



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:45 AM EDT

PDB ID : 4UVJ / pdb_00004uvj
Title : Cohesin subunit Scc3 from yeast, 674-1072
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Deposited on : 2014-08-06
Resolution : 2.10 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

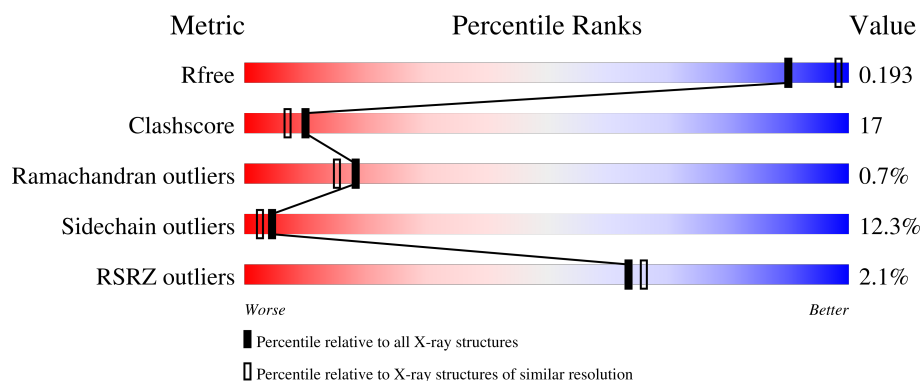
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

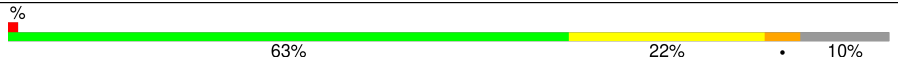
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	406	
1	B	406	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6403 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 COHESIN SUBUNIT SCC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			3001	1965	477	548	11			
1	B	364	Total	C	N	O	S	0	0	0
			3001	1965	477	548	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	673	MET	-	expression tag	UNP P40541
A	1073	HIS	-	expression tag	UNP P40541
A	1074	HIS	-	expression tag	UNP P40541
A	1075	HIS	-	expression tag	UNP P40541
A	1076	HIS	-	expression tag	UNP P40541
A	1077	HIS	-	expression tag	UNP P40541
A	1078	HIS	-	expression tag	UNP P40541
B	673	MET	-	expression tag	UNP P40541
B	1073	HIS	-	expression tag	UNP P40541
B	1074	HIS	-	expression tag	UNP P40541
B	1075	HIS	-	expression tag	UNP P40541
B	1076	HIS	-	expression tag	UNP P40541
B	1077	HIS	-	expression tag	UNP P40541
B	1078	HIS	-	expression tag	UNP P40541

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	192	Total	O	0	0
			192	192		
2	B	209	Total	O	0	0
			209	209		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.79Å 58.02Å 80.18Å 80.68° 82.00° 63.99°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.10) 97.4 (50.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.186 , 0.247 0.189 , 0.193	Depositor DCC
R_{free} test set	2598 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% 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	1.01	1/3060 (0.0%)	1.17	12/4129 (0.3%)
1	B	1.05	1/3060 (0.0%)	1.15	6/4129 (0.1%)
All	All	1.03	2/6120 (0.0%)	1.16	18/8258 (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
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	978	ILE	C-O	-6.03	1.16	1.24
1	A	866	TRP	C-O	-5.12	1.18	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	935	MET	CG-SD-CE	-8.13	83.01	100.90
1	B	900	ILE	CB-CA-C	-6.76	102.88	112.22
1	A	1031	MET	N-CA-C	-6.30	104.33	111.14
1	A	758	ILE	CB-CA-C	-6.18	104.06	111.97
1	B	961	GLU	N-CA-C	5.91	119.75	112.54
1	A	780	HIS	N-CA-C	5.81	117.61	111.28
1	A	985	LEU	N-CA-C	-5.67	105.01	111.14
1	A	824	VAL	N-CA-C	-5.62	100.14	108.45
1	A	1014	GLU	CA-C-N	-5.57	114.55	122.41
1	A	1014	GLU	C-N-CA	-5.57	114.55	122.41
1	A	988	LYS	N-CA-C	-5.51	105.35	111.36
1	B	1010	THR	CB-CA-C	-5.45	98.57	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	837	VAL	N-CA-C	5.35	115.79	110.23
1	B	1040	PHE	N-CA-C	-5.25	105.47	111.14
1	A	875	ILE	N-CA-C	5.19	115.96	110.72
1	A	840	ILE	CA-C-N	-5.16	114.35	119.56
1	A	840	ILE	C-N-CA	-5.16	114.35	119.56
1	A	1043	ARG	N-CA-C	-5.04	105.87	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	877	LYS	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	3001	0	3069	123	0
1	B	3001	0	3069	90	0
2	A	192	0	0	32	0
2	B	209	0	0	29	1
All	All	6403	0	6138	210	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 (210) 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:803:CYS:HB2	2:A:2069:HOH:O	1.28	1.30
1:B:803:CYS:HB2	2:B:2075:HOH:O	1.32	1.25
1:A:810:ILE:HG23	1:A:859:MET:CE	1.72	1.19
1:B:834:ASN:ND2	1:B:902:ARG:HH22	1.42	1.16
1:A:834:ASN:ND2	1:A:902:ARG:HH22	1.47	1.12
1:A:726:ILE:HB	2:A:2019:HOH:O	1.50	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:MET:HE2	2:A:2010:HOH:O	1.53	1.08
1:A:785:LEU:HD23	1:A:789:MET:HE2	1.35	1.05
1:A:1010:THR:HG22	1:A:1012:PHE:H	1.19	1.04
1:A:810:ILE:HG23	1:A:859:MET:HE3	1.37	1.01
1:A:834:ASN:ND2	1:A:902:ARG:NH2	2.09	1.00
1:B:834:ASN:HD22	1:B:902:ARG:NH2	1.59	1.00
1:A:1031:MET:HG2	2:A:2183:HOH:O	1.64	0.98
1:B:785:LEU:HD23	1:B:789:MET:CE	1.96	0.94
1:A:723:LEU:HA	2:A:2019:HOH:O	1.67	0.93
1:A:810:ILE:HG23	1:A:859:MET:HE1	1.51	0.92
1:B:785:LEU:HD23	1:B:789:MET:HE2	1.48	0.91
1:A:995:GLU:H	1:A:1047:ASN:HD21	1.17	0.91
1:B:799:LYS:HE2	2:B:2076:HOH:O	1.68	0.91
1:B:1028:LYS:HD2	2:B:2205:HOH:O	1.70	0.91
1:B:803:CYS:CB	2:B:2075:HOH:O	2.00	0.90
1:A:872:ARG:HD3	2:A:2113:HOH:O	1.70	0.90
1:A:789:MET:HE1	1:A:836:PHE:HB2	1.52	0.89
1:A:834:ASN:HD21	1:A:902:ARG:HH22	1.15	0.88
1:B:674:ASP:N	2:B:2001:HOH:O	2.06	0.88
1:A:1022:LEU:HD12	2:A:2181:HOH:O	1.72	0.88
1:A:785:LEU:CD2	1:A:789:MET:HE2	2.02	0.88
1:B:710:SER:HB2	2:B:2015:HOH:O	1.72	0.88
1:B:813:LEU:HB2	1:B:859:MET:HE2	1.55	0.87
1:A:692:SER:C	2:A:2013:HOH:O	2.16	0.86
1:A:834:ASN:HD22	1:A:902:ARG:NH2	1.72	0.86
1:B:785:LEU:CD2	1:B:789:MET:CE	2.54	0.85
1:A:772:ASN:CG	2:A:2045:HOH:O	2.18	0.85
1:A:1015:ASN:HD22	1:A:1018:THR:H	1.24	0.85
1:A:878:VAL:HG13	1:A:879:ARG:O	1.77	0.83
1:A:772:ASN:OD1	2:A:2045:HOH:O	1.96	0.82
1:A:785:LEU:HD23	1:A:789:MET:CE	2.10	0.82
1:A:1015:ASN:ND2	1:A:1018:THR:H	1.76	0.82
1:A:879:ARG:HA	2:A:2116:HOH:O	1.82	0.80
1:B:995:GLU:H	1:B:1047:ASN:HD21	1.29	0.77
1:A:927:LYS:HB3	1:A:978:ILE:HD11	1.66	0.77
1:B:722:GLU:HG2	2:B:2018:HOH:O	1.86	0.76
1:B:813:LEU:CB	1:B:859:MET:HE2	2.17	0.76
1:A:788:LYS:HE3	2:A:2058:HOH:O	1.85	0.75
1:A:995:GLU:H	1:A:1047:ASN:ND2	1.84	0.75
1:B:871:TRP:CZ2	1:B:892:VAL:HG23	2.22	0.75
1:A:727:THR:HG21	1:A:766:LEU:HD22	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:ASN:ND2	1:B:902:ARG:NH2	2.28	0.74
1:A:785:LEU:CD2	1:A:789:MET:CE	2.64	0.74
1:A:1010:THR:HG21	2:A:2134:HOH:O	1.90	0.72
1:A:741:ASN:HD21	1:A:743:LYS:HB2	1.55	0.72
1:B:834:ASN:HD22	1:B:902:ARG:HH22	0.77	0.72
1:A:803:CYS:CB	2:A:2069:HOH:O	2.05	0.72
1:B:872:ARG:HD3	2:B:2118:HOH:O	1.91	0.70
1:B:1010:THR:HG21	2:B:2127:HOH:O	1.90	0.70
1:A:879:ARG:O	1:A:880:ASP:HB2	1.90	0.69
1:B:757:HIS:HD2	2:B:2005:HOH:O	1.76	0.69
1:B:813:LEU:HB2	1:B:859:MET:CE	2.23	0.69
1:B:729:LYS:HD2	2:B:2022:HOH:O	1.93	0.68
1:A:1001:ASP:CG	1:A:1003:ASN:HB2	2.19	0.68
1:A:674:ASP:HA	2:A:2001:HOH:O	1.92	0.67
1:A:1059:VAL:O	2:A:2192:HOH:O	2.13	0.66
1:B:927:LYS:HB3	1:B:978:ILE:HD11	1.76	0.66
1:A:810:ILE:HD12	1:A:859:MET:HE1	1.76	0.66
1:A:727:THR:HG21	1:A:766:LEU:CD2	2.26	0.65
1:A:977:LYS:HD3	2:A:2157:HOH:O	1.95	0.65
1:B:956:ARG:HG3	2:B:2144:HOH:O	1.95	0.65
1:B:824:VAL:HG22	1:B:828:LEU:HD13	1.78	0.65
1:B:964:PRO:HD2	2:B:2149:HOH:O	1.96	0.65
1:B:812:LYS:HG3	2:B:2080:HOH:O	1.98	0.64
1:A:935:MET:HE1	1:A:1023:PHE:CE1	2.32	0.63
1:A:858:LYS:HE2	2:A:2170:HOH:O	1.97	0.63
1:A:1015:ASN:HD22	1:A:1018:THR:HB	1.63	0.63
1:A:810:ILE:CG2	1:A:859:MET:CE	2.64	0.63
1:B:923:LEU:HD22	1:B:927:LYS:HE3	1.81	0.62
1:B:904:ASN:ND2	1:B:968:HIS:H	1.98	0.62
1:B:709:PHE:HB2	2:B:2013:HOH:O	1.99	0.62
1:B:803:CYS:SG	2:B:2075:HOH:O	2.51	0.60
1:A:880:ASP:N	2:A:2116:HOH:O	2.35	0.60
1:B:789:MET:HE1	1:B:836:PHE:HB2	1.83	0.60
1:A:757:HIS:HD2	2:A:2004:HOH:O	1.85	0.60
1:B:1010:THR:HG22	1:B:1012:PHE:H	1.66	0.59
1:B:995:GLU:H	1:B:1047:ASN:ND2	2.00	0.59
1:A:858:LYS:HD2	2:A:2145:HOH:O	2.01	0.59
1:A:790:ASP:O	1:A:793:ASN:HB2	2.02	0.59
1:A:798:TYR:CG	1:A:843:MET:HG2	2.37	0.58
1:A:1017:GLU:CD	1:B:692:SER:HB2	2.29	0.58
1:A:790:ASP:HB3	1:A:793:ASN:HD22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:772:ASN:HB2	2:B:2051:HOH:O	2.03	0.57
1:B:871:TRP:CZ2	1:B:892:VAL:CG2	2.86	0.57
1:A:948:LEU:HD12	1:A:956:ARG:HG3	1.87	0.57
1:B:932:THR:HG23	1:B:1026:LYS:HE3	1.86	0.57
1:B:785:LEU:CD2	1:B:789:MET:HE1	2.35	0.56
1:A:1018:THR:HG23	1:A:1022:LEU:CD2	2.35	0.56
1:A:878:VAL:CG1	1:A:879:ARG:N	2.68	0.56
1:A:1047:ASN:HD22	1:A:1050:LYS:HD2	1.70	0.56
1:A:904:ASN:ND2	1:A:968:HIS:H	2.03	0.56
1:A:810:ILE:CD1	1:A:859:MET:HE1	2.36	0.56
1:B:703:LEU:O	1:B:707:ILE:HD12	2.06	0.56
1:B:988:LYS:HD3	2:B:2178:HOH:O	2.06	0.55
1:B:1059:VAL:C	2:B:2204:HOH:O	2.49	0.55
1:A:879:ARG:CA	2:A:2116:HOH:O	2.46	0.55
1:B:741:ASN:HD21	1:B:743:LYS:HB2	1.73	0.54
1:A:789:MET:CE	1:A:836:PHE:HB2	2.32	0.54
1:B:698:ILE:HG22	2:B:2147:HOH:O	2.07	0.54
1:A:735:MET:HG3	1:A:773:GLN:HE21	1.73	0.54
1:A:824:VAL:HG22	1:A:828:LEU:HD13	1.88	0.54
1:A:995:GLU:N	1:A:1047:ASN:HD21	1.95	0.54
1:B:956:ARG:HD2	2:B:2144:HOH:O	2.08	0.54
1:B:973:LYS:HE2	2:B:2159:HOH:O	2.08	0.54
1:A:1010:THR:HG22	1:A:1012:PHE:N	2.04	0.53
1:A:692:SER:HB2	1:B:1017:GLU:CD	2.33	0.53
1:B:824:VAL:HG22	1:B:828:LEU:CD1	2.37	0.53
1:B:705:SER:OG	1:B:729:LYS:NZ	2.40	0.53
1:A:997:VAL:HG12	1:A:1000:GLU:OE2	2.08	0.53
1:B:913:THR:HG23	2:B:2103:HOH:O	2.08	0.53
1:A:810:ILE:HA	1:A:859:MET:HE1	1.91	0.52
1:A:880:ASP:HA	2:A:2120:HOH:O	2.09	0.52
1:A:1001:ASP:OD1	1:A:1003:ASN:HB2	2.08	0.52
1:A:798:TYR:CD1	1:A:843:MET:HG2	2.45	0.52
1:A:1018:THR:HG23	1:A:1022:LEU:HD22	1.92	0.52
1:A:810:ILE:CG2	1:A:859:MET:HE1	2.33	0.51
1:B:763:LYS:HG2	1:B:766:LEU:HG	1.91	0.51
1:B:956:ARG:CG	2:B:2144:HOH:O	2.55	0.51
1:B:739:ILE:HD12	1:B:812:LYS:HG2	1.92	0.51
1:B:767:GLN:HE21	1:B:767:GLN:HA	1.75	0.51
1:A:767:GLN:HE21	1:A:767:GLN:HA	1.75	0.51
1:A:879:ARG:C	2:A:2116:HOH:O	2.54	0.51
1:A:874:ILE:O	1:A:878:VAL:HB	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:LEU:HD13	1:A:972:SER:HB2	1.93	0.50
1:A:1039:ARG:NH2	2:A:2185:HOH:O	2.43	0.50
1:A:874:ILE:O	1:A:878:VAL:N	2.46	0.49
1:B:799:LYS:CE	2:B:2076:HOH:O	2.41	0.49
1:A:772:ASN:CB	2:A:2045:HOH:O	2.57	0.48
1:A:1041:ALA:HB2	2:A:2183:HOH:O	2.13	0.48
1:A:1045:ALA:O	1:A:1048:LYS:HG2	2.13	0.48
1:A:722:GLU:HG3	2:A:2144:HOH:O	2.13	0.48
1:B:896:ILE:CG2	1:B:941:ILE:HD11	2.42	0.48
1:B:831:LEU:O	1:B:835:ASN:HB2	2.14	0.48
1:A:928:TRP:HA	1:A:978:ILE:HD13	1.96	0.48
1:A:700:CYS:O	1:A:704:GLU:HB2	2.14	0.47
1:B:935:MET:HE1	1:B:1023:PHE:CE1	2.49	0.47
1:A:1006:ASP:CG	1:A:1006:ASP:O	2.57	0.47
1:A:931:CYS:SG	1:A:978:ILE:HD12	2.54	0.47
1:B:824:VAL:CG2	1:B:828:LEU:HD13	2.43	0.47
1:B:709:PHE:HD1	1:B:710:SER:N	2.13	0.47
1:A:1022:LEU:HD13	1:B:688:LEU:HD13	1.97	0.47
1:A:938:ILE:HG12	1:A:966:TYR:HB3	1.97	0.47
1:A:834:ASN:HD22	1:A:902:ARG:HH21	1.57	0.46
1:A:810:ILE:CG2	1:A:859:MET:HE3	2.25	0.46
1:A:810:ILE:HD12	1:A:859:MET:CE	2.44	0.46
1:B:709:PHE:CD1	1:B:710:SER:N	2.84	0.46
1:B:687:LEU:HB3	1:B:703:LEU:HG	1.96	0.46
1:B:900:ILE:HD13	1:B:900:ILE:HG21	1.66	0.46
1:A:824:VAL:HG22	1:A:828:LEU:CD1	2.45	0.46
1:B:725:LYS:HD3	2:B:2019:HOH:O	2.14	0.46
1:A:684:PHE:CZ	1:A:688:LEU:HD12	2.51	0.45
1:A:759:HIS:HD2	1:A:760:HIS:ND1	2.14	0.45
1:A:1014:GLU:HG2	2:A:2175:HOH:O	2.15	0.45
1:A:1015:ASN:HD22	1:A:1018:THR:N	2.02	0.45
1:A:927:LYS:CB	1:A:978:ILE:HD11	2.42	0.45
1:B:1028:LYS:HE2	1:B:1058:ILE:O	2.17	0.45
1:A:904:ASN:HD21	1:A:968:HIS:H	1.65	0.45
1:B:997:VAL:HG12	1:B:1000:GLU:OE1	2.18	0.44
1:A:935:MET:HE1	1:A:1023:PHE:CZ	2.53	0.44
1:A:942:LYS:HD2	1:A:1035:ILE:HD11	2.00	0.44
1:A:1015:ASN:ND2	1:A:1018:THR:HB	2.32	0.44
1:A:878:VAL:C	1:A:879:ARG:O	2.58	0.44
1:B:1013:PHE:HD1	1:B:1019:GLU:HG2	1.82	0.44
1:A:896:ILE:CG2	1:A:941:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1006:ASP:O	1:B:1006:ASP:CG	2.61	0.44
1:A:799:LYS:HG3	1:A:851:THR:OG1	2.18	0.43
1:B:879:ARG:O	1:B:880:ASP:OD1	2.36	0.43
1:B:942:LYS:HD2	1:B:1035:ILE:HD11	1.99	0.43
1:B:1003:ASN:HB2	2:B:2175:HOH:O	2.18	0.43
1:A:767:GLN:HE21	1:A:767:GLN:CA	2.31	0.43
1:B:919:ASN:OD1	1:B:919:ASN:C	2.61	0.43
1:A:1015:ASN:HD22	1:A:1018:THR:CB	2.31	0.43
1:A:739:ILE:HD12	1:A:812:LYS:HG2	2.00	0.43
1:B:896:ILE:HG21	1:B:941:ILE:HD11	2.00	0.43
1:B:956:ARG:CD	2:B:2144:HOH:O	2.64	0.43
1:A:772:ASN:CA	2:A:2045:HOH:O	2.67	0.43
1:A:763:LYS:NZ	2:A:2017:HOH:O	2.51	0.43
1:A:900:ILE:HD11	1:A:941:ILE:HD12	2.00	0.42
1:B:904:ASN:HD21	1:B:968:HIS:H	1.65	0.42
1:A:709:PHE:HD1	1:A:710:SER:H	1.67	0.42
1:A:805:LEU:HD22	1:A:810:ILE:HG12	2.01	0.42
1:B:1010:THR:HG22	1:B:1012:PHE:HD2	1.85	0.42
1:A:900:ILE:HD11	1:A:941:ILE:CD1	2.49	0.42
1:B:935:MET:HG2	1:B:1030:LEU:HD11	2.01	0.42
1:B:702:LEU:HD23	1:B:702:LEU:HA	1.92	0.41
1:A:964:PRO:HG2	2:A:2147:HOH:O	2.19	0.41
1:B:786:GLN:O	1:B:790:ASP:HB2	2.20	0.41
1:B:890:ARG:HA	1:B:890:ARG:HE	1.85	0.41
1:B:931:CYS:SG	1:B:975:LEU:HD23	2.60	0.41
1:A:945:GLU:HB2	1:A:959:MET:HE1	2.02	0.41
1:B:805:LEU:HD22	1:B:810:ILE:HG12	2.03	0.41
1:A:919:ASN:OD1	1:A:919:ASN:C	2.64	0.41
1:B:710:SER:CB	2:B:2016:HOH:O	2.69	0.41
1:A:767:GLN:HA	1:A:767:GLN:NE2	2.35	0.41
1:A:902:ARG:HD2	1:A:902:ARG:HA	1.89	0.41
1:A:931:CYS:SG	1:A:975:LEU:HD23	2.61	0.41
1:B:709:PHE:CD1	1:B:709:PHE:C	2.99	0.41
1:A:699:LEU:HD21	1:A:751:PHE:CZ	2.56	0.41
1:B:810:ILE:HG23	1:B:859:MET:HE3	2.03	0.41
1:B:995:GLU:N	1:B:1047:ASN:HD21	2.05	0.41
1:A:756:HIS:CE1	1:A:760:HIS:CE1	3.09	0.40
1:B:741:ASN:ND2	1:B:743:LYS:H	2.19	0.40
1:A:790:ASP:HA	1:A:791:PRO:HD3	1.98	0.40
1:B:871:TRP:CE2	1:B:892:VAL:CG2	3.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2053:HOH:O	2:B:2203:HOH:O[1_655]	1.83	0.37

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	356/406 (88%)	344 (97%)	10 (3%)	2 (1%)	21	18
1	B	356/406 (88%)	344 (97%)	9 (2%)	3 (1%)	16	12
All	All	712/812 (88%)	688 (97%)	19 (3%)	5 (1%)	18	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	PHE
1	B	709	PHE
1	B	998	ALA
1	B	1001	ASP
1	A	879	ARG

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	337/377 (89%)	289 (86%)	48 (14%)	3	1
1	B	337/377 (89%)	302 (90%)	35 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	674/754 (89%)	591 (88%)	83 (12%)	4 2

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	678	GLU
1	A	688	LEU
1	A	698	ILE
1	A	700	CYS
1	A	702	LEU
1	A	703	LEU
1	A	705	SER
1	A	707	ILE
1	A	708	THR
1	A	726	ILE
1	A	762	GLU
1	A	767	GLN
1	A	769	LYS
1	A	772	ASN
1	A	782	LYS
1	A	793	ASN
1	A	796	ASP
1	A	805	LEU
1	A	824	VAL
1	A	828	LEU
1	A	845	GLN
1	A	854	GLU
1	A	878	VAL
1	A	890	ARG
1	A	902	ARG
1	A	923	LEU
1	A	934	LEU
1	A	953	THR
1	A	967	LEU
1	A	976	LEU
1	A	988	LYS
1	A	1003	ASN
1	A	1006	ASP
1	A	1009	GLU
1	A	1014	GLU
1	A	1016	ILE
1	A	1018	THR

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Mol	Chain	Res	Type
1	A	1019	GLU
1	A	1022	LEU
1	A	1025	VAL
1	A	1028	LYS
1	A	1032	LYS
1	A	1035	ILE
1	A	1038	GLU
1	A	1042	SER
1	A	1046	LEU
1	A	1054	LEU
1	A	1057	LYS
1	B	676	VAL
1	B	688	LEU
1	B	700	CYS
1	B	703	LEU
1	B	709	PHE
1	B	710	SER
1	B	726	ILE
1	B	744	VAL
1	B	762	GLU
1	B	763	LYS
1	B	767	GLN
1	B	772	ASN
1	B	805	LEU
1	B	824	VAL
1	B	828	LEU
1	B	842	ILE
1	B	845	GLN
1	B	854	GLU
1	B	880	ASP
1	B	889	LEU
1	B	890	ARG
1	B	920	ILE
1	B	923	LEU
1	B	934	LEU
1	B	951	ASP
1	B	961	GLU
1	B	967	LEU
1	B	976	LEU
1	B	1010	THR
1	B	1022	LEU
1	B	1028	LYS

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Mol	Chain	Res	Type
1	B	1039	ARG
1	B	1046	LEU
1	B	1054	LEU
1	B	1057	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	741	ASN
1	A	757	HIS
1	A	759	HIS
1	A	760	HIS
1	A	767	GLN
1	A	773	GLN
1	A	792	ASN
1	A	793	ASN
1	A	830	GLN
1	A	834	ASN
1	A	835	ASN
1	A	904	ASN
1	A	921	ASN
1	A	1003	ASN
1	A	1005	ASN
1	A	1015	ASN
1	A	1047	ASN
1	B	689	ASN
1	B	741	ASN
1	B	756	HIS
1	B	757	HIS
1	B	759	HIS
1	B	767	GLN
1	B	772	ASN
1	B	786	GLN
1	B	792	ASN
1	B	811	ASN
1	B	830	GLN
1	B	834	ASN
1	B	835	ASN
1	B	845	GLN
1	B	904	ASN
1	B	921	ASN
1	B	970	ASN

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Mol	Chain	Res	Type
1	B	1003	ASN
1	B	1047	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 [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	364/406 (89%)	-0.10	9 (2%) 58 61	14, 32, 66, 100	0
1	B	364/406 (89%)	-0.26	6 (1%) 70 73	15, 29, 58, 86	0
All	All	728/812 (89%)	-0.18	15 (2%) 63 66	14, 30, 64, 100	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	709	PHE	5.3
1	B	698	ILE	4.5
1	B	710	SER	4.1
1	A	889	LEU	3.7
1	A	698	ILE	3.2
1	A	878	VAL	3.1
1	A	880	ASP	3.1
1	A	879	ARG	2.7
1	B	957	TYR	2.6
1	B	709	PHE	2.6
1	A	1059	VAL	2.4
1	B	707	ILE	2.4
1	B	964	PRO	2.4
1	A	998	ALA	2.3
1	A	710	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.