2.12	0.48
1:B:548:ARG:HA	1:B:551:ASN:ND2	2.28	0.48
1:B:578:LEU:HB3	1:B:583:ILE:HD11	1.95	0.48
1:A:579:PRO:O	1:A:583:ILE:HG13	2.13	0.48
1:A:653:HIS:HB3	1:B:573:GLY:HA2	1.95	0.48
1:B:627:ARG:HB2	1:B:628:PRO:HD3	1.96	0.48
1:C:539:LEU:O	1:C:543:VAL:HG23	2.14	0.48
1:D:686:SER:O	1:D:689:ILE:HB	2.13	0.48
1:A:498:ALA:O	1:A:502:GLN:HG3	2.14	0.48
1:A:653:HIS:CE1	1:B:571:LYS:HA	2.49	0.48
1:C:666:LEU:O	1:C:670:VAL:HG23	2.14	0.48
1:C:685:ASN:O	1:C:689:ILE:HG13	2.12	0.48
1:B:697:ALA:O	1:B:701:LEU:HG	2.13	0.48
1:A:575:LEU:HD22	1:A:577:PHE:CZ	2.48	0.48
1:D:683:GLU:O	1:D:687:LEU:HG	2.13	0.47
1:A:514:LEU:HB3	1:A:522:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLU:CG	1:A:611:LYS:HE3	2.45	0.47
1:D:548:ARG:HA	1:D:551:ASN:OD1	2.14	0.47
1:A:503:ARG:HD2	1:A:663:THR:HG21	1.96	0.47
1:B:544:ALA:CB	1:B:617:THR:HG21	2.44	0.47
1:B:498:ALA:O	1:B:502:GLN:HG3	2.15	0.47
1:C:465:GLN:NE2	1:C:468:ARG:HH22	2.13	0.47
1:D:585:PRO:HA	1:D:612:PHE:HA	1.97	0.47
1:A:653:HIS:ND1	1:B:571:LYS:HA	2.30	0.46
1:B:707:ASP:O	1:B:711:GLU:HG3	2.15	0.46
1:D:554:VAL:HG22	1:D:578:LEU:H	1.79	0.46
1:D:514:LEU:HD11	1:D:575:LEU:HD12	1.97	0.46
1:A:482:LEU:HD23	1:A:482:LEU:O	2.15	0.46
1:B:556:ASP:OD1	1:B:558:LEU:HB2	2.15	0.46
1:B:461:LEU:HD23	1:B:461:LEU:O	2.15	0.46
1:A:522:ILE:HA	1:A:554:VAL:HG12	1.97	0.46
1:C:541:ILE:HD13	1:C:600:ILE:CG2	2.46	0.46
1:D:611:LYS:O	1:D:615:GLY:HA3	2.15	0.46
1:D:554:VAL:HG22	1:D:578:LEU:N	2.31	0.46
1:B:519:ILE:HG23	1:B:562:LYS:HD2	1.97	0.46
1:C:620:VAL:HG23	1:C:637:THR:HG22	1.98	0.46
1:D:521:GLY:CA	1:D:559:VAL:HG11	2.46	0.46
1:B:611:LYS:O	1:B:615:GLY:HA3	2.16	0.46
1:D:525:THR:OG1	1:D:528:GLU:HG3	2.15	0.46
1:D:527:ALA:HB2	1:D:549:ALA:HB1	1.98	0.45
1:D:685:ASN:O	1:D:689:ILE:HG13	2.16	0.45
1:B:523:TYR:O	1:B:529:LEU:HD21	2.16	0.45
1:C:626:ALA:C	1:C:630:ILE:CG1	2.89	0.45
1:A:612:PHE:HE2	1:B:646:SER:HB2	1.81	0.45
1:B:588:VAL:HG23	1:B:615:GLY:O	2.15	0.45
1:A:533:LYS:HE2	1:A:601:GLU:HG2	1.98	0.45
1:A:627:ARG:HB2	1:A:628:PRO:HD3	1.99	0.45
1:D:558:LEU:O	1:D:562:LYS:HG3	2.17	0.45
1:D:686:SER:HA	1:D:689:ILE:HD12	1.99	0.45
1:A:446:VAL:HG12	1:A:447:VAL:N	2.19	0.45
1:C:633:VAL:HA	1:C:645:ARG:NH1	2.32	0.45
1:D:475:ILE:O	1:D:479:SER:HB2	2.16	0.45
1:D:620:VAL:O	1:D:638:ILE:HG12	2.16	0.45
1:B:525:THR:HA	1:B:551:ASN:O	2.16	0.45
1:A:564:ILE:HD13	1:B:651:GLY:HA3	1.99	0.45
1:A:533:LYS:HE3	1:A:600:ILE:O	2.16	0.45
1:B:554:VAL:HG23	1:B:579:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:ALA:O	1:D:612:PHE:HB3	2.16	0.45
1:A:702:ARG:HB3	1:B:703:ILE:HD13	1.98	0.45
1:B:475:ILE:HD12	1:B:691:LEU:HD12	1.98	0.45
1:D:576:THR:HG23	1:D:576:THR:O	2.16	0.45
1:B:545:LEU:HD21	1:B:614:LEU:HG	2.00	0.44
1:C:607:GLU:CG	1:C:611:LYS:HE3	2.44	0.44
1:D:567:LEU:HB2	1:D:572:LEU:HB2	1.98	0.44
1:B:541:ILE:HD11	1:B:599:VAL:HG23	1.98	0.44
1:B:594:LEU:HD23	1:B:594:LEU:N	2.30	0.44
1:C:489:LEU:C	1:C:491:SER:N	2.75	0.44
1:D:498:ALA:O	1:D:502:GLN:HG3	2.17	0.44
1:C:465:GLN:NE2	1:C:468:ARG:NH2	2.65	0.44
1:C:513:GLU:CD	1:C:572:LEU:HD22	2.42	0.44
1:D:496:LEU:HD23	1:D:496:LEU:C	2.41	0.44
1:D:571:LYS:O	1:D:572:LEU:HD23	2.17	0.44
1:A:612:PHE:CD1	1:A:612:PHE:C	2.96	0.44
1:C:489:LEU:C	1:C:491:SER:H	2.25	0.44
1:D:592:VAL:O	1:D:618:VAL:HG11	2.17	0.44
1:A:580:LEU:CD1	1:A:606:ILE:HG22	2.45	0.44
1:A:583:ILE:HG23	1:A:612:PHE:CD2	2.53	0.44
1:C:493:GLU:HA	1:C:496:LEU:CD2	2.47	0.44
1:D:623:MET:HE1	1:D:641:GLU:OE1	2.17	0.44
1:A:501:ALA:O	1:A:505:VAL:HG23	2.18	0.44
1:A:544:ALA:HB1	1:A:614:LEU:HD22	1.99	0.44
1:A:556:ASP:OD1	1:A:558:LEU:HB2	2.18	0.44
1:D:557:GLU:HG3	1:D:582:LYS:HZ2	1.83	0.44
1:B:669:LYS:O	1:B:673:LEU:HG	2.18	0.44
1:C:654:PHE:HB2	1:D:573:GLY:HA2	1.99	0.44
1:D:585:PRO:HG3	1:D:608:ASN:ND2	2.33	0.44
1:C:626:ALA:O	1:C:630:ILE:HG12	2.18	0.43
1:B:524:GLY:O	1:B:553:VAL:HG22	2.17	0.43
1:C:563:ALA:O	1:C:567:LEU:HG	2.18	0.43
1:D:552:VAL:HG21	1:D:575:LEU:HD13	2.00	0.43
1:C:541:ILE:HD13	1:C:600:ILE:HG22	1.99	0.43
1:C:622:SER:N	1:C:625:GLU:OE1	2.52	0.43
1:D:635:MET:O	1:D:642:LEU:HD12	2.18	0.43
1:B:558:LEU:HD23	1:B:561:GLU:OE1	2.18	0.43
1:D:554:VAL:HG23	1:D:579:PRO:N	2.34	0.43
1:A:575:LEU:HD22	1:A:577:PHE:CE2	2.53	0.43
1:B:558:LEU:O	1:B:562:LYS:HE3	2.18	0.43
1:C:545:LEU:HD21	1:C:614:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:LYS:HD3	1:C:616:ASP:OD2	2.17	0.43
1:D:490:GLU:O	1:D:494:ARG:HG3	2.19	0.43
1:D:503:ARG:HH22	1:D:664:THR:CG2	2.32	0.43
1:A:447:VAL:CG2	1:A:715:ALA:HB1	2.44	0.43
1:A:461:LEU:C	1:A:461:LEU:HD23	2.43	0.43
1:B:464:ILE:HD12	1:B:701:LEU:CD1	2.42	0.43
1:D:632:LYS:HG3	1:D:633:VAL:HG23	2.01	0.43
1:A:502:GLN:HE21	1:B:505:VAL:HG23	1.84	0.42
1:A:535:GLU:HG2	1:A:536:ALA:N	2.34	0.42
1:A:535:GLU:C	1:A:537:TYR:H	2.26	0.42
1:D:566:TYR:CD1	1:D:566:TYR:C	2.97	0.42
1:A:706:SER:O	1:A:710:LYS:HG2	2.19	0.42
1:D:521:GLY:O	1:D:559:VAL:HG11	2.19	0.42
1:A:541:ILE:HD11	1:A:599:VAL:CG2	2.43	0.42
1:B:594:LEU:H	1:B:594:LEU:CD2	2.31	0.42
1:C:514:LEU:HB3	1:C:522:ILE:HD13	2.00	0.42
1:C:586:LYS:O	1:C:615:GLY:HA3	2.20	0.42
1:D:545:LEU:HD21	1:D:614:LEU:HD21	2.00	0.42
1:A:511:ALA:O	1:A:514:LEU:HB2	2.19	0.42
1:A:588:VAL:HG23	1:A:615:GLY:O	2.19	0.42
1:B:567:LEU:HD23	1:B:572:LEU:HD12	2.01	0.42
1:D:705:LEU:C	1:D:707:ASP:N	2.78	0.42
1:C:642:LEU:HB3	1:C:650:THR:HB	2.01	0.42
1:C:714:LEU:HD23	1:C:714:LEU:C	2.44	0.42
1:D:493:GLU:O	1:D:497:ILE:HG13	2.19	0.42
1:D:545:LEU:O	1:D:548:ARG:HB2	2.20	0.42
1:D:557:GLU:HG3	1:D:582:LYS:NZ	2.34	0.42
1:A:535:GLU:HG2	1:A:536:ALA:H	1.84	0.42
1:C:709:LYS:O	1:C:713:GLU:HG3	2.19	0.42
1:D:596:ALA:C	1:D:598:ASP:H	2.28	0.42
1:A:679:ALA:O	1:A:683:GLU:HG3	2.19	0.42
1:A:688:LYS:O	1:A:692:ARG:HG3	2.20	0.42
1:C:592:VAL:HG12	1:C:593:GLY:N	2.34	0.42
1:A:579:PRO:C	1:A:581:ASN:N	2.77	0.41
1:A:703:ILE:H	1:A:703:ILE:HG13	1.63	0.41
1:B:503:ARG:O	1:B:508:ASN:N	2.53	0.41
1:D:567:LEU:HD13	1:D:573:GLY:O	2.20	0.41
1:D:554:VAL:HG23	1:D:579:PRO:CA	2.51	0.41
1:D:620:VAL:HB	1:D:625:GLU:OE1	2.19	0.41
1:B:463:THR:O	1:B:466:ALA:HB3	2.20	0.41
1:B:479:SER:HA	1:B:684:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:GLU:O	1:D:485:VAL:HG23	2.20	0.41
1:B:479:SER:HB3	1:B:684:LEU:HD11	2.02	0.41
1:B:671:GLU:O	1:B:675:ARG:HG3	2.21	0.41
1:A:619:ILE:HA	1:A:636:VAL:HG13	2.02	0.41
1:B:552:VAL:HB	1:B:577:PHE:CD1	2.55	0.41
1:D:554:VAL:HG23	1:D:579:PRO:HA	2.02	0.41
1:C:526:LEU:HD12	1:C:548:ARG:O	2.20	0.41
1:A:556:ASP:HA	1:A:581:ASN:HB3	2.03	0.41
1:B:642:LEU:HB3	1:B:650:THR:HB	2.03	0.41
1:A:567:LEU:HD23	1:A:572:LEU:HD12	2.03	0.41
1:B:496:LEU:HD22	1:B:500:GLU:OE1	2.20	0.41
1:B:523:TYR:CB	1:B:553:VAL:HG23	2.45	0.41
1:B:618:VAL:CG1	1:B:619:ILE:N	2.83	0.41
1:C:517:SER:HB2	1:C:566:TYR:CE2	2.56	0.41
1:D:554:VAL:HG23	1:D:578:LEU:C	2.46	0.41
1:D:554:VAL:HG21	1:D:577:PHE:HB3	2.02	0.41
1:A:526:LEU:HD12	1:A:548:ARG:O	2.21	0.41
1:B:482:LEU:HD23	1:B:482:LEU:O	2.21	0.41
1:A:564:ILE:HD11	1:B:649:ILE:HG22	2.04	0.40
1:A:634:ARG:NH2	1:A:642:LEU:HD21	2.36	0.40
1:C:634:ARG:NH2	1:C:642:LEU:HD21	2.36	0.40
1:D:557:GLU:OE2	1:D:557:GLU:N	2.49	0.40
1:D:580:LEU:HD21	1:D:606:ILE:HG22	2.02	0.40
1:B:507:GLY:O	1:B:510:ALA:HB3	2.21	0.40
1:C:464:ILE:HD12	1:C:701:LEU:HD12	2.02	0.40
1:C:574:ARG:HG3	1:D:651:GLY:O	2.22	0.40
1:D:509:ARG:HH11	1:D:509:ARG:HG3	1.86	0.40
1:D:593:GLY:HA3	1:D:618:VAL:CG1	2.51	0.40
1:C:510:ALA:HB3	1:C:575:LEU:HD11	2.04	0.40
1:A:650:THR:HG23	1:A:650:THR:O	2.21	0.40
1:B:575:LEU:HD23	1:B:576:THR:H	1.87	0.40
1:B:596:ALA:HA	1:B:619:ILE:HD11	2.02	0.40
1:B:597:VAL:HG13	1:B:614:LEU:O	2.21	0.40
1:C:533:LYS:CD	1:C:600:ILE:O	2.67	0.40
1:C:574:ARG:HG3	1:D:651:GLY:C	2.46	0.40
1:A:513:GLU:HB2	1:A:572:LEU:HD13	2.03	0.40
1:C:509:ARG:HG3	1:C:509:ARG:NH1	2.37	0.40
1:D:567:LEU:HD12	1:D:568:LYS:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/276 (96%)	247 (93%)	17 (6%)	2 (1%)	16	49
1	B	262/276 (95%)	237 (90%)	23 (9%)	2 (1%)	16	49
1	C	261/276 (95%)	240 (92%)	21 (8%)	0	100	100
1	D	259/276 (94%)	230 (89%)	25 (10%)	4 (2%)	8	37
All	All	1048/1104 (95%)	954 (91%)	86 (8%)	8 (1%)	16	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	536	ALA
1	A	604	GLN
1	D	533	LYS
1	D	605	LYS
1	A	636	VAL
1	B	546	GLY
1	D	597	VAL
1	D	630	ILE

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	184/232 (79%)	179 (97%)	5 (3%)	39	62
1	B	198/232 (85%)	194 (98%)	4 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	181/232 (78%)	179 (99%)	2 (1%)	65	74
1	D	167/232 (72%)	163 (98%)	4 (2%)	43	64
All	All	730/928 (79%)	715 (98%)	15 (2%)	47	66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	LYS
1	A	537	TYR
1	A	623	MET
1	A	703	ILE
1	A	704	LYS
1	B	496	LEU
1	B	575	LEU
1	B	623	MET
1	B	654	PHE
1	C	533	LYS
1	C	614	LEU
1	D	519	ILE
1	D	574	ARG
1	D	623	MET
1	D	653	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	GLN
1	A	502	GLN
1	A	508	ASN
1	A	547	ASN
1	A	621	ASN
1	A	629	HIS
1	B	465	GLN
1	B	570	HIS
1	B	587	HIS
1	B	608	ASN
1	B	621	ASN
1	C	465	GLN
1	C	629	HIS
1	D	480	ASN

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Mol	Chain	Res	Type
1	D	502	GLN
1	D	508	ASN
1	D	608	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	517:SER	C	518:GLY	N	1.14

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	270/276 (97%)	-0.19	0 100 100	40, 86, 132, 195	26 (9%)
1	B	266/276 (96%)	-0.04	5 (1%) 66 41	48, 79, 131, 157	26 (9%)
1	C	265/276 (96%)	-0.22	2 (0%) 82 60	37, 87, 120, 148	26 (9%)
1	D	263/276 (95%)	-0.15	4 (1%) 72 47	46, 81, 121, 184	26 (9%)
All	All	1064/1104 (96%)	-0.15	11 (1%) 79 56	37, 83, 126, 195	104 (9%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	653	HIS	5.2
1	D	554	VAL	4.4
1	C	653	HIS	4.1
1	D	556	ASP	3.2
1	C	663	THR	3.2
1	B	711	GLU	3.1
1	B	699	PHE	3.1
1	B	520	GLY	2.7
1	B	523	TYR	2.5
1	D	521	GLY	2.4
1	B	537	TYR	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.