



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:36 AM UTC

PDB ID : 6WG6 / pdb_00006wg6
Title : Crystal structure of human SMC1-SMC3 hinge domain heterodimer in north-open conformation
Authors : Shi, Z.B.; Yu, H.
Deposited on : 2020-04-04
Resolution : 3.54 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

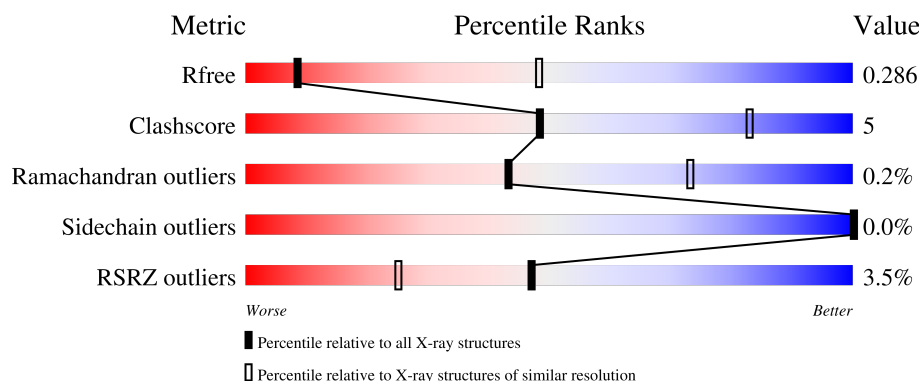
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.54 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	1008 (3.58-3.50)
Clashscore	190562	1062 (3.58-3.50)
Ramachandran outliers	187476	1033 (3.58-3.50)
Sidechain outliers	187428	1034 (3.58-3.50)
RSRZ outliers	180081	1007 (3.58-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	2% 64% 14% 22%
1	C	233	2% 66% 12% 22%
1	E	233	2% 68% 9% 24%
1	G	233	3% 64% 12% 24%
1	I	233	6% 61% 13% 26%

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Mol	Chain	Length	Quality of chain
1	K	233	11%67%8%25%
2	B	256	2%76%16%8%
2	D	256	%80%11%8%
2	F	256	%79%12%8%
2	H	256	81%11%8%
2	J	256	3%80%13%7%
2	L	256	3%79%14%7%
3	M	10	20%80%
3	N	10	10%10%80%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20038 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 Structural maintenance of chromosomes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1446	910	262	268	6			
1	C	182	Total	C	N	O	S	0	0	0
			1446	910	262	268	6			
1	E	178	Total	C	N	O	S	0	0	0
			1409	886	256	261	6			
1	G	178	Total	C	N	O	S	0	0	0
			1409	886	256	261	6			
1	I	173	Total	C	N	O	S	0	0	0
			1376	866	250	254	6			
1	K	175	Total	C	N	O	S	0	0	0
			1390	875	253	256	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	GLY	-	expression tag	UNP G8JLG1
A	471	PRO	-	expression tag	UNP G8JLG1
C	470	GLY	-	expression tag	UNP G8JLG1
C	471	PRO	-	expression tag	UNP G8JLG1
E	470	GLY	-	expression tag	UNP G8JLG1
E	471	PRO	-	expression tag	UNP G8JLG1
G	470	GLY	-	expression tag	UNP G8JLG1
G	471	PRO	-	expression tag	UNP G8JLG1
I	470	GLY	-	expression tag	UNP G8JLG1
I	471	PRO	-	expression tag	UNP G8JLG1
K	470	GLY	-	expression tag	UNP G8JLG1
K	471	PRO	-	expression tag	UNP G8JLG1

- Molecule 2 is a protein called Structural maintenance of chromosomes protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1908	1194	343	361	10			
2	D	235	Total	C	N	O	S	0	0	0
			1902	1189	345	358	10			
2	F	235	Total	C	N	O	S	0	0	0
			1899	1189	342	358	10			
2	H	236	Total	C	N	O	S	0	0	0
			1908	1194	343	361	10			
2	J	238	Total	C	N	O	S	0	0	0
			1927	1206	348	363	10			
2	L	239	Total	C	N	O	S	0	0	0
			1938	1212	352	364	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	457	GLY	-	expression tag	UNP Q9UQE7
B	458	PRO	-	expression tag	UNP Q9UQE7
B	459	LEU	-	expression tag	UNP Q9UQE7
B	460	GLY	-	expression tag	UNP Q9UQE7
B	461	SER	-	expression tag	UNP Q9UQE7
B	462	GLY	-	expression tag	UNP Q9UQE7
B	463	ARG	-	expression tag	UNP Q9UQE7
B	464	PRO	-	expression tag	UNP Q9UQE7
D	457	GLY	-	expression tag	UNP Q9UQE7
D	458	PRO	-	expression tag	UNP Q9UQE7
D	459	LEU	-	expression tag	UNP Q9UQE7
D	460	GLY	-	expression tag	UNP Q9UQE7
D	461	SER	-	expression tag	UNP Q9UQE7
D	462	GLY	-	expression tag	UNP Q9UQE7
D	463	ARG	-	expression tag	UNP Q9UQE7
D	464	PRO	-	expression tag	UNP Q9UQE7
F	457	GLY	-	expression tag	UNP Q9UQE7
F	458	PRO	-	expression tag	UNP Q9UQE7
F	459	LEU	-	expression tag	UNP Q9UQE7
F	460	GLY	-	expression tag	UNP Q9UQE7
F	461	SER	-	expression tag	UNP Q9UQE7
F	462	GLY	-	expression tag	UNP Q9UQE7
F	463	ARG	-	expression tag	UNP Q9UQE7
F	464	PRO	-	expression tag	UNP Q9UQE7
H	457	GLY	-	expression tag	UNP Q9UQE7
H	458	PRO	-	expression tag	UNP Q9UQE7
H	459	LEU	-	expression tag	UNP Q9UQE7
H	460	GLY	-	expression tag	UNP Q9UQE7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	461	SER	-	expression tag	UNP Q9UQE7
H	462	GLY	-	expression tag	UNP Q9UQE7
H	463	ARG	-	expression tag	UNP Q9UQE7
H	464	PRO	-	expression tag	UNP Q9UQE7
J	457	GLY	-	expression tag	UNP Q9UQE7
J	458	PRO	-	expression tag	UNP Q9UQE7
J	459	LEU	-	expression tag	UNP Q9UQE7
J	460	GLY	-	expression tag	UNP Q9UQE7
J	461	SER	-	expression tag	UNP Q9UQE7
J	462	GLY	-	expression tag	UNP Q9UQE7
J	463	ARG	-	expression tag	UNP Q9UQE7
J	464	PRO	-	expression tag	UNP Q9UQE7
L	457	GLY	-	expression tag	UNP Q9UQE7
L	458	PRO	-	expression tag	UNP Q9UQE7
L	459	LEU	-	expression tag	UNP Q9UQE7
L	460	GLY	-	expression tag	UNP Q9UQE7
L	461	SER	-	expression tag	UNP Q9UQE7
L	462	GLY	-	expression tag	UNP Q9UQE7
L	463	ARG	-	expression tag	UNP Q9UQE7
L	464	PRO	-	expression tag	UNP Q9UQE7

- Molecule 3 is a DNA chain called poly(dT).

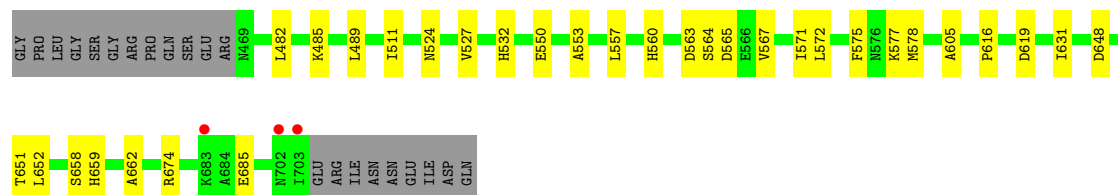
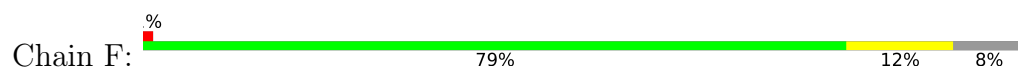
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	P	0	0	0
			40	20	4	14	2			
3	N	2	Total	C	N	O	P	0	0	0
			40	20	4	14	2			

- Molecule 1: Structural maintenance of chromosomes protein.

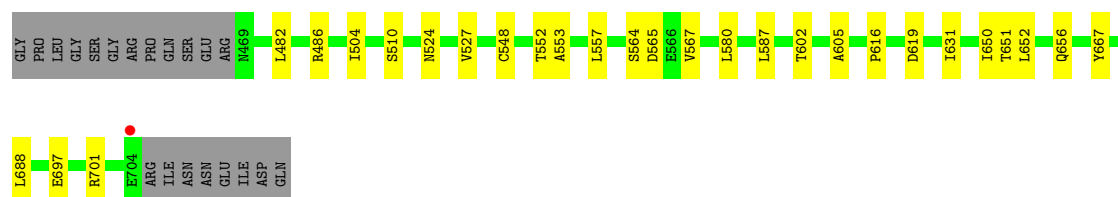
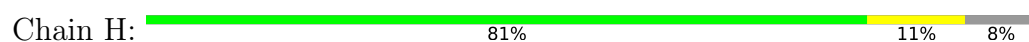




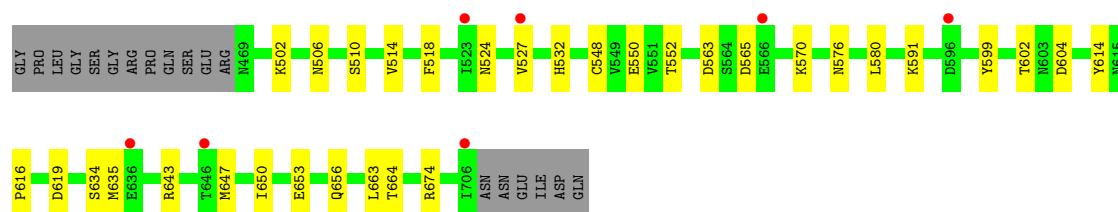
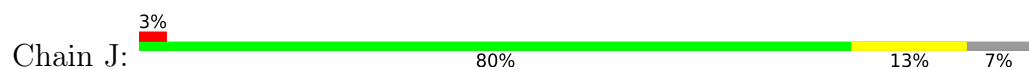
• Molecule 2: Structural maintenance of chromosomes protein 3



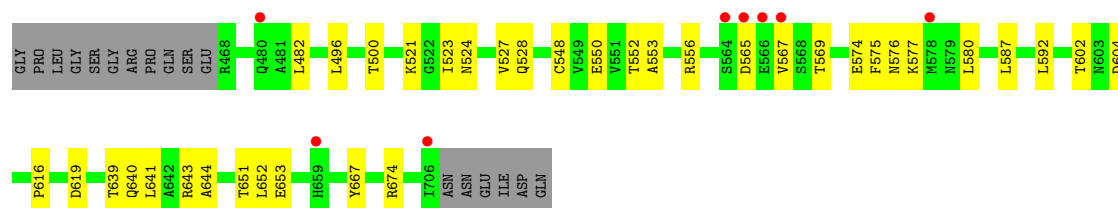
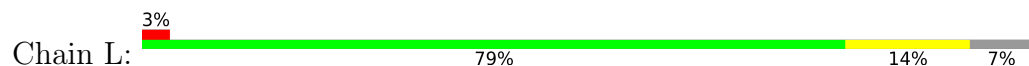
• Molecule 2: Structural maintenance of chromosomes protein 3



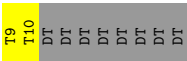
• Molecule 2: Structural maintenance of chromosomes protein 3



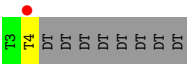
• Molecule 2: Structural maintenance of chromosomes protein 3



● Molecule 3: poly(dT)



● Molecule 3: poly(dT)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.98Å 145.02Å 315.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 3.54 49.50 – 3.54	Depositor EDS
% Data completeness (in resolution range)	87.3 (49.50-3.54) 73.1 (49.50-3.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.252 , 0.288 0.252 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	20038	wwPDB-VP
Average B, all atoms (Å ²)	79.0	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 45.84 % 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 1.2465e-04. 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/1467	0.51	0/1968
1	C	0.19	0/1467	0.50	1/1968 (0.1%)
1	E	0.18	0/1430	0.44	0/1920
1	G	0.16	0/1430	0.44	0/1920
1	I	0.23	0/1397	0.49	0/1876
1	K	0.17	0/1411	0.43	0/1894
2	B	0.21	0/1939	0.45	0/2609
2	D	0.18	0/1933	0.42	0/2600
2	F	0.18	0/1930	0.43	0/2597
2	H	0.18	0/1939	0.42	0/2609
2	J	0.17	0/1958	0.40	0/2634
2	L	0.17	0/1969	0.41	0/2648
3	M	0.36	0/43	0.77	0/64
3	N	0.44	0/43	0.88	0/64
All	All	0.19	0/20356	0.44	1/27371 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	597	VAL	N-CA-C	-5.13	107.83	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1446	0	1497	22	0
1	C	1446	0	1497	21	0
1	E	1409	0	1455	12	0
1	G	1409	0	1455	18	0
1	I	1376	0	1418	19	0
1	K	1390	0	1436	11	0
2	B	1908	0	1897	28	0
2	D	1902	0	1893	23	0
2	F	1899	0	1891	19	0
2	H	1908	0	1897	17	0
2	J	1927	0	1921	23	0
2	L	1938	0	1934	24	0
3	M	40	0	25	2	0
3	N	40	0	25	1	0
All	All	20038	0	20241	221	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 5.

All (221) 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)
2:J:514:VAL:O	2:J:518:PHE:HB2	1.94	0.67
1:K:561:LYS:HA	2:L:667:TYR:HB2	1.77	0.65
2:H:486:ARG:HG2	2:H:688:LEU:HD11	1.78	0.65
2:D:532:HIS:NE2	2:D:563:ASP:OD1	2.31	0.64
2:L:575:PHE:HA	2:L:580:LEU:HD23	1.81	0.63
2:H:616:PRO:O	2:H:619:ASP:HB2	1.99	0.63
1:I:504:MET:HE1	1:I:517:GLY:HA2	1.80	0.63
2:F:527:VAL:HG13	2:F:567:VAL:HG23	1.81	0.62
1:C:522:LEU:HD23	1:C:605:ILE:HD13	1.81	0.62
1:A:573:LEU:HD21	1:A:605:ILE:HA	1.81	0.62
1:I:591:ALA:HB3	1:I:617:LEU:HD23	1.82	0.61
2:B:518:PHE:HE2	2:B:524:ASN:HB2	1.65	0.61
1:C:600:TYR:CD2	1:C:609:LEU:HD12	2.37	0.60
1:A:588:LEU:HD13	1:A:589:LYS:N	2.17	0.60
1:C:600:TYR:HD2	1:C:609:LEU:HD12	1.66	0.60
2:L:616:PRO:O	2:L:619:ASP:HB2	2.01	0.60
2:J:616:PRO:O	2:J:619:ASP:HB2	2.03	0.59
1:A:598:ILE:HD12	1:A:609:LEU:HD13	1.83	0.59
2:D:486:ARG:NH1	2:J:580:LEU:O	2.35	0.59
1:K:550:GLU:OE1	1:K:554:ARG:NE	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:661:ALA:HA	1:G:664:ARG:HE	1.69	0.58
3:M:9:DT:H2''	3:M:10:DT:H5'	1.85	0.58
1:G:518:ARG:HA	1:G:545:ILE:HA	1.85	0.58
2:D:695:LEU:HD23	2:J:576:ASN:HD22	1.69	0.58
1:G:582:ASP:HB3	1:G:585:LEU:HG	1.85	0.57
2:H:527:VAL:HG13	2:H:567:VAL:HG23	1.87	0.56
2:D:527:VAL:HG13	2:D:567:VAL:HG23	1.86	0.56
2:B:602:THR:HG21	2:B:641:LEU:HD11	1.88	0.56
2:B:644:ALA:O	1:G:554:ARG:NH2	2.38	0.56
2:L:587:LEU:HD22	2:L:592:LEU:HD11	1.87	0.56
1:C:512:PRO:HB3	2:H:602:THR:HB	1.88	0.56
1:E:518:ARG:NH2	1:E:568:GLU:OE1	2.39	0.56
2:J:532:HIS:NE2	2:J:563:ASP:OD1	2.38	0.56
2:B:553:ALA:O	2:B:556:ARG:HB2	2.05	0.56
2:L:524:ASN:HB3	2:L:527:VAL:HB	1.88	0.56
1:E:582:ASP:HB3	1:E:585:LEU:HG	1.88	0.56
1:I:561:LYS:NZ	2:J:653:GLU:OE2	2.36	0.55
2:D:502:LYS:H	2:D:502:LYS:HD3	1.70	0.55
2:F:658:SER:HB3	2:F:662:ALA:H	1.72	0.55
1:G:621:ASN:ND2	1:G:624:ASP:OD1	2.40	0.55
2:L:521:LYS:HD3	2:L:523:ILE:HD11	1.89	0.55
2:B:472:TRP:O	2:B:476:ASN:ND2	2.35	0.55
1:A:519:LEU:HD21	1:A:609:LEU:HD21	1.88	0.55
1:I:535:THR:HG23	1:I:662:LYS:HE2	1.88	0.55
2:F:524:ASN:HB3	2:F:527:VAL:HB	1.89	0.54
1:I:525:PRO:HG2	1:I:531:GLN:HA	1.89	0.54
1:C:620:ASP:OD2	1:C:620:ASP:N	2.41	0.54
2:L:639:THR:OG1	2:L:643:ARG:NH2	2.41	0.54
1:G:564:ARG:NH2	2:H:667:TYR:OH	2.41	0.53
2:F:511:ILE:HD12	2:F:560:HIS:HD2	1.73	0.53
2:B:604:ASP:OD2	2:B:633:ARG:NH2	2.42	0.53
2:D:527:VAL:HG22	2:D:567:VAL:HA	1.90	0.53
1:G:518:ARG:NH2	1:G:568:GLU:OE1	2.41	0.53
2:H:564:SER:OG	2:H:565:ASP:N	2.42	0.53
1:K:561:LYS:NZ	2:L:653:GLU:OE2	2.38	0.53
2:B:514:VAL:O	2:B:518:PHE:HB2	2.10	0.52
2:F:564:SER:OG	2:F:565:ASP:N	2.40	0.52
1:C:550:GLU:OE1	1:C:554:ARG:NE	2.31	0.52
1:C:588:LEU:HD13	1:C:589:LYS:H	1.75	0.52
1:A:522:LEU:HD21	1:A:605:ILE:HG21	1.91	0.52
1:A:536:LYS:HD3	1:A:659:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:PRO:HD3	1:A:666:TRP:HE1	1.75	0.52
2:H:650:ILE:HD12	2:H:656:GLN:HG2	1.90	0.52
1:I:577:GLU:OE1	2:J:643:ARG:NE	2.42	0.51
2:F:616:PRO:O	2:F:619:ASP:HB2	2.09	0.51
2:H:651:THR:OG1	2:H:652:LEU:N	2.44	0.51
1:K:543:ASP:OD2	1:K:665:ARG:NH1	2.44	0.51
1:K:533:ALA:HB2	1:K:641:LEU:HA	1.91	0.51
2:B:648:ASP:OD1	2:B:659:HIS:ND1	2.32	0.51
1:I:525:PRO:HD2	1:I:531:GLN:HG2	1.92	0.51
2:J:604:ASP:OD1	2:J:604:ASP:N	2.44	0.51
2:J:548:CYS:O	2:J:552:THR:OG1	2.24	0.51
1:E:504:MET:HE3	1:E:518:ARG:HG2	1.93	0.51
1:C:594:VAL:O	1:C:597:VAL:HB	2.10	0.51
1:E:518:ARG:HA	1:E:545:ILE:HA	1.92	0.50
2:J:565:ASP:OD1	2:J:565:ASP:N	2.44	0.50
2:L:574:GLU:OE1	2:L:577:LYS:NZ	2.37	0.50
1:K:573:LEU:O	1:K:607:LYS:NZ	2.36	0.50
2:J:524:ASN:HB3	2:J:527:VAL:HB	1.93	0.50
2:J:550:GLU:OE2	2:J:674:ARG:N	2.44	0.50
1:G:538:LEU:O	1:G:541:ASN:HB2	2.12	0.50
1:A:518:ARG:NH2	1:A:568:GLU:OE1	2.45	0.50
1:A:561:LYS:NZ	2:B:653:GLU:OE2	2.36	0.50
1:G:588:LEU:HD13	1:G:590:GLY:H	1.77	0.49
1:I:582:ASP:HB3	1:I:585:LEU:HG	1.93	0.49
1:I:642:ASP:HB3	1:I:644:THR:HG22	1.93	0.49
1:I:581:THR:HG23	1:I:610:GLN:HG2	1.92	0.49
2:F:532:HIS:NE2	2:F:563:ASP:OD2	2.43	0.49
2:H:553:ALA:HB3	2:H:557:LEU:HD13	1.94	0.49
2:B:614:TYR:HE1	2:B:619:ASP:HA	1.78	0.48
1:K:628:ILE:HD11	1:K:638:THR:HG21	1.96	0.48
2:L:602:THR:HG21	2:L:641:LEU:HD21	1.95	0.48
1:C:551:LYS:NZ	1:C:555:ASP:OD1	2.47	0.48
1:A:504:MET:HE3	1:A:508:LYS:HE2	1.95	0.48
2:B:616:PRO:O	2:B:619:ASP:HB2	2.14	0.48
1:I:518:ARG:NH2	1:I:568:GLU:OE1	2.47	0.48
2:L:565:ASP:OD1	2:L:565:ASP:N	2.39	0.48
2:F:648:ASP:OD1	2:F:659:HIS:ND1	2.39	0.48
2:H:548:CYS:O	2:H:552:THR:OG1	2.22	0.48
1:C:582:ASP:HB3	1:C:585:LEU:HG	1.96	0.48
2:B:485:LYS:NZ	2:B:687:GLU:OE1	2.42	0.48
1:A:656:ALA:HA	1:A:659:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:585:LEU:HA	1:I:588:LEU:HD23	1.95	0.47
2:F:605:ALA:HA	2:F:631:ILE:O	2.15	0.47
1:A:588:LEU:HD13	1:A:589:LYS:H	1.78	0.47
1:E:665:ARG:O	1:E:669:LYS:N	2.47	0.47
2:H:524:ASN:HB3	2:H:527:VAL:HB	1.96	0.47
1:I:496:ARG:HA	1:I:499:ARG:HD2	1.97	0.47
1:I:572:PRO:HG3	2:J:663:LEU:HD23	1.97	0.47
2:F:571:ILE:O	2:F:575:PHE:HB2	2.14	0.47
2:D:548:CYS:O	2:D:552:THR:OG1	2.28	0.46
2:F:489:LEU:HD21	2:F:685:GLU:HG3	1.95	0.46
2:L:550:GLU:OE2	2:L:674:ARG:N	2.46	0.46
2:D:602:THR:OG1	2:D:604:ASP:OD1	2.30	0.46
2:B:531:TYR:HA	2:B:562:VAL:HG12	1.96	0.46
2:J:599:TYR:HA	2:J:647:MET:HE1	1.98	0.46
1:C:588:LEU:HD12	1:C:591:ALA:HB3	1.96	0.46
2:F:511:ILE:HD12	2:F:560:HIS:CD2	2.49	0.46
1:C:573:LEU:HD21	1:C:605:ILE:HA	1.98	0.46
1:C:591:ALA:HB2	1:C:628:ILE:HD13	1.98	0.46
2:J:614:TYR:HE1	2:J:619:ASP:HA	1.80	0.46
2:B:565:ASP:OD1	2:B:565:ASP:N	2.40	0.46
1:I:574:ASP:OD1	1:I:574:ASP:N	2.46	0.46
2:B:527:VAL:HG13	2:B:567:VAL:HG23	1.97	0.46
1:G:504:MET:HE1	1:G:518:ARG:H	1.81	0.45
1:G:573:LEU:HD21	1:G:605:ILE:HA	1.98	0.45
2:H:697:GLU:OE2	2:H:701:ARG:NH1	2.49	0.45
1:G:649:SER:HB2	1:G:651:VAL:HG23	1.98	0.45
2:L:553:ALA:HB1	2:L:556:ARG:HB2	1.98	0.45
2:D:468:ARG:HB3	2:J:591:LYS:HD2	1.98	0.45
2:D:648:ASP:OD1	2:D:648:ASP:N	2.50	0.45
2:L:548:CYS:O	2:L:552:THR:OG1	2.31	0.45
2:F:482:LEU:HD23	2:F:482:LEU:HA	1.81	0.45
2:F:572:LEU:HD13	2:F:572:LEU:HA	1.69	0.45
1:A:525:PRO:HD3	1:A:666:TRP:NE1	2.32	0.45
2:L:527:VAL:HG13	2:L:567:VAL:HG23	1.98	0.45
2:D:567:VAL:O	2:D:571:ILE:HG12	2.17	0.44
1:E:618:VAL:HA	1:E:639:VAL:O	2.16	0.44
2:J:634:SER:OG	2:J:635:MET:N	2.51	0.44
2:B:643:ARG:HD2	2:B:643:ARG:HA	1.79	0.44
1:C:525:PRO:HA	1:C:598:ILE:HA	1.99	0.44
1:C:600:TYR:HB2	1:C:605:ILE:HD11	2.00	0.44
2:J:502:LYS:HD3	2:J:502:LYS:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ILE:O	1:A:669:LYS:HE3	2.17	0.44
2:H:510:SER:HB2	2:H:580:LEU:HD23	1.98	0.44
1:K:518:ARG:HA	1:K:545:ILE:HA	1.99	0.44
1:A:504:MET:HE2	1:A:518:ARG:HG3	1.99	0.44
2:B:638:SER:HB2	2:B:649:CYS:HB3	1.99	0.44
2:D:575:PHE:HA	2:D:580:LEU:HD23	1.98	0.44
2:J:656:GLN:N	2:J:664:THR:O	2.46	0.44
2:B:514:VAL:HG23	2:B:580:LEU:HD11	1.99	0.44
2:D:565:ASP:OD1	2:D:565:ASP:N	2.43	0.44
3:N:4:DT:H6	3:N:4:DT:H2'	1.67	0.44
2:F:577:LYS:HD3	2:F:578:MET:HG3	2.00	0.43
2:F:651:THR:OG1	2:F:652:LEU:N	2.51	0.43
2:D:482:LEU:HD13	2:D:486:ARG:HH21	1.84	0.43
1:E:591:ALA:HB2	1:E:619:CYS:SG	2.58	0.43
2:L:651:THR:OG1	2:L:652:LEU:N	2.52	0.43
2:B:695:LEU:HD12	2:L:576:ASN:ND2	2.32	0.43
2:H:587:LEU:HD23	2:H:587:LEU:HA	1.89	0.43
2:F:485:LYS:HA	2:F:485:LYS:HD3	1.80	0.43
2:H:605:ALA:HA	2:H:631:ILE:O	2.19	0.43
1:A:600:TYR:CD1	1:A:609:LEU:HD12	2.54	0.43
2:B:516:ASP:O	2:B:520:ARG:HG2	2.18	0.43
2:D:550:GLU:HG3	2:D:557:LEU:HD21	2.00	0.43
1:G:529:LYS:HB3	1:G:641:LEU:HD21	2.00	0.43
1:G:574:ASP:OD1	1:G:574:ASP:N	2.49	0.43
2:D:554:GLY:O	2:D:557:LEU:HB2	2.19	0.43
1:A:645:LEU:HB3	1:A:653:SER:HB3	2.00	0.43
1:E:590:GLY:HA3	1:E:628:ILE:HD11	2.01	0.43
1:I:529:LYS:H	1:I:529:LYS:HG2	1.49	0.43
2:B:515:LEU:HD23	2:B:515:LEU:HA	1.83	0.42
2:B:572:LEU:HA	2:B:575:PHE:HB2	2.01	0.42
2:B:695:LEU:HD12	2:L:576:ASN:HD21	1.84	0.42
2:J:506:ASN:O	2:J:510:SER:OG	2.28	0.42
1:K:649:SER:HB2	1:K:651:VAL:HG22	2.00	0.42
2:D:572:LEU:HD23	2:D:572:LEU:HA	1.90	0.42
2:D:679:LYS:HD2	2:D:679:LYS:HA	1.72	0.42
2:B:496:LEU:O	2:B:500:THR:OG1	2.32	0.42
2:D:587:LEU:HD23	2:D:587:LEU:HA	1.92	0.42
1:G:526:THR:HG23	1:G:597:VAL:O	2.19	0.42
2:L:496:LEU:O	2:L:500:THR:OG1	2.32	0.42
1:C:572:PRO:O	1:C:576:LEU:HB2	2.20	0.42
2:B:699:LEU:HD22	2:L:569:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:656:ALA:HA	1:G:659:LEU:HB2	2.02	0.42
2:H:482:LEU:HD23	2:H:482:LEU:HA	1.81	0.42
1:K:526:THR:HG23	1:K:597:VAL:O	2.20	0.42
1:A:572:PRO:HB2	1:A:575:TYR:HB3	2.02	0.41
2:F:553:ALA:HB3	2:F:557:LEU:CD1	2.50	0.41
2:B:611:LYS:HA	2:B:611:LYS:HD2	1.89	0.41
1:C:585:LEU:HD12	1:C:615:ASN:HB3	2.02	0.41
1:K:656:ALA:HB1	1:K:659:LEU:HB2	2.02	0.41
2:L:482:LEU:HD23	2:L:482:LEU:HA	1.84	0.41
1:E:576:LEU:HD21	1:E:611:TYR:HB2	2.01	0.41
2:D:553:ALA:HB3	2:D:557:LEU:HD13	2.01	0.41
2:D:644:ALA:O	1:E:554:ARG:NH2	2.42	0.41
2:J:602:THR:OG1	2:J:604:ASP:OD1	2.39	0.41
1:E:550:GLU:OE1	1:E:554:ARG:NE	2.41	0.41
1:I:594:VAL:O	1:I:598:ILE:HG13	2.21	0.41
2:L:523:ILE:O	2:L:528:GLN:NE2	2.51	0.41
2:L:604:ASP:OD1	2:L:604:ASP:N	2.54	0.41
1:I:525:PRO:HB3	1:I:597:VAL:HG12	2.03	0.41
1:G:661:ALA:HB2	1:G:664:ARG:HH11	1.86	0.41
2:J:524:ASN:OD1	2:J:570:LYS:NZ	2.40	0.41
1:A:532:ILE:O	1:A:535:THR:OG1	2.35	0.41
1:A:538:LEU:O	1:A:541:ASN:HB2	2.20	0.41
2:B:651:THR:HG23	2:B:653:GLU:H	1.86	0.41
1:E:574:ASP:OD1	1:E:574:ASP:N	2.45	0.41
1:A:564:ARG:NH2	2:B:667:TYR:OH	2.54	0.41
1:C:649:SER:HB2	1:C:651:VAL:HG23	2.02	0.41
2:F:550:GLU:OE2	2:F:674:ARG:N	2.50	0.41
1:C:575:TYR:HE1	2:D:643:ARG:HB2	1.86	0.40
1:C:600:TYR:HD2	1:C:609:LEU:CD1	2.33	0.40
2:H:504:ILE:H	2:H:504:ILE:HG12	1.67	0.40
2:L:640:GLN:O	2:L:644:ALA:HB2	2.21	0.40
1:C:561:LYS:HB2	1:C:561:LYS:HE3	1.91	0.40
1:G:588:LEU:HD22	1:G:589:LYS:H	1.86	0.40
2:J:650:ILE:HD12	2:J:656:GLN:HG2	2.03	0.40
2:D:648:ASP:OD1	2:D:659:HIS:ND1	2.51	0.40
1:A:603:PRO:HB3	3:M:9:DT:H6	1.84	0.40
1:I:624:ASP:O	1:I:628:ILE:HG13	2.21	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	180/233 (77%)	171 (95%)	7 (4%)	2 (1%)	11	44
1	C	180/233 (77%)	170 (94%)	10 (6%)	0	100	100
1	E	176/233 (76%)	168 (96%)	7 (4%)	1 (1%)	21	55
1	G	176/233 (76%)	165 (94%)	10 (6%)	1 (1%)	21	55
1	I	171/233 (73%)	160 (94%)	11 (6%)	0	100	100
1	K	173/233 (74%)	163 (94%)	10 (6%)	0	100	100
2	B	234/256 (91%)	227 (97%)	6 (3%)	1 (0%)	30	61
2	D	233/256 (91%)	226 (97%)	6 (3%)	1 (0%)	30	61
2	F	233/256 (91%)	228 (98%)	5 (2%)	0	100	100
2	H	234/256 (91%)	225 (96%)	9 (4%)	0	100	100
2	J	236/256 (92%)	228 (97%)	8 (3%)	0	100	100
2	L	237/256 (93%)	231 (98%)	6 (2%)	0	100	100
All	All	2463/2934 (84%)	2362 (96%)	95 (4%)	6 (0%)	43	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	646	THR
1	A	601	GLU
2	B	524	ASN
1	A	655	GLY
1	G	590	GLY
1	E	605	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	155/201 (77%)	155 (100%)	0	100	100
1	C	155/201 (77%)	155 (100%)	0	100	100
1	E	151/201 (75%)	151 (100%)	0	100	100
1	G	151/201 (75%)	151 (100%)	0	100	100
1	I	147/201 (73%)	146 (99%)	1 (1%)	76	78
1	K	148/201 (74%)	148 (100%)	0	100	100
2	B	206/223 (92%)	206 (100%)	0	100	100
2	D	205/223 (92%)	205 (100%)	0	100	100
2	F	205/223 (92%)	205 (100%)	0	100	100
2	H	206/223 (92%)	206 (100%)	0	100	100
2	J	208/223 (93%)	208 (100%)	0	100	100
2	L	209/223 (94%)	209 (100%)	0	100	100
All	All	2146/2544 (84%)	2145 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	599	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	527	GLN
2	B	528	GLN
1	C	524	GLN
1	C	531	GLN
1	C	615	ASN
1	C	621	ASN
1	C	633	HIS
2	D	528	GLN
1	E	636	HIS
2	F	493	GLN
2	F	525	GLN

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Mol	Chain	Res	Type
2	F	579	ASN
2	F	590	ASN
2	H	576	ASN
2	H	678	GLN
1	I	563	GLN
2	J	590	ASN
2	J	678	GLN
2	L	525	GLN
2	L	538	ASN
2	L	696	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/233 (78%)	0.37	4 (2%) 62 34	22, 70, 117, 140	0
1	C	182/233 (78%)	0.42	5 (2%) 56 30	25, 66, 113, 132	0
1	E	178/233 (76%)	0.59	5 (2%) 55 30	40, 98, 138, 155	0
1	G	178/233 (76%)	0.65	7 (3%) 43 22	50, 100, 136, 147	0
1	I	173/233 (74%)	1.10	13 (7%) 20 12	73, 128, 160, 177	0
1	K	175/233 (75%)	1.26	25 (14%) 6 4	107, 146, 175, 189	0
2	B	236/256 (92%)	0.30	4 (1%) 69 40	26, 52, 108, 154	0
2	D	235/256 (91%)	0.20	3 (1%) 75 47	20, 49, 105, 141	0
2	F	235/256 (91%)	0.19	3 (1%) 75 47	22, 48, 90, 113	0
2	H	236/256 (92%)	0.13	1 (0%) 88 69	17, 47, 93, 118	0
2	J	238/256 (92%)	0.47	7 (2%) 53 29	41, 73, 114, 142	0
2	L	239/256 (93%)	0.51	8 (3%) 49 26	44, 79, 113, 143	0
3	M	2/10 (20%)	1.60	0 100 100	86, 86, 86, 113	0
3	N	2/10 (20%)	1.55	1 (50%) 0 1	91, 91, 91, 120	0
All	All	2491/2954 (84%)	0.48	86 (3%) 47 25	17, 72, 147, 189	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	517	GLY	6.1
2	L	706	ILE	5.0
1	C	601	GLU	3.5
2	J	566	GLU	3.4
1	I	622	VAL	3.3
1	I	652	ILE	3.2
1	K	630	PHE	3.2
1	C	642	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	575	TYR	3.2
2	L	578	MET	3.2
1	K	517	GLY	3.0
1	G	671	VAL	2.9
2	D	700	ARG	2.9
1	K	575	TYR	2.9
1	K	629	ALA	2.9
2	H	704	GLU	2.9
1	K	605	ILE	2.8
2	J	636	GLU	2.8
2	B	700	ARG	2.8
1	K	639	VAL	2.8
2	L	566	GLU	2.8
1	K	622	VAL	2.7
1	K	651	VAL	2.7
1	K	608	ALA	2.7
1	C	629	ALA	2.6
1	K	613	CYS	2.6
1	E	548	ASP	2.6
1	A	674	LEU	2.6
2	L	565	ASP	2.6
1	K	546	ILE	2.5
1	K	611	TYR	2.5
1	C	655	GLY	2.5
1	E	671	VAL	2.5
2	J	646	THR	2.5
2	L	567	VAL	2.5
2	J	706	ILE	2.5
1	I	496	ARG	2.5
1	K	563	GLN	2.5
1	G	601	GLU	2.4
1	A	629	ALA	2.4
1	K	580	PRO	2.4
1	I	630	PHE	2.4
1	K	637	LYS	2.4
1	I	659	LEU	2.4
1	K	530	TYR	2.4
2	D	526	HIS	2.4
2	F	702	ASN	2.4
1	E	579	LYS	2.4
1	I	643	GLY	2.3
2	J	527	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	592	LYS	2.3
1	I	511	TYR	2.3
1	I	636	HIS	2.2
1	K	584	LYS	2.2
2	B	526	HIS	2.2
1	G	591	ALA	2.2
1	G	514	SER	2.2
1	G	662	LYS	2.2
3	N	4	DT	2.1
2	D	702	ASN	2.1
1	K	578	VAL	2.1
1	K	648	LYS	2.1
1	K	595	ILE	2.1
1	E	521	ASP	2.1
1	I	637	LYS	2.1
1	K	585	LEU	2.1
1	K	631	GLY	2.1
1	K	644	THR	2.1
1	I	516	TYR	2.1
2	F	703	ILE	2.1
1	K	646	PHE	2.1
1	C	674	LEU	2.1
1	G	516	TYR	2.0
2	L	659	HIS	2.0
2	F	683	LYS	2.0
1	K	612	ALA	2.0
2	L	564	SER	2.0
1	A	671	VAL	2.0
2	L	480	GLN	2.0
2	B	469	ASN	2.0
2	B	576	ASN	2.0
1	I	644	THR	2.0
2	J	596	ASP	2.0
2	J	523	ILE	2.0
1	A	583	GLU	2.0
1	G	521	ASP	2.0

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

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

6.3 Carbohydrates [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.