



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:54 PM UTC

PDB ID : 6QNX / pdb_00006qnx
Title : Structure of the SA2/SCC1/CTCF complex
Authors : Li, Y.; Muir, K.W.; Panne, D.
Deposited on : 2019-02-12
Resolution : 2.70 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

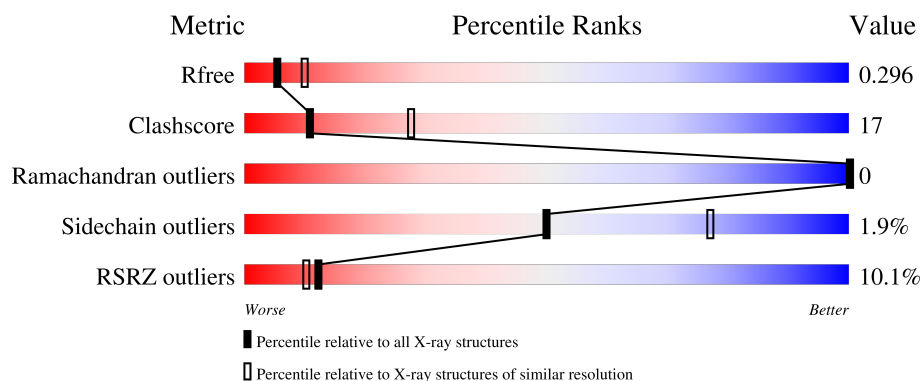
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	981	10% 64% 30% • 5%
2	B	140	% 42% 11% 47%
3	C	10	20% 90% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16469 atoms, of which 8240 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 Cohesin subunit SA-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	928	Total	C	H	N	O	S	0	0	0
			15088	4808	7539	1258	1428	55			

- Molecule 2 is a protein called 64-kDa C-terminal product.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	74	Total	C	H	N	O	S	0	0	0
			1235	385	639	101	107	3			

- Molecule 3 is a protein called Transcriptional repressor CTCF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O	0	0	0
			140	50	62	9	19			

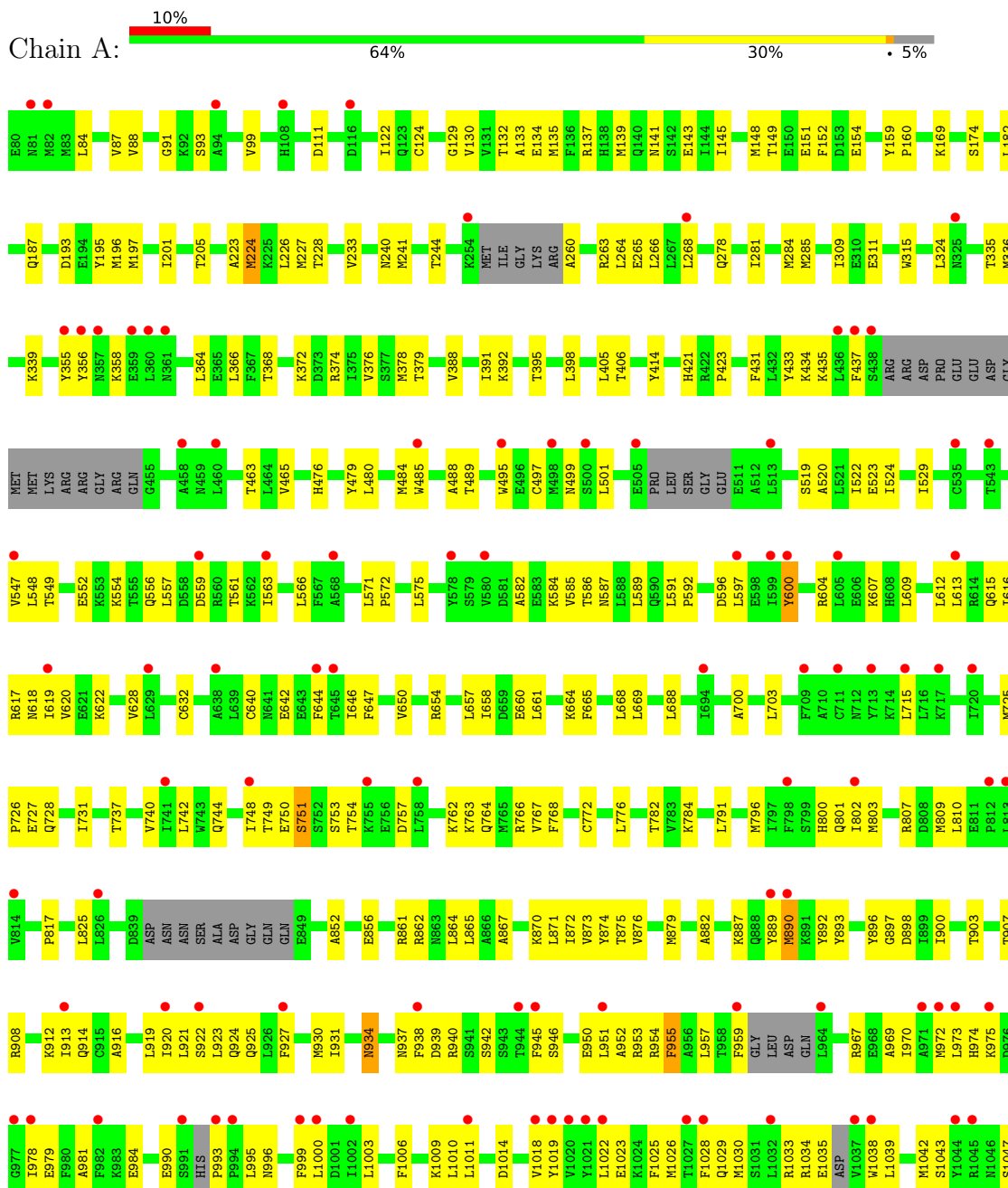
- Molecule 4 is water.

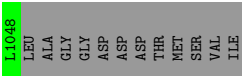
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0

3 Residue-property plots

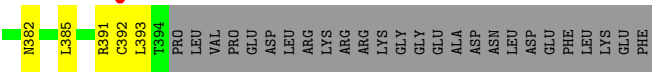
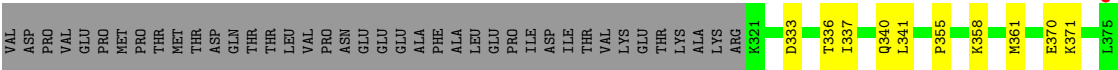
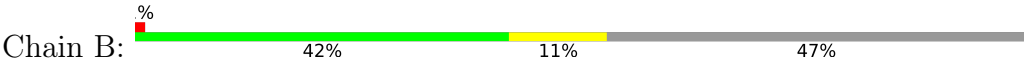
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cohesin subunit SA-2

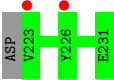
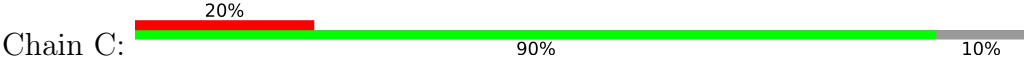




• Molecule 2: 64-kDa C-terminal product



• Molecule 3: Transcriptional repressor CTCF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.03Å 107.25Å 176.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 2.70 45.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.80-2.70) 99.6 (45.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.275 , 0.296	Depositor DCC
R_{free} test set	2741 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16469	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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	0.53	4/7677 (0.1%)	0.77	8/10341 (0.1%)
2	B	0.36	0/606	0.59	0/818
3	C	0.20	0/79	0.27	0/106
All	All	0.52	4/8362 (0.0%)	0.76	8/11265 (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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1039	LEU	C-N	7.76	1.51	1.33
1	A	952	ALA	CA-CB	-6.53	1.43	1.53
1	A	889	TYR	C-O	-5.19	1.18	1.24
1	A	224	MET	SD-CE	5.10	1.92	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	MET	CA-CB-CG	-7.66	98.79	114.10
1	A	1039	LEU	CA-C-N	7.29	128.95	119.84
1	A	1039	LEU	C-N-CA	7.29	128.95	119.84
1	A	955	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	227	MET	CB-CG-SD	6.17	131.22	112.70
1	A	955	PHE	CB-CA-C	-5.86	101.07	110.79
1	A	1039	LEU	O-C-N	-5.72	115.19	120.51
1	A	945	PHE	N-CA-C	-5.53	105.16	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	751	SER	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	7549	7539	7538	269	1
2	B	596	639	639	11	0
3	C	78	62	62	0	0
4	A	6	0	0	2	0
All	All	8229	8240	8239	273	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (273) 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:187:GLN:O	4:A:1301:HOH:O	1.82	0.96
1:A:993:PRO:N	1:A:1038:TRP:CZ2	2.37	0.91
1:A:197:MET:HB3	1:A:284:MET:HE2	1.52	0.91
1:A:803:MET:HA	1:A:807:ARG:HB2	1.54	0.90
1:A:224:MET:CE	1:A:315:TRP:CH2	2.58	0.87
1:A:993:PRO:HD3	1:A:1038:TRP:NE1	1.91	0.84
1:A:224:MET:HE2	1:A:315:TRP:CH2	2.14	0.83
1:A:642:GLU:HG2	1:A:647:PHE:CE2	2.14	0.82
1:A:132:THR:HG23	1:A:135:MET:HE3	1.62	0.81
1:A:224:MET:HE3	1:A:315:TRP:CZ2	2.14	0.81
1:A:547:VAL:HG12	1:A:548:LEU:H	1.46	0.80
1:A:993:PRO:N	1:A:1038:TRP:HZ2	1.80	0.79
1:A:201:ILE:O	1:A:205:THR:HG22	1.82	0.79
1:A:501:LEU:HD23	1:A:501:LEU:O	1.83	0.78
1:A:224:MET:CE	1:A:315:TRP:CZ2	2.66	0.78
1:A:129:GLY:C	1:A:148:MET:HE1	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:OG1	1:A:311:GLU:OE1	2.03	0.77
1:A:642:GLU:HG2	1:A:647:PHE:HE2	1.47	0.76
1:A:224:MET:CE	1:A:315:TRP:HH2	1.99	0.75
1:A:519:SER:HB3	1:A:584:LYS:HE3	1.70	0.74
1:A:134:GLU:OE1	1:A:137:ARG:NH1	2.20	0.74
1:A:934:ASN:N	1:A:934:ASN:OD1	2.21	0.73
1:A:993:PRO:HD3	1:A:1038:TRP:HE1	1.50	0.73
1:A:927:PHE:CD1	1:A:999:PHE:HD1	2.07	0.72
1:A:374:ARG:HG3	1:A:378:MET:HE2	1.71	0.72
1:A:571:LEU:HD23	1:A:612:LEU:HD22	1.72	0.71
1:A:364:LEU:O	1:A:368:THR:HG23	1.90	0.71
1:A:908:ARG:HG2	1:A:912:LYS:HD3	1.69	0.71
1:A:224:MET:HE3	1:A:315:TRP:HZ2	1.53	0.71
1:A:572:PRO:HG3	1:A:612:LEU:HB2	1.72	0.71
1:A:913:ILE:HD11	1:A:972:MET:HB3	1.73	0.70
1:A:975:LYS:HA	1:A:978:ILE:HG12	1.72	0.70
1:A:600:TYR:HB3	1:A:646:ILE:HD11	1.73	0.70
1:A:796:MET:HE2	1:A:871:LEU:HD23	1.74	0.70
1:A:920:ILE:HD13	1:A:923:LEU:HD12	1.73	0.69
1:A:1014:ASP:O	1:A:1018:VAL:HG13	1.91	0.69
1:A:437:PHE:HE1	1:A:463:THR:HB	1.57	0.69
1:A:197:MET:CB	1:A:284:MET:HE2	2.22	0.69
1:A:376:VAL:O	1:A:379:THR:HG23	1.93	0.68
1:A:664:LYS:O	1:A:668:LEU:HD12	1.93	0.68
1:A:974:HIS:O	1:A:978:ILE:HG23	1.93	0.68
1:A:240:ASN:O	1:A:244:THR:HG23	1.94	0.68
1:A:130:VAL:N	1:A:148:MET:HE1	2.09	0.68
1:A:111:ASP:OD1	1:A:195:TYR:OH	2.11	0.67
1:A:609:LEU:HD21	1:A:646:ILE:HG21	1.77	0.66
1:A:309:ILE:HG13	1:A:335:THR:HG21	1.77	0.66
1:A:646:ILE:HG22	1:A:650:VAL:HG23	1.76	0.66
1:A:920:ILE:HG12	1:A:973:LEU:HD11	1.78	0.66
1:A:613:LEU:HD11	1:A:650:VAL:HG22	1.77	0.66
1:A:355:TYR:OH	1:A:368:THR:HG21	1.96	0.65
1:A:620:VAL:HG12	1:A:632:CYS:SG	2.36	0.65
1:A:921:LEU:HD13	1:A:921:LEU:O	1.96	0.65
1:A:993:PRO:CD	1:A:1038:TRP:CZ2	2.79	0.65
1:A:224:MET:HE2	1:A:315:TRP:HH2	1.59	0.65
1:A:391:ILE:O	1:A:395:THR:HG23	1.96	0.64
1:A:715:LEU:HD21	1:A:725:MET:SD	2.37	0.64
1:A:927:PHE:CD1	1:A:999:PHE:CD1	2.84	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LEU:HD12	1:A:612:LEU:HD11	1.78	0.64
1:A:398:LEU:HD12	1:A:405:LEU:HD12	1.80	0.64
1:A:751:SER:OG	1:A:809:MET:HE1	1.98	0.64
1:A:984:GLU:HB3	1:A:995:LEU:HD12	1.80	0.63
1:A:575:LEU:HD12	1:A:612:LEU:CD1	2.27	0.63
1:A:921:LEU:HA	1:A:924:GLN:HB2	1.81	0.63
1:A:993:PRO:HD3	1:A:1038:TRP:CE2	2.34	0.63
1:A:1010:LEU:HD21	1:A:1018:VAL:HG11	1.80	0.63
1:A:398:LEU:CD1	1:A:405:LEU:HD12	2.28	0.63
1:A:942:SER:O	1:A:946:SER:OG	2.13	0.62
1:A:609:LEU:HD22	1:A:646:ILE:HD13	1.81	0.62
1:A:993:PRO:CA	1:A:1038:TRP:CZ2	2.83	0.61
1:A:970:ILE:HD12	1:A:973:LEU:HD23	1.82	0.61
1:A:646:ILE:HG22	1:A:646:ILE:O	2.01	0.61
1:A:772:CYS:CB	1:A:791:LEU:HD13	2.31	0.61
1:A:970:ILE:O	1:A:973:LEU:HB3	2.01	0.60
1:A:414:TYR:OH	1:A:435:LYS:HG2	2.01	0.60
1:A:1010:LEU:HD21	1:A:1018:VAL:CG1	2.31	0.60
1:A:791:LEU:HD23	1:A:825:LEU:HD21	1.83	0.60
1:A:796:MET:CE	1:A:871:LEU:HD23	2.33	0.59
1:A:547:VAL:HG12	1:A:548:LEU:N	2.17	0.59
1:A:124:CYS:O	1:A:160:PRO:HG2	2.01	0.59
1:A:556:GLN:O	1:A:556:GLN:HG2	2.03	0.58
1:A:879:MET:HE1	1:A:914:GLN:C	2.28	0.58
1:A:87:VAL:O	1:A:91:GLY:N	2.37	0.57
1:A:763:LYS:O	1:A:767:VAL:HG12	2.04	0.57
1:A:405:LEU:O	1:A:406:THR:HB	2.03	0.57
1:A:993:PRO:CD	1:A:1038:TRP:CE2	2.87	0.57
1:A:575:LEU:CD1	1:A:612:LEU:HD11	2.34	0.57
1:A:589:LEU:HD11	1:A:619:ILE:HD12	1.87	0.57
1:A:981:ALA:HA	1:A:996:ASN:HB2	1.84	0.57
1:A:522:ILE:HG13	1:A:523:GLU:H	1.69	0.56
1:A:589:LEU:HD11	1:A:619:ILE:CD1	2.36	0.56
1:A:522:ILE:HG13	1:A:523:GLU:N	2.21	0.56
1:A:597:LEU:HB2	1:A:644:PHE:CD1	2.41	0.56
1:A:1023:GLU:HA	1:A:1026:MET:HG2	1.87	0.56
1:A:264:LEU:HD12	1:A:265:GLU:N	2.22	0.55
1:A:900:ILE:O	1:A:903:THR:HG22	2.06	0.55
1:A:1026:MET:HG3	1:A:1026:MET:O	2.06	0.55
1:A:480:LEU:HD11	1:A:484:MET:HE1	1.89	0.55
1:A:727:GLU:HG3	1:A:728:GLN:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:ILE:HD11	1:A:972:MET:CB	2.36	0.55
1:A:586:THR:HG22	1:A:628:VAL:HA	1.88	0.54
1:A:973:LEU:HD21	1:A:1006:PHE:CD2	2.42	0.54
1:A:873:VAL:HG23	1:A:874:TYR:CD2	2.42	0.54
1:A:1019:TYR:HA	1:A:1022:LEU:HB3	1.89	0.54
1:A:754:THR:HG21	1:A:757:ASP:HB2	1.90	0.54
1:A:978:ILE:HG13	1:A:979:GLU:H	1.73	0.54
1:A:224:MET:HE2	1:A:315:TRP:CZ2	2.37	0.54
1:A:749:THR:HG23	1:A:750:GLU:H	1.73	0.53
1:A:950:GLU:OE1	1:A:950:GLU:HA	2.07	0.53
1:A:665:PHE:O	1:A:669:LEU:HD23	2.08	0.53
1:A:887:LYS:NZ	1:A:925:GLN:OE1	2.27	0.53
1:A:921:LEU:HD22	1:A:924:GLN:HB2	1.90	0.53
1:A:122:ILE:HG21	1:A:148:MET:HE2	1.90	0.53
1:A:224:MET:HG3	1:A:311:GLU:CB	2.39	0.53
1:A:1022:LEU:HG	1:A:1026:MET:HE3	1.91	0.53
1:A:557:LEU:O	1:A:561:THR:HG23	2.08	0.52
1:A:549:THR:N	1:A:552:GLU:OE1	2.40	0.52
1:A:913:ILE:HD12	1:A:969:ALA:HA	1.90	0.52
1:A:975:LYS:HG3	1:A:975:LYS:O	2.10	0.52
1:A:559:ASP:O	1:A:563:ILE:HG13	2.09	0.52
1:A:1019:TYR:O	1:A:1023:GLU:N	2.38	0.52
1:A:600:TYR:CB	1:A:646:ILE:HD11	2.39	0.52
1:A:753:SER:OG	1:A:754:THR:HG22	2.08	0.51
1:A:776:LEU:O	1:A:776:LEU:HD23	2.11	0.51
2:B:333:ASP:CG	2:B:336:THR:HG23	2.35	0.51
1:A:88:VAL:HG13	1:A:174:SER:HB3	1.93	0.51
1:A:867:ALA:HA	1:A:870:LYS:HE2	1.93	0.51
1:A:803:MET:HA	1:A:807:ARG:CB	2.34	0.51
1:A:395:THR:HG22	1:A:431:PHE:HD2	1.74	0.50
1:A:772:CYS:HB3	1:A:791:LEU:HD13	1.92	0.50
1:A:920:ILE:CG1	1:A:973:LEU:HD11	2.40	0.50
1:A:281:ILE:O	1:A:285:MET:HG3	2.12	0.50
1:A:476:HIS:NE2	2:B:361:MET:HE2	2.27	0.50
1:A:751:SER:OG	1:A:809:MET:CE	2.58	0.50
1:A:1019:TYR:HD1	1:A:1023:GLU:OE2	1.95	0.50
1:A:356:TYR:HD1	1:A:356:TYR:O	1.95	0.49
1:A:609:LEU:CD2	1:A:646:ILE:HG21	2.41	0.49
1:A:916:ALA:HB1	1:A:973:LEU:HD13	1.93	0.49
1:A:921:LEU:HD13	1:A:921:LEU:C	2.37	0.49
1:A:336:MET:SD	1:A:378:MET:HE1	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ALA:O	1:A:586:THR:HG23	2.11	0.49
1:A:1000:LEU:HD22	1:A:1003:LEU:HD23	1.94	0.49
1:A:374:ARG:HG3	1:A:378:MET:CE	2.38	0.49
1:A:264:LEU:HD12	1:A:264:LEU:C	2.38	0.49
1:A:566:LEU:HD23	1:A:566:LEU:O	2.12	0.49
1:A:737:THR:HG21	1:A:768:PHE:CD1	2.47	0.49
1:A:742:LEU:HB3	2:B:385:LEU:HD22	1.95	0.49
1:A:890:MET:HB2	1:A:951:LEU:HD13	1.93	0.49
1:A:715:LEU:O	1:A:715:LEU:HD23	2.13	0.48
1:A:800:HIS:NE2	1:A:875:THR:OG1	2.45	0.48
1:A:224:MET:CE	1:A:315:TRP:HZ2	2.18	0.48
1:A:495:TRP:O	1:A:499:ASN:N	2.35	0.48
1:A:196:MET:HG3	4:A:1304:HOH:O	2.13	0.48
1:A:903:THR:O	1:A:907:THR:HG23	2.13	0.48
1:A:193:ASP:OD1	1:A:193:ASP:C	2.55	0.48
1:A:801:GLN:O	1:A:807:ARG:NH2	2.46	0.48
1:A:223:ALA:O	1:A:226:LEU:HB3	2.14	0.48
1:A:547:VAL:CG1	1:A:548:LEU:H	2.22	0.48
1:A:154:GLU:CD	1:A:154:GLU:H	2.20	0.48
1:A:751:SER:C	1:A:753:SER:N	2.71	0.48
1:A:1018:VAL:HG23	1:A:1019:TYR:N	2.28	0.48
2:B:337:ILE:O	2:B:341:LEU:HG	2.13	0.48
1:A:465:VAL:HG22	1:A:524:ILE:HD12	1.96	0.47
1:A:566:LEU:HD23	1:A:566:LEU:C	2.39	0.47
1:A:802:ILE:HG12	1:A:802:ILE:O	2.14	0.47
1:A:196:MET:HG3	1:A:197:MET:N	2.28	0.47
1:A:197:MET:HB3	1:A:284:MET:CE	2.34	0.47
1:A:324:LEU:HD12	1:A:324:LEU:HA	1.73	0.47
1:A:762:LYS:HE3	1:A:766:ARG:HH12	1.78	0.47
1:A:339:LYS:HE2	2:B:340:GLN:HG2	1.96	0.47
1:A:421:HIS:CD2	1:A:423:PRO:HD2	2.49	0.47
1:A:908:ARG:CZ	1:A:912:LYS:HZ2	2.27	0.47
1:A:748:ILE:HG22	1:A:810:LEU:HD21	1.97	0.47
1:A:993:PRO:HA	1:A:1038:TRP:CH2	2.50	0.47
1:A:861:ARG:HA	1:A:864:LEU:HD12	1.97	0.47
1:A:99:VAL:CG1	1:A:182:LEU:HA	2.45	0.46
1:A:139:MET:HG2	1:A:143:GLU:HB2	1.98	0.46
1:A:763:LYS:HG3	1:A:764:GLN:N	2.29	0.46
1:A:658:ILE:HD13	1:A:703:LEU:CD2	2.44	0.46
1:A:772:CYS:HB2	1:A:791:LEU:HD13	1.97	0.46
1:A:133:ALA:O	1:A:137:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:VAL:HG13	1:A:520:ALA:HB3	1.98	0.46
1:A:978:ILE:HG13	1:A:979:GLU:N	2.29	0.46
1:A:874:TYR:CE2	2:B:393:LEU:HD22	2.50	0.46
1:A:523:GLU:OE1	2:B:358:LYS:CE	2.63	0.46
1:A:169:LYS:HE2	1:A:169:LYS:HA	1.97	0.46
1:A:197:MET:CG	1:A:284:MET:HE2	2.46	0.46
1:A:726:PRO:O	1:A:727:GLU:C	2.59	0.46
1:A:740:VAL:O	1:A:744:GLN:OE1	2.34	0.46
1:A:657:LEU:O	1:A:661:LEU:HD12	2.16	0.46
1:A:731:ILE:HD11	1:A:782:THR:OG1	2.16	0.46
2:B:370:GLU:HG2	2:B:371:LYS:H	1.80	0.46
1:A:559:ASP:OD2	1:A:559:ASP:N	2.50	0.45
1:A:715:LEU:HD23	1:A:715:LEU:C	2.40	0.45
1:A:803:MET:HA	1:A:807:ARG:HE	1.81	0.45
1:A:990:GLU:CD	1:A:990:GLU:H	2.24	0.45
1:A:817:PRO:HG3	1:A:876:VAL:HG12	1.98	0.45
1:A:497:CYS:O	1:A:501:LEU:HB2	2.16	0.45
1:A:529:ILE:HG23	1:A:563:ILE:HD13	1.98	0.45
1:A:688:LEU:HD11	1:A:728:GLN:HB3	1.99	0.45
1:A:748:ILE:HG22	1:A:748:ILE:O	2.16	0.45
1:A:519:SER:O	1:A:522:ILE:HG13	2.17	0.45
1:A:591:LEU:HB2	1:A:592:PRO:HD3	1.99	0.45
1:A:388:VAL:CG1	1:A:392:LYS:HD2	2.47	0.44
1:A:398:LEU:HD13	1:A:405:LEU:HD12	1.99	0.44
1:A:852:ALA:O	1:A:856:GLU:HG3	2.17	0.44
1:A:919:LEU:O	1:A:922:SER:HB2	2.18	0.44
1:A:930:MET:O	1:A:930:MET:HG3	2.17	0.44
1:A:862:ARG:NH2	1:A:898:ASP:OD2	2.50	0.44
1:A:953:ARG:NH1	1:A:957:LEU:HD11	2.33	0.44
1:A:433:TYR:CE1	1:A:488:ALA:HB2	2.52	0.44
1:A:616:ILE:O	1:A:620:VAL:HG13	2.18	0.44
1:A:84:LEU:HD12	1:A:84:LEU:O	2.18	0.44
1:A:938:PHE:O	1:A:938:PHE:CD2	2.70	0.44
1:A:266:LEU:O	1:A:266:LEU:HD22	2.18	0.44
1:A:776:LEU:O	1:A:784:LYS:HE2	2.17	0.44
1:A:865:LEU:HD12	1:A:865:LEU:O	2.18	0.44
1:A:959:PHE:HB2	1:A:1009:LYS:HD3	1.99	0.44
1:A:993:PRO:CG	1:A:1038:TRP:CE2	3.00	0.44
1:A:872:ILE:HD13	1:A:882:ALA:HB2	2.00	0.43
1:A:938:PHE:CD2	1:A:938:PHE:C	2.96	0.43
1:A:421:HIS:CG	1:A:423:PRO:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:LYS:HE3	1:A:766:ARG:NH1	2.33	0.43
1:A:159:TYR:HB2	1:A:160:PRO:HD2	2.00	0.43
1:A:920:ILE:HG12	1:A:973:LEU:CD1	2.47	0.43
1:A:355:TYR:O	1:A:358:LYS:HB3	2.18	0.43
1:A:612:LEU:O	1:A:615:GLN:N	2.51	0.43
1:A:892:TYR:HB3	1:A:896:TYR:HD2	1.83	0.43
1:A:978:ILE:CD1	1:A:1025:PHE:CE1	3.02	0.43
1:A:187:GLN:HB2	1:A:233:VAL:HG22	2.01	0.43
1:A:224:MET:HG3	1:A:311:GLU:HB2	2.01	0.43
1:A:604:ARG:CG	1:A:604:ARG:O	2.67	0.43
1:A:615:GLN:O	1:A:619:ILE:HG23	2.19	0.43
1:A:366:LEU:HD12	1:A:366:LEU:O	2.19	0.43
1:A:993:PRO:HG3	1:A:1038:TRP:CE2	2.54	0.43
1:A:1019:TYR:O	1:A:1022:LEU:HB3	2.19	0.43
1:A:1026:MET:HB2	1:A:1030:MET:CE	2.49	0.42
1:A:260:ALA:HA	1:A:263:ARG:HE	1.84	0.42
1:A:618:ASN:O	1:A:622:LYS:HG3	2.19	0.42
1:A:141:ASN:O	1:A:145:ILE:HG13	2.19	0.42
1:A:368:THR:O	1:A:372:LYS:HB2	2.19	0.42
1:A:893:TYR:O	1:A:897:GLY:N	2.51	0.42
1:A:972:MET:HA	1:A:975:LYS:HB3	2.01	0.42
1:A:617:ARG:NH2	1:A:660:GLU:OE1	2.53	0.42
1:A:993:PRO:CD	1:A:1038:TRP:NE1	2.75	0.42
1:A:485:TRP:O	1:A:489:THR:HB	2.20	0.42
1:A:522:ILE:HD12	1:A:587:ASN:CB	2.50	0.42
1:A:437:PHE:CE1	1:A:463:THR:HB	2.46	0.42
1:A:646:ILE:O	1:A:646:ILE:CG2	2.66	0.42
1:A:1043:SER:O	1:A:1047:SER:OG	2.38	0.42
1:A:241:MET:HE1	1:A:278:GLN:CD	2.45	0.42
1:A:640:CYS:CB	1:A:654:ARG:HH21	2.33	0.42
1:A:893:TYR:O	1:A:897:GLY:HA3	2.19	0.42
1:A:616:ILE:O	1:A:619:ILE:HG12	2.19	0.41
1:A:91:GLY:C	1:A:93:SER:N	2.79	0.41
1:A:434:LYS:HE2	1:A:434:LYS:HB2	1.76	0.41
1:A:547:VAL:CG1	1:A:548:LEU:N	2.83	0.41
1:A:874:TYR:C	1:A:875:THR:HG23	2.44	0.41
2:B:391:ARG:HG3	2:B:392:CYS:SG	2.60	0.41
1:A:582:ALA:HA	1:A:585:VAL:HG22	2.03	0.41
1:A:749:THR:HG23	1:A:750:GLU:N	2.35	0.41
1:A:920:ILE:CG1	1:A:973:LEU:CD1	2.98	0.41
1:A:619:ILE:HG13	1:A:620:VAL:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:ARG:HB3	1:A:1011:LEU:HD21	2.03	0.41
1:A:265:GLU:HA	1:A:268:LEU:CD2	2.51	0.41
1:A:700:ALA:HA	2:B:382:ASN:HB2	2.02	0.41
1:A:658:ILE:HD13	1:A:703:LEU:HD22	2.02	0.41
1:A:1026:MET:HB2	1:A:1030:MET:HE2	2.03	0.40
1:A:145:ILE:O	1:A:149:THR:HG23	2.20	0.40
1:A:154:GLU:CD	1:A:154:GLU:N	2.80	0.40
1:A:309:ILE:HD13	1:A:309:ILE:HA	1.96	0.40
1:A:479:TYR:CZ	2:B:355:PRO:HD2	2.56	0.40
1:A:879:MET:HE2	1:A:914:GLN:HG2	2.02	0.40
1:A:151:GLU:O	1:A:152:PHE:C	2.64	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:LYS:NZ	1:A:938:PHE:N[1_455]	2.01	0.19

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	911/981 (93%)	862 (95%)	49 (5%)	0	100	100
2	B	72/140 (51%)	69 (96%)	3 (4%)	0	100	100
3	C	7/10 (70%)	7 (100%)	0	0	100	100
All	All	990/1131 (88%)	938 (95%)	52 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	839/882 (95%)	822 (98%)	17 (2%)	48	76
2	B	69/129 (54%)	69 (100%)	0	100	100
3	C	9/10 (90%)	9 (100%)	0	100	100
All	All	917/1021 (90%)	900 (98%)	17 (2%)	50	77

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	596	ASP
1	A	600	TYR
1	A	607	LYS
1	A	890	MET
1	A	931	ILE
1	A	934	ASN
1	A	937	ASN
1	A	939	ASP
1	A	940	ARG
1	A	954	ARG
1	A	955	PHE
1	A	1028	PHE
1	A	1029	GLN
1	A	1033	ARG
1	A	1034	ARG
1	A	1035	GLU
1	A	1042	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	261	ASN
1	A	674	GLN
1	A	701	HIS

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Mol	Chain	Res	Type
1	A	728	GLN
1	A	770	GLN
1	A	928	ASN
1	A	996	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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	993:PRO	C	994:PRO	N	3.08

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	928/981 (94%)	0.84	98 (10%) 11 9	53, 113, 168, 205	0
2	B	74/140 (52%)	0.55	2 (2%) 56 53	55, 95, 134, 141	0
3	C	9/10 (90%)	1.31	2 (22%) 2 2	98, 113, 130, 138	0
All	All	1011/1131 (89%)	0.83	102 (10%) 12 10	53, 111, 165, 205	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ASN	6.4
1	A	1028	PHE	5.3
1	A	999	PHE	5.1
1	A	973	LEU	4.7
1	A	82	MET	4.6
1	A	813	LEU	4.3
3	C	223	VAL	4.3
1	A	982	PHE	4.1
1	A	715	LEU	3.9
1	A	361	ASN	3.7
1	A	360	LEU	3.6
1	A	355	TYR	3.5
1	A	513	LEU	3.4
1	A	991	SER	3.4
1	A	959	PHE	3.4
1	A	978	ILE	3.4
1	A	1000	LEU	3.4
1	A	1037	VAL	3.3
1	A	485	TRP	3.3
1	A	720	ILE	3.2
1	A	1018	VAL	3.2
1	A	356	TYR	3.1
1	A	325	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	812	PRO	3.1
1	A	600	TYR	3.1
1	A	605	LEU	3.1
1	A	1044	TYR	3.0
1	A	927	PHE	3.0
1	A	436	LEU	3.0
1	A	580	VAL	3.0
1	A	645	THR	2.9
1	A	644	PHE	2.9
1	A	945	PHE	2.9
3	C	226	TYR	2.9
1	A	977	GLY	2.9
1	A	1032	LEU	2.8
1	A	547	VAL	2.8
1	A	964	LEU	2.7
1	A	814	VAL	2.7
1	A	94	ALA	2.7
1	A	971	ALA	2.7
1	A	713	TYR	2.7
1	A	913	ILE	2.7
1	A	1038	TRP	2.7
1	A	758	LEU	2.7
1	A	709	PHE	2.7
1	A	1011	LEU	2.6
1	A	438	SER	2.6
1	A	495	TRP	2.6
1	A	437	PHE	2.6
1	A	1022	LEU	2.6
1	A	975	LYS	2.6
1	A	357	ASN	2.6
1	A	568	ALA	2.5
1	A	972	MET	2.5
1	A	694	ILE	2.5
1	A	748	ILE	2.5
1	A	460	LEU	2.5
1	A	951	LEU	2.5
1	A	505	GLU	2.4
1	A	944	THR	2.4
1	A	500	SER	2.4
1	A	498	MET	2.4
1	A	798	PHE	2.4
1	A	890	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	638	ALA	2.4
1	A	920	ILE	2.3
1	A	1027	THR	2.3
1	A	993	PRO	2.3
1	A	1045	ARG	2.3
1	A	535	CYS	2.3
1	A	938	PHE	2.3
1	A	458	ALA	2.3
1	A	755	LYS	2.3
1	A	922	SER	2.3
2	B	375	LEU	2.3
1	A	108	HIS	2.2
1	A	254	LYS	2.2
1	A	563	ILE	2.2
1	A	619	ILE	2.2
1	A	717	LYS	2.2
1	A	802	ILE	2.2
1	A	578	TYR	2.2
1	A	1021	TYR	2.2
1	A	826	LEU	2.2
1	A	1020	VAL	2.2
1	A	597	LEU	2.1
1	A	543	THR	2.1
1	A	613	LEU	2.1
1	A	359	GLU	2.1
1	A	994	PRO	2.1
1	A	711	CYS	2.1
2	B	392	CYS	2.1
1	A	1019	TYR	2.1
1	A	1002	ILE	2.1
1	A	629	LEU	2.1
1	A	599	ILE	2.1
1	A	741	ILE	2.1
1	A	116	ASP	2.0
1	A	889	TYR	2.0
1	A	559	ASP	2.0
1	A	268	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.