



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:31 AM UTC

PDB ID : 5C6G / pdb_00005c6g
Title : Structural Insights into the Scc2-Scc4 Cohesin Loader
Authors : Singleton, M.R.; Chao, W.C.H.
Deposited on : 2015-06-23
Resolution : 2.60 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

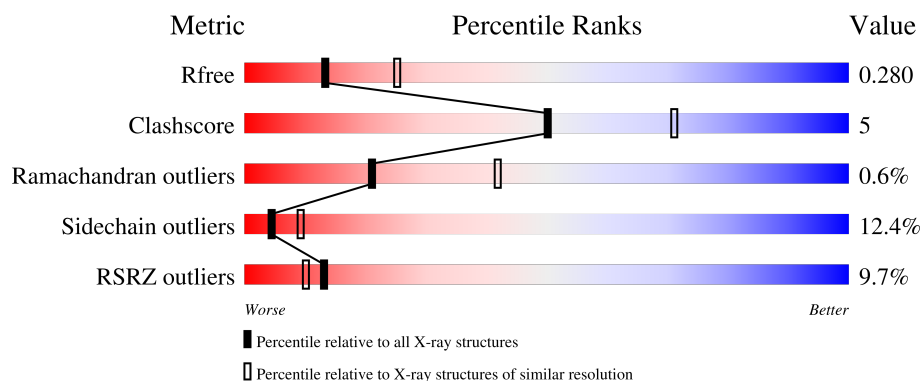
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	620	3% 77% 17% • •
1	C	620	16% 75% 17% • 5%
2	B	218	4% 39% 11% 7% 42%
2	D	218	7% 41% 12% • 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11563 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 AGR133Cp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	0	0
			4854	3097	833	901	23			
1	C	588	Total	C	N	O	S	0	0	0
			4725	3016	811	875	23			

- Molecule 2 is a protein called Sister chromatid cohesion protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			1006	629	180	195	2			
2	D	121	Total	C	N	O	S	0	0	0
			968	606	174	186	2			

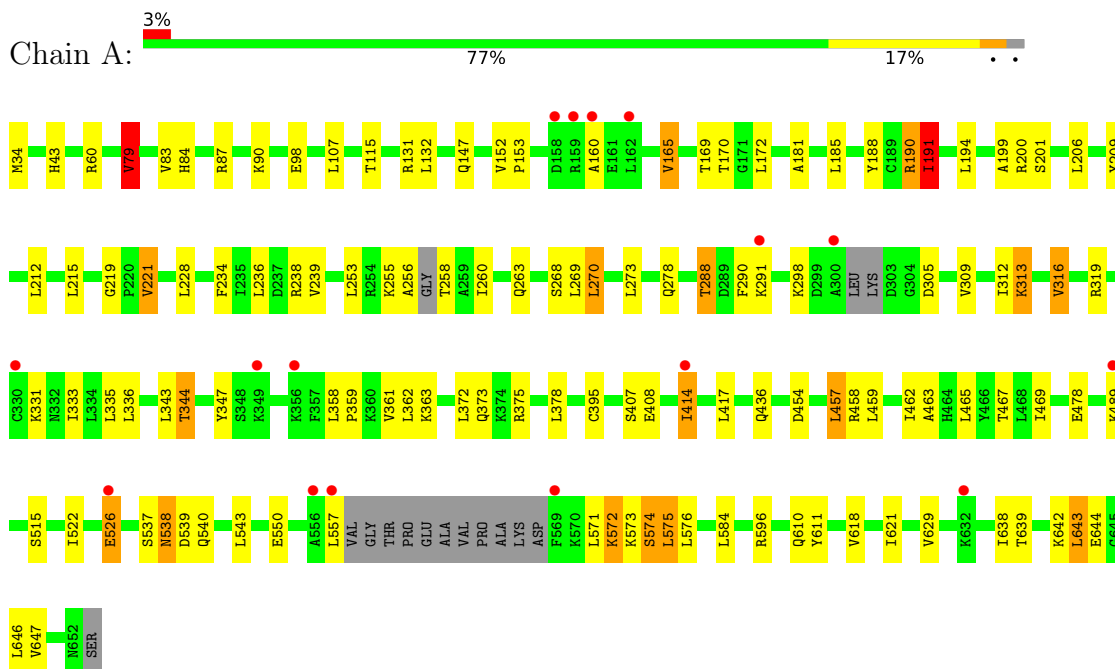
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	3	Total	O	0	0
			3	3		
3	C	4	Total	O	0	0
			4	4		
3	D	1	Total	O	0	0
			1	1		

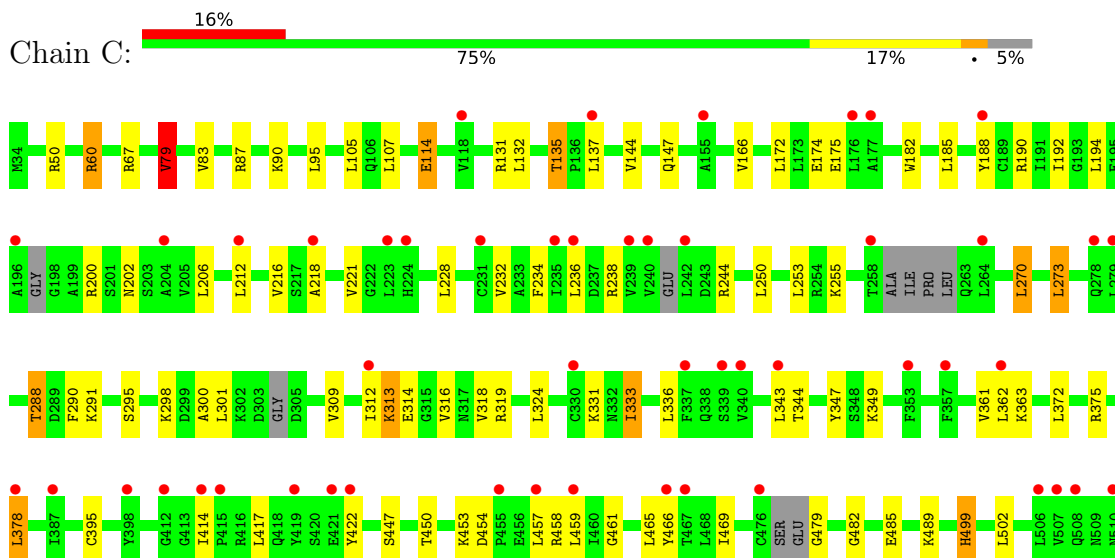
3 Residue-property plots

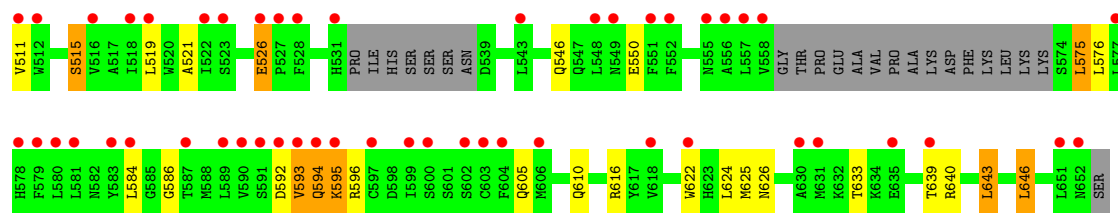
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: AGR133Cp

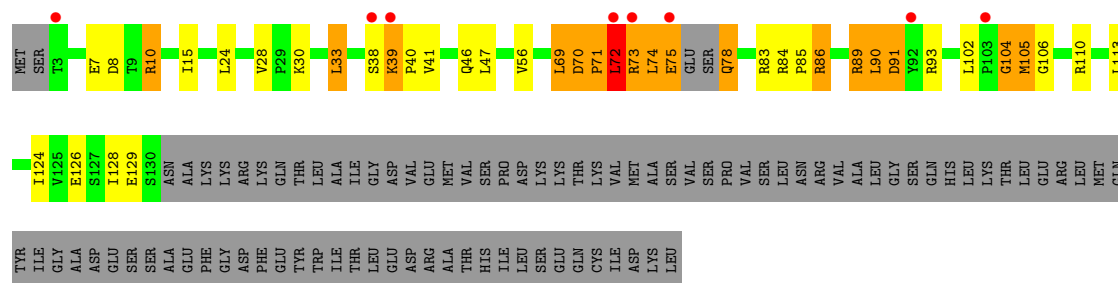
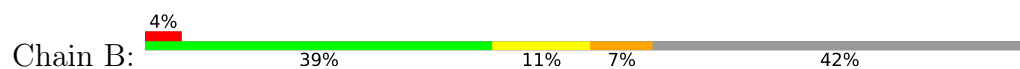


• Molecule 1: AGR133Cp

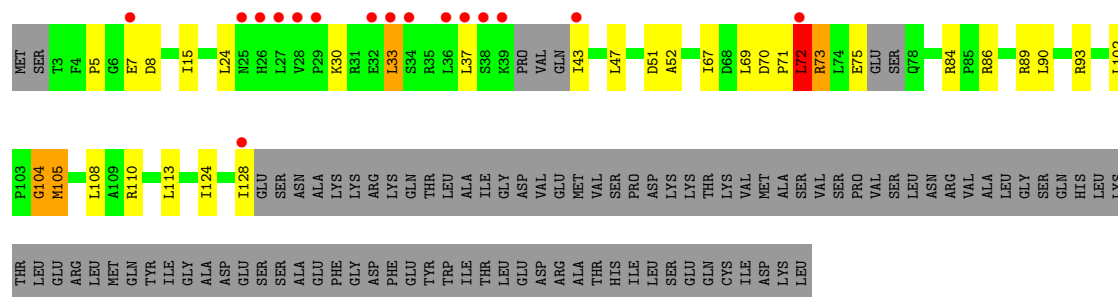




• Molecule 2: Sister chromatid cohesion protein 2



• Molecule 2: Sister chromatid cohesion protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.24Å 88.81Å 116.00Å 90.00° 118.49° 90.00°	Depositor
Resolution (Å)	98.65 – 2.60 98.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (98.65-2.60) 96.7 (98.65-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.227 , 0.274 0.235 , 0.280	Depositor DCC
R_{free} test set	3198 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-l,k,h 0.008 for l,k,-h-l 0.018 for h,-k,-h-l 0.017 for -h-l,-k,l 0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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	0.74	2/4939 (0.0%)	0.99	8/6684 (0.1%)
1	C	0.48	1/4802 (0.0%)	0.84	5/6493 (0.1%)
2	B	0.70	0/1026	1.11	8/1391 (0.6%)
2	D	0.48	0/986	0.89	4/1334 (0.3%)
All	All	0.62	3/11753 (0.0%)	0.93	25/15902 (0.2%)

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
2	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	VAL	CA-CB	5.62	1.61	1.54
1	A	191	ILE	CA-CB	5.17	1.60	1.54
1	A	79	VAL	CA-CB	5.13	1.61	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	GLU	CA-C-N	-9.22	108.80	118.85
1	A	526	GLU	C-N-CA	-9.22	108.80	118.85
2	B	73	ARG	N-CA-C	8.85	123.33	112.54
2	B	71	PRO	CA-C-O	-8.14	115.28	121.31
2	D	73	ARG	N-CA-C	7.84	122.42	113.01
2	B	70	ASP	CA-C-N	-7.72	111.48	121.91
2	B	70	ASP	C-N-CA	-7.72	111.48	121.91
1	A	571	LEU	N-CA-C	7.40	119.86	110.24
2	B	69	LEU	N-CA-C	-7.36	101.04	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	LYS	N-CA-C	6.46	120.74	112.34
2	D	104	GLY	CA-C-N	6.13	132.74	121.70
2	D	104	GLY	C-N-CA	6.13	132.74	121.70
2	B	104	GLY	CA-C-N	6.07	132.62	121.70
2	B	104	GLY	C-N-CA	6.07	132.62	121.70
2	B	28	VAL	N-CA-C	6.05	114.54	107.77
2	D	69	LEU	N-CA-C	-5.64	101.35	110.32
1	C	526	GLU	CA-C-N	-5.43	114.08	119.56
1	C	526	GLU	C-N-CA	-5.43	114.08	119.56
1	C	633	THR	N-CA-C	5.32	118.00	111.82
1	C	479	GLY	CA-C-N	5.31	124.76	119.24
1	C	479	GLY	C-N-CA	5.31	124.76	119.24
1	A	414	ILE	CA-C-N	5.20	125.12	119.76
1	A	414	ILE	C-N-CA	5.20	125.12	119.76
1	A	152	VAL	CA-C-N	-5.02	114.44	119.56
1	A	152	VAL	C-N-CA	-5.02	114.44	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	72	LEU	Peptide

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	4854	0	4922	46	0
1	C	4725	0	4792	48	0
2	B	1006	0	999	25	0
2	D	968	0	963	14	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	2	0
3	D	1	0	0	0	0
All	All	11563	0	11676	124	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 (124) 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:181:ALA:HB1	1:A:312:ILE:HD12	1.66	0.77
1:C:309:VAL:HG12	1:C:319:ARG:HG2	1.76	0.68
1:A:309:VAL:HG12	1:A:319:ARG:HG2	1.77	0.66
1:C:135:THR:HG23	1:C:137:LEU:H	1.61	0.66
1:A:221:VAL:HG13	1:A:260:ILE:HD13	1.79	0.65
2:D:104:GLY:HA2	2:D:105:MET:HB3	1.78	0.64
1:C:422:TYR:HE1	1:C:457:LEU:HD11	1.64	0.62
1:A:199:ALA:C	1:A:201:SER:H	2.07	0.61
1:C:616:ARG:HD3	1:C:646:LEU:HD11	1.82	0.61
1:A:170:THR:OG1	1:A:190:ARG:NH1	2.34	0.61
1:A:465:LEU:O	1:A:469:ILE:HG12	2.01	0.60
1:C:234:PHE:HE1	1:C:238:ARG:HH11	1.49	0.60
2:B:30:LYS:O	2:B:33:LEU:HB2	2.00	0.60
1:C:67:ARG:HH11	2:D:93:ARG:HH12	1.49	0.59
2:B:84:ARG:NH1	2:B:124:ILE:O	2.37	0.58
1:A:191:ILE:HD13	1:A:209:TYR:CZ	2.39	0.57
1:C:465:LEU:O	1:C:469:ILE:HG12	2.06	0.56
1:A:361:VAL:HG23	1:A:395:CYS:SG	2.45	0.56
2:B:84:ARG:HB2	2:B:124:ILE:HG22	1.87	0.56
2:B:38:SER:O	2:B:38:SER:OG	2.20	0.56
2:B:75:GLU:O	2:B:78:GLN:N	2.38	0.56
2:D:70:ASP:OD1	2:D:73:ARG:N	2.40	0.55
2:D:105:MET:O	2:D:110:ARG:NH1	2.40	0.55
1:C:624:LEU:HD23	1:C:625:MET:HE2	1.89	0.54
1:C:232:VAL:HG21	1:C:250:LEU:HD13	1.90	0.53
1:C:575:LEU:HD23	1:C:610:GLN:HG2	1.90	0.53
2:B:38:SER:O	2:B:40:PRO:HD3	2.07	0.53
2:B:70:ASP:OD1	2:B:73:ARG:N	2.42	0.53
1:C:270:LEU:HD13	1:C:290:PHE:HZ	1.73	0.53
1:C:288:THR:HA	1:C:291:LYS:HD2	1.91	0.53
1:A:618:VAL:HG21	2:B:15:ILE:HD12	1.91	0.52
2:B:89:ARG:NH2	2:B:91:ASP:HB2	2.25	0.52
1:A:537:SER:N	1:A:538:ASN:HA	2.25	0.51
2:B:89:ARG:O	2:B:89:ARG:HG3	2.10	0.51
1:C:270:LEU:HD13	1:C:290:PHE:CZ	2.47	0.50
1:C:640:ARG:HG3	2:D:5:PRO:HG3	1.93	0.50
1:A:572:LYS:O	1:A:573:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLU:HA	1:C:175:GLU:HA	1.61	0.49
2:D:84:ARG:NH1	2:D:124:ILE:O	2.46	0.49
1:A:43:HIS:HB3	2:B:56:VAL:HG12	1.95	0.49
2:B:39:LYS:HD3	2:B:39:LYS:H	1.78	0.48
2:B:86:ARG:HH11	2:B:126:GLU:HB3	1.78	0.48
1:C:216:VAL:C	1:C:218:ALA:H	2.20	0.48
1:A:153:PRO:HG3	1:A:165:VAL:HG21	1.94	0.48
2:D:7:GLU:O	2:D:8:ASP:HB2	2.14	0.48
1:A:263:GLN:NE2	1:A:305:ASP:O	2.47	0.47
1:A:373:GLN:HG3	1:A:375:ARG:HH22	1.78	0.47
1:C:466:TYR:HE2	1:C:519:LEU:HB3	1.78	0.47
1:A:256:ALA:O	1:A:258:THR:N	2.47	0.47
1:A:288:THR:HA	1:A:291:LYS:HD2	1.96	0.47
2:B:7:GLU:O	2:B:8:ASP:CG	2.57	0.47
1:C:295:SER:HA	1:C:298:LYS:HG3	1.97	0.47
1:A:335:LEU:HB3	1:A:361:VAL:CG1	2.45	0.47
1:A:160:ALA:HB1	2:D:8:ASP:HB3	1.97	0.46
1:A:373:GLN:HG3	1:A:375:ARG:NH2	2.30	0.46
1:A:199:ALA:C	1:A:201:SER:N	2.73	0.46
1:C:461:GLY:O	1:C:465:LEU:HB2	2.15	0.46
2:D:67:ILE:HD12	2:D:108:LEU:HD11	1.97	0.46
2:B:106:GLY:O	2:B:110:ARG:HG3	2.16	0.46
2:D:84:ARG:HB2	2:D:124:ILE:HG22	1.98	0.46
1:C:511:VAL:O	1:C:515:SER:OG	2.30	0.46
1:A:313:LYS:HD2	1:A:316:VAL:HG13	1.98	0.46
1:C:188:TYR:O	1:C:192:ILE:HG12	2.16	0.46
2:B:71:PRO:O	2:B:72:LEU:HD23	2.16	0.45
2:B:72:LEU:HD12	2:B:73:ARG:HG2	1.98	0.45
1:C:79:VAL:O	1:C:83:VAL:HG23	2.17	0.45
1:A:188:TYR:O	1:A:191:ILE:HG13	2.16	0.45
1:A:458:ARG:O	1:A:462:ILE:HG13	2.15	0.45
1:A:269:LEU:HG	1:A:290:PHE:CE2	2.51	0.45
1:C:592:ASP:OD1	1:C:594:GLN:N	2.49	0.45
1:A:185:LEU:HD11	1:A:312:ILE:HD13	1.98	0.45
2:B:10:ARG:H	2:B:10:ARG:HG3	1.51	0.45
1:A:347:TYR:CZ	1:A:575:LEU:HD13	2.51	0.45
1:A:239:VAL:HG12	1:A:278:GLN:NE2	2.33	0.44
2:B:104:GLY:HA2	2:B:105:MET:HB3	1.99	0.44
1:C:521:ALA:HB3	1:C:584:LEU:HD21	1.97	0.44
1:A:269:LEU:HG	1:A:290:PHE:CZ	2.52	0.44
2:B:90:LEU:HD12	2:B:90:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:HE21	1:A:375:ARG:HH22	1.66	0.44
1:C:361:VAL:HG23	1:C:395:CYS:SG	2.58	0.44
1:C:454:ASP:HB3	1:C:457:LEU:HB2	1.99	0.44
1:A:234:PHE:CE1	1:A:238:ARG:HD3	2.53	0.44
1:A:643:LEU:O	1:A:647:VAL:HG13	2.18	0.44
2:B:91:ASP:OD1	2:B:93:ARG:HG2	2.17	0.44
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.89	0.43
1:C:626:ASN:ND2	3:C:701:HOH:O	2.50	0.43
1:A:115:THR:O	2:B:83:ARG:NE	2.47	0.43
1:C:319:ARG:O	2:D:43:ILE:HA	2.18	0.43
1:C:575:LEU:HD12	1:C:575:LEU:HA	1.77	0.43
1:C:166:VAL:HG13	1:C:190:ARG:HG3	2.00	0.43
1:C:50:ARG:HD3	1:C:50:ARG:HA	1.72	0.42
1:C:185:LEU:HD21	1:C:318:VAL:HG21	2.00	0.42
1:C:333:ILE:HD13	2:D:37:LEU:HD21	2.00	0.42
1:C:596:ARG:O	3:C:701:HOH:O	2.21	0.42
1:C:499:HIS:HA	1:C:502:LEU:HD12	2.01	0.42
1:A:537:SER:H	1:A:538:ASN:HA	1.83	0.42
1:A:639:THR:HG22	1:A:643:LEU:HD22	2.00	0.42
1:C:593:VAL:HG13	1:C:596:ARG:NH2	2.35	0.42
1:A:344:THR:HG21	1:A:574:SER:OG	2.18	0.42
1:A:454:ASP:HB3	1:A:457:LEU:HB2	2.00	0.42
1:A:638:ILE:HG13	1:A:642:LYS:HE3	2.02	0.41
1:C:105:LEU:HD21	1:C:144:VAL:HG22	2.01	0.41
1:A:408:GLU:HB2	1:A:611:TYR:CZ	2.55	0.41
1:C:60:ARG:NH2	1:C:114:GLU:OE1	2.35	0.41
1:A:358:LEU:N	1:A:359:PRO:HD2	2.35	0.41
1:C:312:ILE:HG13	1:C:313:LYS:N	2.36	0.41
2:B:84:ARG:HA	2:B:85:PRO:HD3	1.92	0.41
1:A:270:LEU:HD13	1:A:290:PHE:HZ	1.85	0.41
2:B:39:LYS:O	2:B:39:LYS:NZ	2.37	0.41
1:C:447:SER:O	1:C:450:THR:OG1	2.39	0.41
1:C:592:ASP:HB3	1:C:595:LYS:HG2	2.02	0.41
1:A:575:LEU:HD23	1:A:610:GLN:HG2	2.03	0.41
1:C:586:GLY:HA3	1:C:622:TRP:HH2	1.86	0.41
2:D:71:PRO:O	2:D:72:LEU:HD23	2.21	0.41
1:C:349:LYS:HD2	1:C:349:LYS:HA	1.93	0.40
1:A:270:LEU:HD13	1:A:290:PHE:CZ	2.56	0.40
1:A:463:ALA:O	1:A:467:THR:HG23	2.21	0.40
1:C:347:TYR:CE2	1:C:575:LEU:HD22	2.56	0.40
1:C:639:THR:O	1:C:643:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:HIS:NE2	2:B:74:LEU:HD13	2.36	0.40
1:C:482:GLY:O	1:C:485:GLU:HG2	2.21	0.40
1:A:79:VAL:O	1:A:83:VAL:HG23	2.22	0.40
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.80	0.40
2:D:30:LYS:O	2:D:33:LEU:HB2	2.21	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	597/620 (96%)	576 (96%)	20 (3%)	1 (0%)	43	66
1	C	572/620 (92%)	552 (96%)	19 (3%)	1 (0%)	43	66
2	B	122/218 (56%)	111 (91%)	8 (7%)	3 (2%)	4	8
2	D	115/218 (53%)	103 (90%)	8 (7%)	4 (4%)	3	4
All	All	1406/1676 (84%)	1342 (95%)	55 (4%)	9 (1%)	21	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	GLY
2	B	72	LEU
2	D	72	LEU
2	D	51	ASP
2	B	105	MET
1	C	300	ALA
2	D	52	ALA
2	D	105	MET
2	B	41	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	541/552 (98%)	473 (87%)	68 (13%)	4	9
1	C	526/552 (95%)	465 (88%)	61 (12%)	5	11
2	B	113/194 (58%)	94 (83%)	19 (17%)	2	4
2	D	108/194 (56%)	96 (89%)	12 (11%)	6	12
All	All	1288/1492 (86%)	1128 (88%)	160 (12%)	4	9

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	MET
1	A	60	ARG
1	A	79	VAL
1	A	87	ARG
1	A	90	LYS
1	A	98	GLU
1	A	107	LEU
1	A	131	ARG
1	A	132	LEU
1	A	147	GLN
1	A	165	VAL
1	A	169	THR
1	A	172	LEU
1	A	190	ARG
1	A	191	ILE
1	A	194	LEU
1	A	200	ARG
1	A	206	LEU
1	A	212	LEU
1	A	215	LEU
1	A	221	VAL
1	A	228	LEU
1	A	236	LEU
1	A	253	LEU

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Mol	Chain	Res	Type
1	A	255	LYS
1	A	268	SER
1	A	270	LEU
1	A	273	LEU
1	A	288	THR
1	A	298	LYS
1	A	313	LYS
1	A	316	VAL
1	A	331	LYS
1	A	333	ILE
1	A	336	LEU
1	A	343	LEU
1	A	344	THR
1	A	362	LEU
1	A	363	LYS
1	A	372	LEU
1	A	378	LEU
1	A	407	SER
1	A	414	ILE
1	A	417	LEU
1	A	436	GLN
1	A	457	LEU
1	A	459	LEU
1	A	478	GLU
1	A	489	LYS
1	A	515	SER
1	A	522	ILE
1	A	526	GLU
1	A	538	ASN
1	A	539	ASP
1	A	540	GLN
1	A	543	LEU
1	A	550	GLU
1	A	557	LEU
1	A	574	SER
1	A	575	LEU
1	A	576	LEU
1	A	584	LEU
1	A	596	ARG
1	A	621	ILE
1	A	629	VAL
1	A	643	LEU

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Mol	Chain	Res	Type
1	A	644	GLU
1	A	646	LEU
2	B	10	ARG
2	B	24	LEU
2	B	33	LEU
2	B	39	LYS
2	B	46	GLN
2	B	47	LEU
2	B	69	LEU
2	B	72	LEU
2	B	74	LEU
2	B	75	GLU
2	B	78	GLN
2	B	86	ARG
2	B	89	ARG
2	B	90	LEU
2	B	91	ASP
2	B	102	LEU
2	B	113	LEU
2	B	128	ILE
2	B	129	GLU
1	C	60	ARG
1	C	79	VAL
1	C	87	ARG
1	C	90	LYS
1	C	95	LEU
1	C	107	LEU
1	C	114	GLU
1	C	131	ARG
1	C	132	LEU
1	C	135	THR
1	C	147	GLN
1	C	172	LEU
1	C	182	TRP
1	C	194	LEU
1	C	200	ARG
1	C	202	ASN
1	C	206	LEU
1	C	212	LEU
1	C	221	VAL
1	C	228	LEU
1	C	236	LEU

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Mol	Chain	Res	Type
1	C	244	ARG
1	C	253	LEU
1	C	255	LYS
1	C	270	LEU
1	C	273	LEU
1	C	288	THR
1	C	301	LEU
1	C	313	LYS
1	C	314	GLU
1	C	316	VAL
1	C	324	LEU
1	C	331	LYS
1	C	333	ILE
1	C	336	LEU
1	C	343	LEU
1	C	344	THR
1	C	362	LEU
1	C	363	LYS
1	C	372	LEU
1	C	375	ARG
1	C	378	LEU
1	C	414	ILE
1	C	417	LEU
1	C	453	LYS
1	C	458	ARG
1	C	459	LEU
1	C	489	LYS
1	C	499	HIS
1	C	515	SER
1	C	526	GLU
1	C	546	GLN
1	C	550	GLU
1	C	575	LEU
1	C	576	LEU
1	C	593	VAL
1	C	594	GLN
1	C	595	LYS
1	C	605	GLN
1	C	643	LEU
1	C	646	LEU
2	D	15	ILE
2	D	24	LEU

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Mol	Chain	Res	Type
2	D	33	LEU
2	D	47	LEU
2	D	72	LEU
2	D	75	GLU
2	D	86	ARG
2	D	89	ARG
2	D	90	LEU
2	D	102	LEU
2	D	113	LEU
2	D	128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	53	GLN
1	A	106	GLN
1	A	147	GLN
1	A	278	GLN
1	A	297	HIS
1	A	317	ASN
1	A	366	GLN
1	A	373	GLN
1	A	380	HIS
1	A	382	GLN
1	A	386	ASN
1	A	441	HIS
1	A	541	GLN
1	A	549	ASN
2	B	21	HIS
2	B	42	GLN
2	B	46	GLN
1	C	43	HIS
1	C	263	GLN
1	C	366	GLN
1	C	441	HIS
1	C	531	HIS
1	C	546	GLN
1	C	549	ASN
2	D	26	HIS

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	605/620 (97%)	0.21	16 (2%) 57 51	46, 65, 102, 136	0
1	C	588/620 (94%)	1.23	100 (17%) 4 3	61, 116, 150, 179	0
2	B	126/218 (57%)	0.49	8 (6%) 26 20	49, 70, 112, 137	0
2	D	121/218 (55%)	0.98	16 (13%) 7 5	70, 106, 143, 162	0
All	All	1440/1676 (85%)	0.72	140 (9%) 13 10	46, 88, 141, 179	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	ALA	5.5
1	C	595	LYS	5.4
1	A	557	LEU	5.4
1	C	552	PHE	4.8
1	A	162	LEU	4.7
1	C	581	LEU	4.7
2	D	128	ILE	4.5
1	C	577	LEU	4.1
1	C	592	ASP	4.0
2	D	29	PRO	3.8
1	C	278	GLN	3.7
1	C	240	VAL	3.6
1	C	639	THR	3.6
1	C	548	LEU	3.6
1	C	196	ALA	3.5
1	C	635	GLU	3.5
2	B	72	LEU	3.5
2	D	28	VAL	3.4
1	C	527	PRO	3.4
1	C	557	LEU	3.4
1	C	531	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	236	LEU	3.4
1	C	590	VAL	3.4
1	C	506	LEU	3.3
1	C	522	ILE	3.2
1	C	584	LEU	3.2
2	D	26	HIS	3.2
1	C	357	PHE	3.2
1	C	593	VAL	3.2
1	A	159	ARG	3.2
2	D	27	LEU	3.2
2	B	3	THR	3.2
2	D	34	SER	3.1
1	C	580	LEU	3.1
1	C	523	SER	3.1
1	C	630	ALA	3.0
1	C	419	TYR	3.0
1	C	622	TRP	3.0
2	D	72	LEU	2.9
1	C	353	PHE	2.9
1	C	558	VAL	2.9
1	C	422	TYR	2.9
2	D	36	LEU	2.9
1	C	512	TRP	2.9
1	C	337	PHE	2.9
1	C	378	LEU	2.9
2	B	38	SER	2.9
1	C	242	LEU	2.9
2	D	39	LYS	2.9
1	C	455	PRO	2.8
1	C	543	LEU	2.8
1	A	569	PHE	2.8
1	C	312	ILE	2.8
1	C	518	ILE	2.8
1	C	600	SER	2.8
1	C	583	TYR	2.8
1	C	603	CYS	2.7
1	C	387	ILE	2.7
2	D	43	ILE	2.7
1	C	118	VAL	2.7
1	A	349	LYS	2.7
1	C	204	ALA	2.7
1	C	604	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	414	ILE	2.7
1	C	651	LEU	2.7
1	C	176	LEU	2.6
1	C	589	LEU	2.6
1	A	330	CYS	2.6
1	C	556	ALA	2.6
1	C	606	MET	2.6
1	C	511	VAL	2.6
1	C	421	GLU	2.6
1	C	597	CYS	2.6
1	C	591	SER	2.5
1	A	158	ASP	2.5
1	C	137	LEU	2.5
1	C	507	VAL	2.5
1	A	556	ALA	2.5
1	C	223	LEU	2.5
1	C	415	PRO	2.5
1	C	258	THR	2.5
1	C	330	CYS	2.5
1	C	476	CYS	2.5
1	C	155	ALA	2.5
1	C	599	ILE	2.4
1	C	578	HIS	2.4
1	C	526	GLU	2.4
1	C	618	VAL	2.4
1	C	459	LEU	2.4
1	A	526	GLU	2.4
1	C	466	TYR	2.4
1	C	218	ALA	2.4
2	B	73	ARG	2.4
1	A	489	LYS	2.4
1	C	224	HIS	2.3
1	C	231	CYS	2.3
1	C	340	VAL	2.3
1	C	343	LEU	2.3
1	C	579	PHE	2.3
2	D	7	GLU	2.3
2	D	25	ASN	2.3
1	C	551	PHE	2.3
2	B	92	TYR	2.2
1	C	212	LEU	2.2
1	C	339	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	32	GLU	2.2
1	C	398	TYR	2.2
1	C	508	GLN	2.2
1	A	291	LYS	2.2
1	C	519	LEU	2.2
1	C	652	ASN	2.2
1	C	594	GLN	2.2
1	C	516	VAL	2.2
2	D	38	SER	2.2
1	A	356	LYS	2.1
1	A	632	LYS	2.1
1	C	457	LEU	2.1
1	A	414	ILE	2.1
1	C	467	THR	2.1
1	C	555	ASN	2.1
1	C	528	PHE	2.1
1	C	602	SER	2.1
1	A	160	ALA	2.1
1	C	177	ALA	2.1
2	B	75	GLU	2.1
1	C	264	LEU	2.1
1	C	279	LEU	2.1
1	C	510	ASN	2.1
1	C	188	TYR	2.1
1	C	412	GLY	2.1
1	C	587	THR	2.1
2	B	103	PRO	2.1
1	C	631	MET	2.1
2	D	37	LEU	2.1
1	C	549	ASN	2.1
2	B	39	LYS	2.0
1	C	235	ILE	2.0
1	C	239	VAL	2.0
1	C	362	LEU	2.0
2	D	33	LEU	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.