

Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 03:32 pm BST

PDB ID	:	6QNX
Title	:	Structure of the SA2/SCC1/CTCF complex
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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122(2.70-2.70)
Ramachandran outliers	138981	3069(2.70-2.70)
Sidechain outliers	138945	3069(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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length		Quality	of chain		
1	А	1231	50	1%	24%	•	25%
2	В	631	9% •		88%		
3	С	727	•	9	9%		



2 Entry composition (i)

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			Aton	ns	ZeroOcc	AltConf	Trace		
1	А	928	Total 15088	C 4808	H 7539	N 1258	O 1428	${ m S}{55}$	0	0	0

• Molecule 2 is a protein called Double-strand-break repair protein rad21 homolog.

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

• Molecule 3 is a protein called Transcriptional repressor CTCF.

Mol	Chain	Residues		\mathbf{At}	\mathbf{oms}			ZeroOcc	AltConf	Trace
3	С	9	Total 140	$\begin{array}{c} \mathrm{C} \\ 50 \end{array}$	H 62	N 9	O 19	0	0	0

• Molecule 4 is water.

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



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are colorcoded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Cohesin subunit SA-2



• Molecule 2: Double-strand-break repair protein rad21 homolog

С	ha	in	B:		9%	•												8	8%														
MET	TYR	ALA HIS	PHE		LYS	GLY PRO	LEU	LYS	TRP TRP	LEU ALA	ALA	TRP	ASP LYS	T EU		LYS	SIH	VAL	GLU CYS	ASN T FTI	OTO OT	H S S S S S S S S S S S S S S S S S S S	GLU	SER	ILE SEP	PRO 1 VS	VAL	LYS MET	ALA LEU	ARG THR	SER	HIS	NEW
LEU	GLY VAL	VAL ARG	ILE	SIH	ARG LYS ALA	LYS TYR	LEU	ALA	ASP CYS	ASN GLU	ALA	ILE	LYS ILE	LYS	ALA	PHE ARG	PRO	VAL	VAL ASP	LEU	GLU	ASN	ARG GLU	AL.A AL.A	TYR	ALA	THR	LEU PRO	GLU GLU	PHE	ASP PHE	ASP GLN DRO	011.1
LEU	PRO ASP	LEU ASP	ASP	ASP	VAL ALA GLN	GLN	SER	ASN	GLN SER	ARG VAL	GLU	ILE	THR MET	ARG	GLU	VAL GLY	ASN	SER	ILEU	GLN GLN	ASN	PHE	GLY ASP	PHE	MET	ASP	GLU	NET	ARG GLU	GLY SER	AL.A PHE	GLU ASP ASP	TCH
ASP	MET LEU	VAL SER	THR	THT I	ASN LEU	LEU	GLU	GLU	GLN SER	THR SER	ASN	ASN	GLU GLU	ILE	HIS	LEU GLU	TYR	ASP	GLN TYR	LYS	ASP	PHE	GLU	GLY ASN	ASP	ATT D	LEU	ASP ASP	LEU	ILE SER	ASN	ASP GLY GLY	1115
ILE	ASP	ASP PRO	PRO AT A		GLU ALA	GLY VAL	MET	PRO	GLU	PRO ALA	SIH	ASP	MET ASP	GLU	ASP	ASN VAL	SER	GLY	GLY PRO	ASP SFR	PRO	SER	VAL ASP	PRO VAL	GLU	MET	THR	MET THR	ASP GLN	THR THR	LEU VAL	PRO ASN	010
GLU	GLU ALA	PHE ALA	LEU	PRO	ASP	THR VAL	TYS	THR	LYS ALA	LYS ARG	K321	D333	T336	1337	<mark>q340</mark>	L341	P355	K358	M361	F370	K371	N382	L385	R.301	C392 1 202	T394 DBD	LEU	VAL. PRO	GLU ASP	L.EU ARG	LYS ARG	ARG LYS GTV	115
GLY	GLU ALA	ASP	LEU	GLU	LEU LEU	GLU PHE	GLU	PRO	GLU VAL	PRO ARG	GLU	GLN	GLIN	GLN	NTID	GLN ARG	ASP	VAL	ASP GLU	PRO TIF	ILE	GLU	PRO SER	ARG LEU	GLN	SER	MET	GLU ALA	SER ARG	THR ASN	ILE ASP	GLU SER	Nut
MET	Oud Oud	DRQ PRO	PRO CT M	GLY	VAL LYS ARG	LYS	GLY	ILE	ASP PRO	GLU PRO	VAL	PRO	PRO GLN	GLN	GLU	GLN	GLU	- DRG	PRO VAL	GLU T FII	DRG	GLU	GLU PRO	PRO ASN	ILE	GLN 1 FII	ILE	PR0 GLU	GLU	LIEU	PRO GLU	OTD OTD STT	011
GLU	0TD GTU	GLU	TIS	ASP	GLU GLU	GLU GLU	ASP	ASP	AL.A SER	GLY GLY	ASP	ASP	GLU GLU	GLU	ARG	ASN	SVI	THR	0LIN GLIN	NET T FII	SIH	LEU LEU	GLN	ALA LEU	AL.A T VS	THR	ALA	GLU SER	ILE SER	LEU	GLU LEU	CYS ARG	NT C14
THR	ASN ARG	G LN G LN	ALA	ALA	PHE	SER PHE	LEU	LEU	TYS LYS	GLN	ALA	GLU	LEU THR	GLN	GLU	PRO TYR	SER	ASF	ILE ALA	THR	GLY	ARG	PHE	ILE ILE									
•	М	ole	ecu	le	3: '	Tra	ns	scr	ipt	ioı	1a	l re	epi	res	so	r (СЛ	C	F														
С	ha	in	C:		-	-	_	_	-	_	_	_	-	_	-	_	99	%	-	_	-	-	_	_	_	-	_	-	-	-			
MET	GLU	ASP ALA	VAL	ALA	VAL	GLU SER	GLU	THK	LYS	GLY GLY	GLU	LYS	THR TYR	GLN	ARG	GLU	GLY 6	GLN	G L U	ASP	CYS	LEU LEU	0 ILN	ASN	THR	GLY	GLU	VAL VAL	GLN ASP	VAL. ASN	SER	VAL GLN MFT	Terri
VAL	MET	GLU	LEU	PRO	LEU LEU	GLN	LYS	GLU	VAL MET	GLU GLY	THR	ALA	PRO GLU	ALA	ALA	ALA VAL	ASP	THR	GLN	THE	LEU	VAL	VAL. ASN	MET GLU	GLU	PRO	ASN	ILE GLY	G LU	GLN	VAL	VAL PRO VAT	TTTA
DRQ	VAL	VAL PRO	VAL	HEL I	SER VAL	GLU	LEU	GLY	ALA TYR	GLU ASN	GLU	SER	GLU SYJ	GLY GLY	ALA	GLU	GLU	MET	TLE CYS	SIH	TEU	LEU	GLU	GLY PHE	GLN	VAL	VAL	GLY ALA	ASN GLY	GLU VAL	GLU	GLU GLU	MITTO
GLY	CTU GTU	PRO PRO	0 TI	ASP	FRU SER TRP	CTN GLN	ASP	ASP	TYR GLN	PRO PRO	ALA	CI T SA T	THR LYS	LYS	LYS	LYS	T N	ARG	TYR THR	GLU	GLY 5 U	ASP	ASP	V223	E231 GIN	NID	GLY	LEU	SER GLU	VAL. ASN	ALA GLU	LYS VAL VAT	714 4
GLY	ASN	LYS PRO	DRQ T VS	PRO	LYS LYS	LYS	LYS	VAL	TYS LYS	THR PHE	GLN	GLU	LEU	SER	THR	CYS	ARG	SER	ASN LEU	ASP	SIH	LYS	SER	ASP	GLU	PRO	SYJ	CYS	LEU CYS	GLY ARG	ALA PHE	ARG THR VAI	THAN I



THR LEU LEU ARG ARG ARM HIS HIS HIS CUS CUS CUS CUS CUS CUS CUS CUS CUS CU	ALA PALA VALE STRR STRR STRR STRR STRR CULU LYS ALA ALA CULU LYS ALA ALA CULU CULU CULU CULU CULU CULU C	LEU
LYS ARG ARG ARG ARG ARG CIV CIV CIV CIV CIV CIV CIV CIV CIV CIV	THR THR TYR TYR TYR TYR MET TRR MET TYR TYR TYR TYR TYR TYR TRR MET TR	HIS ILE
LEU GLN GLN HIS HIR GLU GLN GLN GLU ASN ASN HIS PHE HIS PHE HIS PHE HIS CVS CVS ASP CVS TAP TAP TAP TAP TAP TAP TAP TAP SCORTAN	SER ASE ASE ASE ASE ASE ASE ASE ASE ASE ASE	GLN
LYS SER HITS HITS LYS ASN GUU GUU GUN GUN GUN GUN GUN GUN GUN GU	NET THE MET HIS LITS LITS LITS LITS HIS HIS CITY CITY ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	TYR HIS
ASP PRO ASN VAL PRO PRO PRO ALA ALA CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	MET ARG ARG ARG ARG ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	LYS LYS
9,000 ASP SSR SSR SSR SSR SSR SSR SSR SSR ASP 0,010 ASP 0,010 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP 0 CSL ASP CSL AS	VAL 1112 1	ASN GLN
PRO THR THR THE THE THE VAL CLN CLN CLN CLN CLN CLN CLN CLN CLN CL	CLU CLU REA REA ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	MET ASP
ARG		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	79.03Å 107.25 Å 176.49 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	45.80 - 2.70	Depositor
Resolution (A)	47.19 - 2.46	EDS
% Data completeness	99.6 (45.80-2.70)	Depositor
(in resolution range)	99.1 (47.19 - 2.46)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.96 (at 2.45 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
D D.	(Not available) , (Not available)	Depositor
Π, Π_{free}	0.276 , 0.296	DCC
R_{free} test set	2741 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	75.9	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38 , 61.2	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.52	1/7677~(0.0%)	0.69	9/10341~(0.1%)
2	В	0.41	0/606	0.63	0/818
3	С	0.33	0/79	0.36	0/106
All	All	0.51	1/8362~(0.0%)	0.68	9/11265~(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	А	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	1039	LEU	C-N	9.34	1.51	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	227	MET	CA-CB-CG	-8.54	98.79	113.30
1	А	997	LEU	CB-CG-CD2	-7.02	99.07	111.00
1	А	224	MET	CG-SD-CE	6.80	111.08	100.20
1	А	973	LEU	CB-CG-CD2	6.36	121.81	111.00
1	А	221	LEU	CB-CG-CD2	6.31	121.73	111.00
1	А	227	MET	CB-CG-SD	6.28	131.22	112.40
1	А	559	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	997	LEU	CB-CG-CD1	5.98	121.17	111.00
1	А	360	LEU	CA-CB-CG	5.95	128.99	115.30

There are no chirality outliers.



All (1) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	751	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	7549	7539	7538	259	1
2	В	596	639	639	12	0
3	С	78	62	62	0	0
4	А	6	0	0	2	0
All	All	8229	8240	8239	263	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 16.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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: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:224:MET:HE2	1:A:315:TRP:CH2	2.11	0.86
1:A:993:PRO:HD3	1:A:1038:TRP:NE1	1.91	0.84
1:A:642:GLU:HG2	1:A:647:PHE:CE2	2.14	0.82
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:O	1:A:501:LEU:HD23	1.83	0.78
1:A:224:MET:CE	1:A:315:TRP:CZ2	2.66	0.78
1:A:197:MET:HB3	1:A:284:MET:HE2	1.64	0.78
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:224:MET:HE3	1:A:315:TRP:CZ2	2.22	0.74



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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:OD1	1:A:934:ASN:N	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: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: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	0.69
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: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:224:MET:HE2	1:A:315:TRP:CZ2	2.29	0.68
1:A:240:ASN:O	1:A:244:THR:HG23	1.94	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	1.61	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
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: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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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:942:SER:O	1:A:946:SER:OG	2.13	0.61
1:A:646:ILE:HG22	1:A:646:ILE:O	2.01	0.61
1:A:970:ILE:HD12	1:A:973:LEU:HD23	1.82	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:224:MET:HE3	1:A:315:TRP:HZ2	1.62	0.60
1:A:241:MET:HE1	1:A:278:GLN:HB2	1.84	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:HG2	1:A:556:GLN:O	2.03	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:993:PRO:CD	1:A:1038:TRP:CE2	2.87	0.57
1:A:405:LEU:O	1:A:406:THR:HB	2.03	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:879:MET:HE1	1:A:914:GLN:C	2.25	0.57
1:A:197:MET:HB3	1:A:284:MET:CE	2.34	0.56
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:1023:GLU:HA	1:A:1026:MET:HG2	1.87	0.56
1:A:597:LEU:HB2	1:A:644:PHE:CD1	2.41	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:O	1:A:1026:MET:HG3	2.06	0.55
1:A:132:THR:HG23	1:A:135:MET:HE3	1.89	0.55
1:A:727:GLU:HG3	1:A:728:GLN:N	2.22	0.55
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:1019:TYR:HA	1:A:1022:LEU:HB3	1.89	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:873:VAL:HG23	1:A:874:TYR:CD2	2.42	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: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:374:ARG:HG3	1:A:378:MET:CE	2.38	0.53
1:A:921:LEU:HD22	1:A:924:GLN:HB2	1.90	0.53
1:A:224:MET:HG3	1:A:311:GLU:CB	2.39	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:O	1:A:975:LYS:HG3	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
1:A:751:SER:OG	1:A:809:MET:CE	2.58	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:129:GLY:HA3	1:A:148:MET:HE3	1.93	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:1019:TYR:HD1	1:A:1023:GLU:OE2	1.95	0.50
1:A:356:TYR:O	1:A:356:TYR:HD1	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:1000:LEU:HD22	1:A:1003:LEU:HD23	1.94	0.49
1:A:582:ALA:O	1:A:586:THR:HG23	2.11	0.49
1:A:566:LEU:O	1:A:566:LEU:HD23	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:HD23	1:A:715:LEU:O	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



		Interatomic	Clash
Atom-1	Atom-2	$distance (m \AA)$	overlap (Å)
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: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:374:ARG:HG3	1:A:378:MET:HE2	1.95	0.48
1:A:547:VAL:CG1	1:A:548:LEU:H	2.22	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:196:MET:HG3	1:A:197:MET:N	2.28	0.48
1:A:465:VAL:HG22	1:A:524:ILE:HD12	1.96	0.47
1:A:802:ILE:HG12	1:A:802:ILE:O	2.14	0.47
1:A:324:LEU:HA	1:A:324:LEU:HD12	1.73	0.47
1:A:762:LYS:HE3	1:A:766:ARG:HH12	1.78	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:339:LYS:HE2	2:B:340:GLN:HG2	1.96	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:1026:MET:HB2	1:A:1030:MET:HE2	1.96	0.47
1:A:763:LYS:HG3	1:A:764:GLN:N	2.29	0.47
1:A:139:MET:HG2	1:A:143:GLU:HB2	1.98	0.46
1:A:99:VAL:CG1	1:A:182:LEU:HA	2.45	0.46
2:B:333:ASP:CG	2:B:336:THR:HG23	2.35	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
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:HA	1:A:169:LYS:HE2	1.97	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:803:MET:HA	1:A:807:ARG:HE	1.81	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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:921:LEU:C	1:A:921:LEU:HD13	2.37	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:264:LEU:C	1:A:264:LEU:HD12	2.38	0.44
1:A:930:MET:HG3	1:A:930:MET:O	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:CD2	1:A:938:PHE:O	2.70	0.44
1:A:959:PHE:HB2	1:A:1009:LYS:HD3	1.99	0.44
1:A:266:LEU:HD22	1:A:266:LEU:O	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:993:PRO:CG	1:A:1038:TRP:CE2	3.00	0.44
1:A:193:ASP:C	1:A:193:ASP:OD1	2.55	0.43
1:A:872:ILE:HD13	1:A:882:ALA:HB2	2.00	0.43
1:A:421:HIS:CG	1:A:423:PRO:HD2	2.53	0.43
1:A:762:LYS:HE3	1:A:766:ARG:NH1	2.33	0.43
1:A:154:GLU:H	1:A:154:GLU:CD	2.20	0.43
1:A:159:TYR:HB2	1:A:160:PRO:HD2	2.00	0.43
1:A:751:SER:C	1:A:753:SER:N	2.71	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:566:LEU:C	1:A:566:LEU:HD23	2.39	0.43
1:A:604:ARG:O	1:A:604:ARG:CG	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1019:TYR:O	1:A:1022:LEU:HB3	2.19	0.43
1:A:993:PRO:HG3	1:A:1038:TRP:CE2	2.54	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:619:ILE:HG13	1:A:620:VAL:N	2.34	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:129:GLY:C	1:A:148:MET:HE1	2.39	0.42
1:A:993:PRO:CD	1:A:1038:TRP:NE1	2.75	0.42
1:A:617:ARG:NH2	1:A:660:GLU:OE1	2.53	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:1043:SER:O	1:A:1047:SER:OG	2.38	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:476:HIS:CE1	2:B:361:MET:HE2	2.55	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: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
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: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:726:PRO:O	1:A:727:GLU:C	2.59	0.41
1:A:700:ALA:HA	2:B:382:ASN:HB2	2.02	0.41
1:A:715:LEU:HD23	1:A:715:LEU:C	2.40	0.41
1:A:129:GLY:C	1:A:148:MET:CE	2.90	0.41
1:A:658:ILE:HD13	1:A:703:LEU:HD22	2.02	0.41
1:A:132:THR:HG23	1:A:135:MET:CE	2.51	0.40
1:A:476:HIS:NE2	2:B:361:MET:HE2	2.36	0.40
1:A:145:ILE:O	1:A:149:THR:HG23	2.20	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:990:GLU:CD	1:A:990:GLU:H	2.24	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-1 Atom-2		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	А	911/1231~(74%)	862~(95%)	49~(5%)	0	100 100
2	В	72/631~(11%)	69~(96%)	3 (4%)	0	100 100
3	С	7/727~(1%)	7 (100%)	0	0	100 100
All	All	990/2589~(38%)	938~(95%)	52 (5%)	0	100 100

There are no Ramachandran outliers to report.

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	Percentile	es
1	А	839/1106~(76%)	796~(95%)	43~(5%)	24 50	
2	В	69/566~(12%)	69~(100%)	0	100 100)
3	С	9/647~(1%)	9~(100%)	0	100 100)
All	All	917/2319 (40%)	874 (95%)	43 (5%)	26 54	

All (43) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	202	SER
1	А	232	ASN
1	А	263	ARG
1	А	296	ARG
1	А	319	TYR
1	А	346	LYS
1	А	356	TYR
1	А	369	SER
1	А	419	SER
1	А	434	LYS
1	А	459	ASN
1	А	474	HIS
1	А	535	CYS
1	A	596	ASP
1	A	600	TYR
1	А	634	LYS
1	А	636	TYR
1	А	663	ASP
1	А	675	GLU
1	А	705	LYS
1	А	744	GLN
1	А	751	SER
1	А	752	SER
1	А	756	GLU
1	А	763	LYS
1	А	766	ARG
1	А	890	MET
1	А	931	ILE
1	А	934	ASN
1	A	937	ASN
1	А	939	ASP
1	A	940	ARG
1	A	954	ARG
1	A	955	PHE
1	A	1009	LYS
1	A	1019	TYR
1	A	1028	PHE
1	A	1029	GLN
1	A	1033	ARG
1	A	1034	ARG
1	A	1035	GLU
1	A	1042	MET
1	А	1045	ARG



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	А	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	993:PRO	С	994:PRO	Ν	3.08



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

