Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2023 – 04:08 AM EDT

PDB ID	:	4RSJ
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:

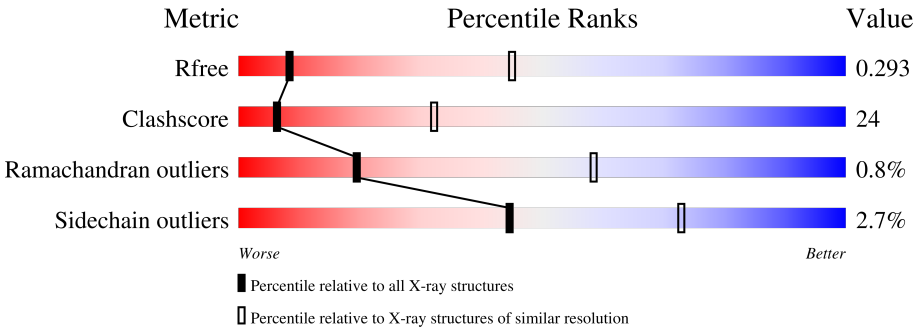
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	276	60% 37%
1	B	276	53% 41%
1	C	276	62% 33%
1	D	276	58% 36% 5%

2 Entry composition (i)

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.

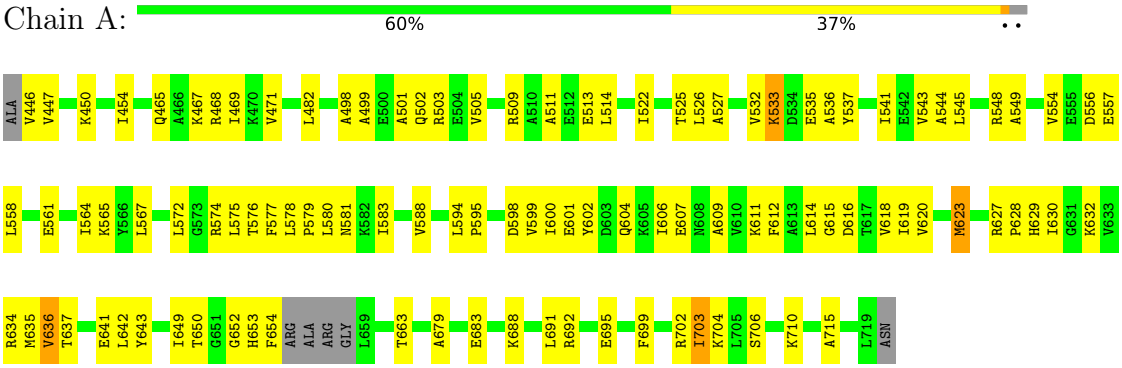
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	30	0	0
			1954	1217	346	389	2			
1	B	266	Total	C	N	O	S	36	0	0
			1994	1246	360	386	2			
1	C	265	Total	C	N	O	S	32	0	0
			1908	1187	336	383	2			
1	D	263	Total	C	N	O	S	36	0	0
			1859	1155	340	362	2			

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. 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. 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.

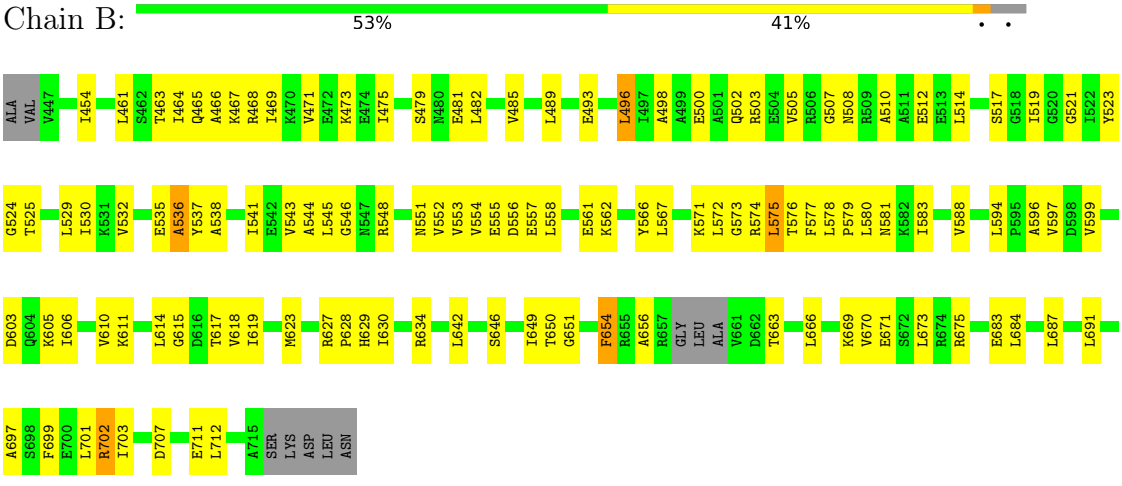
• Molecule 1: Chromosome partition protein Smc

Chain A:



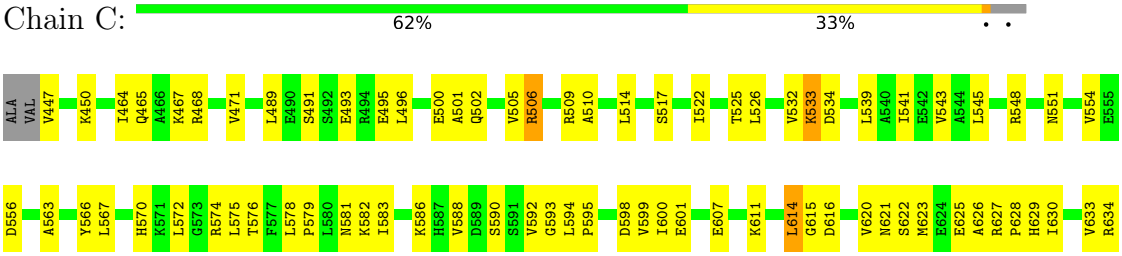
• Molecule 1: Chromosome partition protein Smc

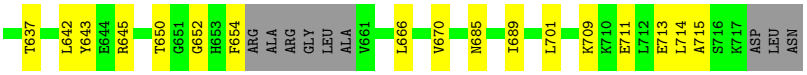
Chain B:



• Molecule 1: Chromosome partition protein Smc

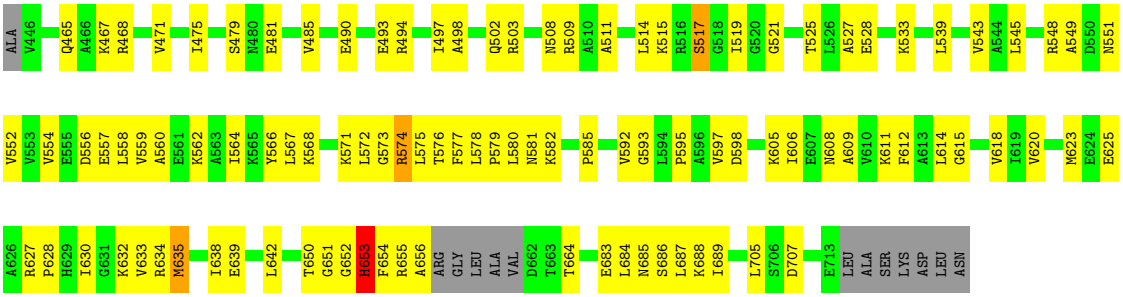
Chain C:





• Molecule 1: Chromosome partition protein Smc

Chain D:



4 Data and refinement statistics (i)

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 37.63 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.50) 73.5 (37.63-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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)	0.29 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/1969	0.46	0/2661
1	B	0.24	0/2009	0.48	0/2705
1	C	0.24	0/1922	0.48	0/2598
1	D	0.43	2/1873 (0.1%)	0.66	4/2535 (0.2%)
All	All	0.30	2/7773 (0.0%)	0.52	4/10499 (0.0%)

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	11.06	1.59	1.34
1	D	517	SER	C-N	-10.31	1.14	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	653	HIS	O-C-N	-17.11	95.33	122.70
1	D	653	HIS	CA-C-N	12.02	143.65	117.20
1	D	653	HIS	C-N-CA	7.43	140.28	121.70
1	D	517	SER	O-C-N	-7.20	110.96	123.20

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	Mainchain,Peptide

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	103	0
1	B	1994	0	1990	116	0
1	C	1908	0	1818	81	0
1	D	1859	0	1746	85	0
All	All	7715	0	7415	362	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 24.

All (362) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:699:PHE:O	1:B:703:ILE:HG13	1.94	0.67
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:541:ILE:HD11	1:C:599:VAL:HG23	1.78	0.65
1:B:469:ILE:HG22	1:B:473:LYS:HE3	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:533:LYS:O	1:C:534:ASP:HB2	2.01	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: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:519:ILE:HD12	1:D:562:LYS:HZ1	1.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:519:ILE:HD12	1:D:562:LYS:HZ2	1.68	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:629:HIS:O	1:B:630:ILE:C	2.45	0.52
1:C:574:ARG:HA	1:D:652:GLY:HA3	1.91	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:482:LEU:C	1:A:482:LEU:HD23	2.34	0.48
1:A:525:THR:HG22	1:A:527:ALA:N	2.28	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:B:537:TYR:O	1:B:538:ALA:C	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:ASP:OD1	1:B:558:LEU:HB2	2.15	0.46
1:D:705:LEU:C	1:D:707:ASP:H	2.18	0.46
1:B:461:LEU:O	1:B:461:LEU:HD23	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:C:626:ALA:C	1:C:630:ILE:HG13	2.36	0.45
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: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
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:D:498:ALA:O	1:D:502:GLN:HG3	2.17	0.44
1:B:461:LEU:HD23	1:B:461:LEU:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:GLN:NE2	1:C:468:ARG:NH2	2.65	0.44
1:D:571:LYS:O	1:D:572:LEU:HD23	2.17	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:642:LEU:HB3	1:C:650:THR:HB	2.01	0.42
1:A:623:MET:HE2	1:A:643:TYR:CZ	2.54	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: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: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
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:C:626:ALA:C	1:C:630:ILE:CG1	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:513:GLU:HB2	1:A:572:LEU:HD13	2.03	0.40
1:C:489:LEU:C	1:C:491:SER:N	2.75	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 (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	266/276 (96%)	247 (93%)	17 (6%)	2 (1%)	19	58
1	B	262/276 (95%)	237 (90%)	23 (9%)	2 (1%)	19	58
1	C	261/276 (95%)	240 (92%)	21 (8%)	0	100	100
1	D	259/276 (94%)	230 (89%)	25 (10%)	4 (2%)	10	45
All	All	1048/1104 (95%)	954 (91%)	86 (8%)	8 (1%)	19	58

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 (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	184/232 (79%)	178 (97%)	6 (3%)	38	68
1	B	198/232 (85%)	193 (98%)	5 (2%)	47	75
1	C	181/232 (78%)	178 (98%)	3 (2%)	60	82
1	D	167/232 (72%)	161 (96%)	6 (4%)	35	66
All	All	730/928 (79%)	710 (97%)	20 (3%)	44	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	LYS
1	A	537	TYR
1	A	557	GLU
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	B	702	ARG
1	C	506	ARG
1	C	533	LYS
1	C	614	LEU

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Mol	Chain	Res	Type
1	D	566	TYR
1	D	574	ARG
1	D	623	MET
1	D	635	MET
1	D	653	HIS
1	D	654	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	581	ASN
1	B	465	GLN
1	B	570	HIS
1	B	587	HIS
1	C	465	GLN
1	D	480	ASN
1	D	502	GLN
1	D	508	ASN
1	D	608	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.