Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:03 am BST

PDB ID	:	6QJ4
Title	:	Crystal structure of the C. thermophilum condensin Ycs4-Brn1 subcomplex bound to the Smc4 ATPase head in complex with the C-terminal domain of Brn1
Authors	:	Hassler, M.; Haering, C.H.; Kschonsak, M.
Deposited on	:	2019-01-22
Resolution	:	5.80 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 following versions of software and data (see references ①) were used in the production of this report:

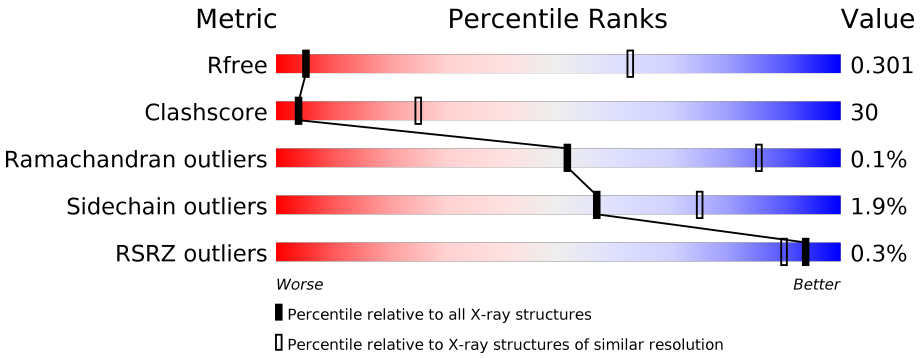
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.80 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}	130704	1008 (7.70-3.86)
Clashscore	141614	1035 (7.70-3.90)
Ramachandran outliers	138981	1003 (7.70-3.86)
Sidechain outliers	138945	1006 (7.78-3.82)
RSRZ outliers	127900	1009 (7.82-3.78)

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% 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	1155	41% 41% • 17%
2	B	197	% 12% 13% 75%
3	C	403	31% 44% 24%
4	D	23	87% 9% •
5	E	135	27% 24% • 47%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10778 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 Condensin complex subunit 1,Condensin complex subunit 1,Condensin complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	963	7240	4571	1260	1361	48	0	0	0

There are 121 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP G0SB82
A	?	-	CYS	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	ILE	deletion	UNP G0SB82
A	?	-	PHE	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	PHE	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	TYR	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	ILE	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	VAL	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	MET	deletion	UNP G0SB82

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ILE	deletion	UNP G0SB82
A	?	-	GLU	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	VAL	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	PRO	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ASN	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	ASP	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	HIS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	LEU	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	ALA	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	THR	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	ARG	deletion	UNP G0SB82

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	GLY	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	ASN	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	SER	deletion	UNP G0SB82
A	?	-	LYS	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82
A	?	-	GLN	deletion	UNP G0SB82

- Molecule 2 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	50	Total	C	N	O	S	0	0	0
			392	256	62	73	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	222	GLY	-	expression tag	UNP G0SBJ6
B	223	HIS	-	expression tag	UNP G0SBJ6
B	224	MET	-	expression tag	UNP G0SBJ6

- Molecule 3 is a protein called Uncharacterized protein,Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	306	Total	C	N	O	S	0	0	0
			2443	1563	419	450	11			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	261	MET	-	initiating methionine	UNP G0S2G2
C	262	ALA	-	expression tag	UNP G0S2G2
C	1360	SER	-	linker	UNP G0S2G2
C	1361	GLY	-	linker	UNP G0S2G2
C	1362	GLY	-	linker	UNP G0S2G2
C	1363	SER	-	linker	UNP G0S2G2
C	1364	GLY	-	linker	UNP G0S2G2
C	1365	GLY	-	linker	UNP G0S2G2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1366	SER	ALA	conflict	UNP G0S2G2
C	1543	GLY	-	expression tag	UNP G0S2G2
C	1544	ILE	-	expression tag	UNP G0S2G2
C	1545	SER	-	expression tag	UNP G0S2G2
C	1546	SER	-	expression tag	UNP G0S2G2
C	1547	ALA	-	expression tag	UNP G0S2G2
C	1548	SER	-	expression tag	UNP G0S2G2
C	1549	HIS	-	expression tag	UNP G0S2G2
C	1550	HIS	-	expression tag	UNP G0S2G2
C	1551	HIS	-	expression tag	UNP G0S2G2
C	1552	HIS	-	expression tag	UNP G0S2G2
C	1553	HIS	-	expression tag	UNP G0S2G2
C	1554	HIS	-	expression tag	UNP G0S2G2
C	1555	HIS	-	expression tag	UNP G0S2G2
C	1556	HIS	-	expression tag	UNP G0S2G2

- Molecule 4 is a protein called Brn1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	22	Total	C	N	O	0	0	0
			110	66	22	22			

- Molecule 5 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	71	Total	C	N	O	S	0	0	0
			593	379	100	110	4			

There is a discrepancy between the modelled and reference sequences:

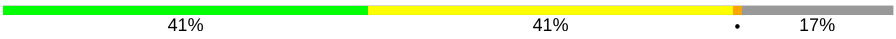
Chain	Residue	Modelled	Actual	Comment	Reference
E	764	MET	VAL	conflict	UNP G0SBJ6

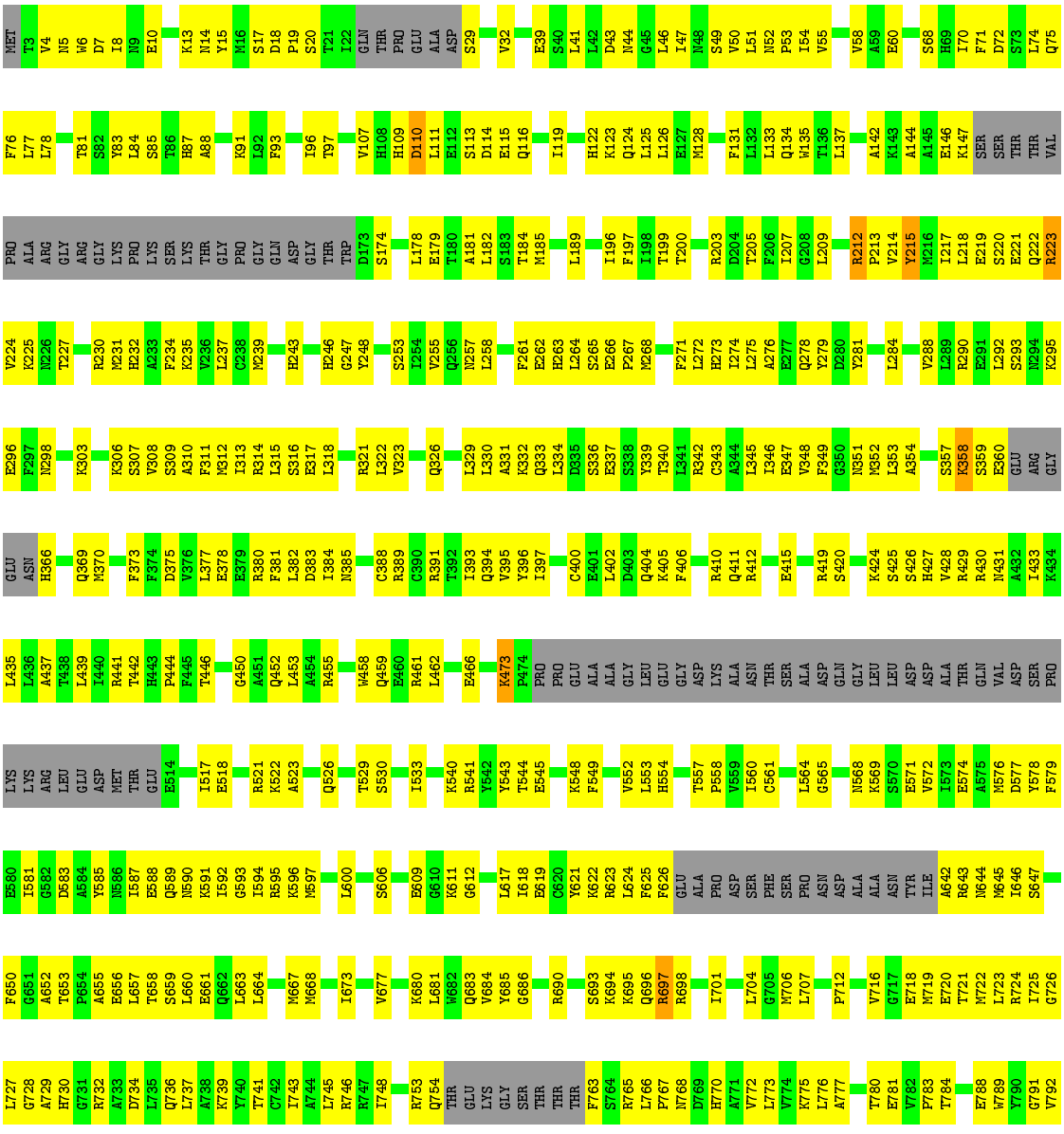
3 Residue-property plots (i)

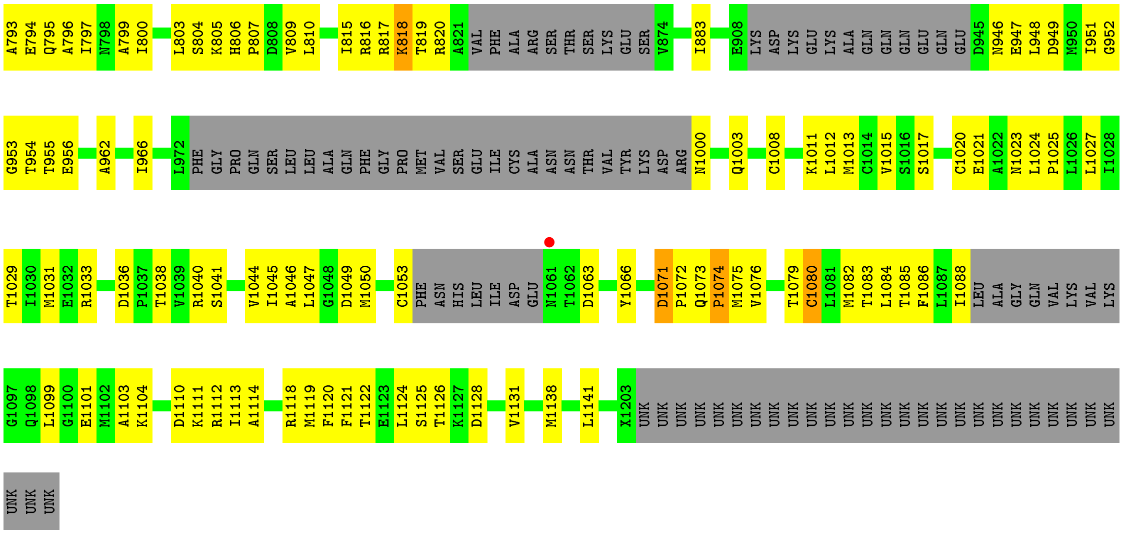
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Condensin complex subunit 1,Condensin complex subunit 1,Condensin complex subunit 1

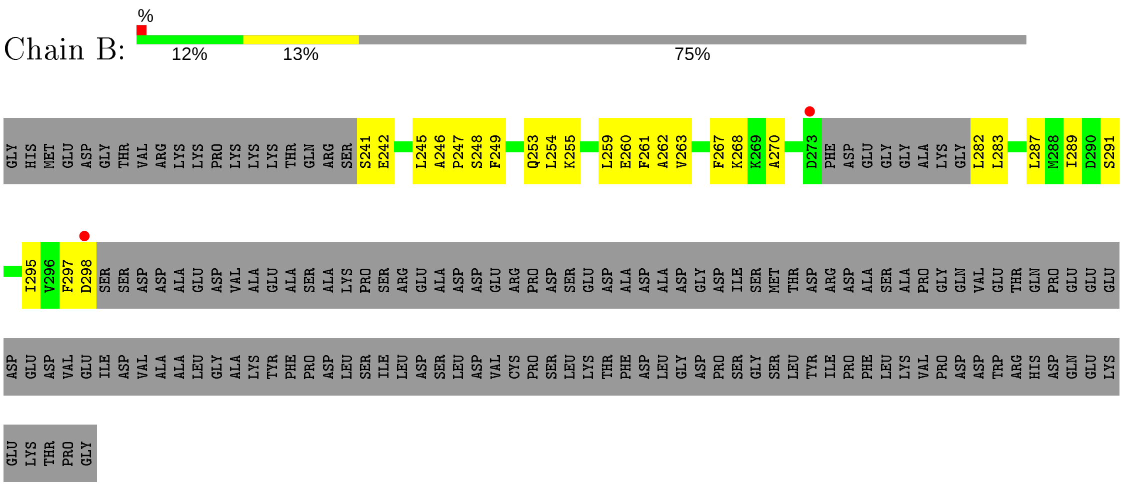
Chain A:



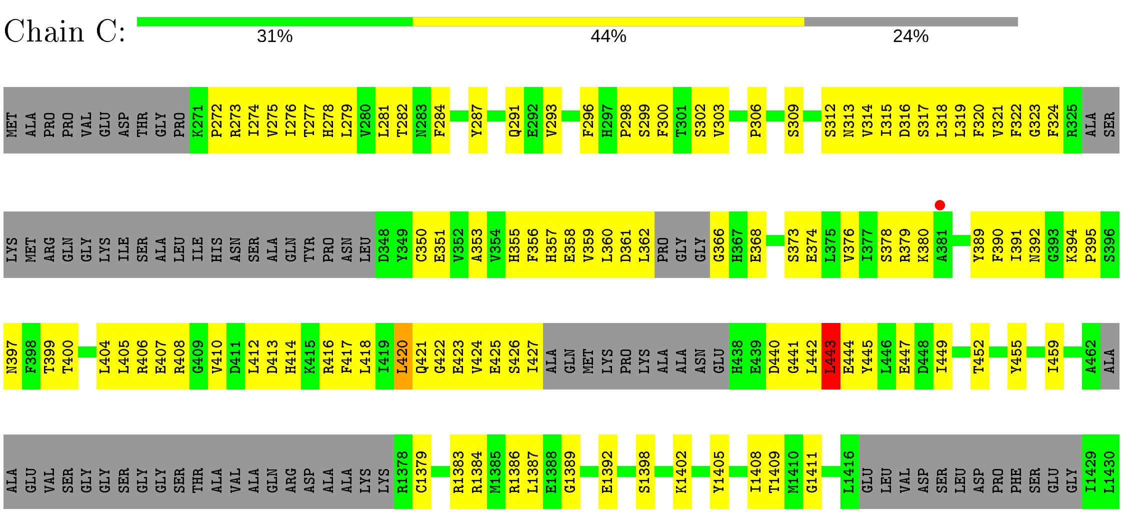


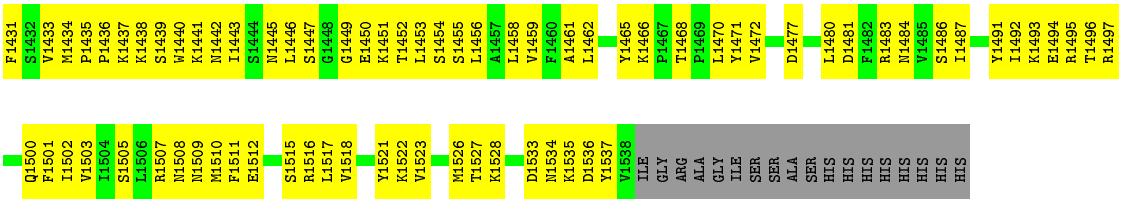


• Molecule 2: Condensin complex subunit 2



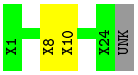
• Molecule 3: Uncharacterized protein,Uncharacterized protein





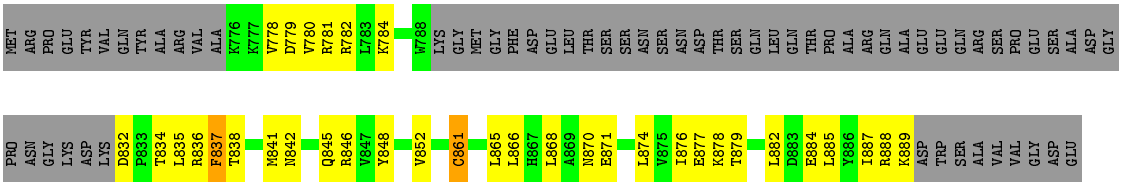
• Molecule 4: Brn1

Chain D:



• Molecule 5: Condensin complex subunit 2

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.41Å 82.38Å 177.83Å 90.00° 98.77° 90.00°	Depositor
Resolution (Å)	47.74 – 5.80 47.74 – 5.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.74-5.80) 96.5 (47.74-5.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 5.73Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.292 , 0.301 0.292 , 0.301	Depositor DCC
R_{free} test set	296 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å^2)	327.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 259.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10778	wwPDB-VP
Average B, all atoms (Å^2)	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.29	0/7199	0.45	0/9737
2	B	0.29	0/398	0.52	0/534
3	C	0.30	0/2489	0.48	1/3352 (0.0%)
5	E	0.27	0/601	0.44	0/808
All	All	0.29	0/10687	0.46	1/14431 (0.0%)

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	2
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	443	LEU	C-N-CA	5.43	135.27	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1071	ASP	Peptide
1	A	243	HIS	Peptide
3	C	443	LEU	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	A	7240	0	6987	442	1
2	B	392	0	398	34	0
3	C	2443	0	2454	163	0
4	D	110	0	31	1	0
5	E	593	0	610	31	0
All	All	10778	0	10480	644	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 30.

All (644) 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)
3:C:356:PHE:O	3:C:374:GLU:HA	1.71	0.90
3:C:1494:GLU:HA	3:C:1497:ARG:HH22	1.43	0.83
1:A:265:SER:HB3	1:A:311:PHE:HB2	1.61	0.83
1:A:723:LEU:HA	1:A:727:LEU:HB2	1.59	0.82
1:A:266:GLU:OE1	1:A:314:ARG:HB2	1.78	0.82
1:A:189:LEU:HD22	1:A:239:MET:HB3	1.64	0.79
1:A:382:LEU:HD22	2:B:248:SER:HA	1.64	0.79
3:C:420:LEU:HD23	3:C:422:GLY:H	1.46	0.79
1:A:783:PRO:O	1:A:784:THR:HG23	1.83	0.79
1:A:298:ASN:HA	1:A:337:GLU:HB3	1.63	0.78
1:A:29:SER:N	1:A:75:GLN:OE1	2.17	0.77
1:A:788:GLU:HA	2:B:291:SER:HB2	1.67	0.77
1:A:336:SER:O	1:A:342:ARG:NH1	2.17	0.77
1:A:377:LEU:H	1:A:377:LEU:HD12	1.50	0.77
3:C:1477:ASP:OD2	3:C:1507:ARG:HG2	1.85	0.76
3:C:1409:THR:HB	3:C:1436:PRO:HG3	1.67	0.75
1:A:220:SER:HB2	1:A:223:ARG:HE	1.51	0.75
5:E:841:MET:SD	5:E:845:GLN:NE2	2.59	0.75
3:C:319:LEU:O	3:C:323:GLY:N	2.18	0.74
1:A:1063:ASP:HA	1:A:1066:TYR:HD2	1.52	0.74
3:C:1450:GLU:HA	3:C:1453:LEU:HD13	1.67	0.74
1:A:227:THR:HA	1:A:230:ARG:HB3	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:320:PHE:O	3:C:379:ARG:NH1	2.22	0.72
1:A:384:ILE:O	1:A:389:ARG:NH2	2.23	0.71
1:A:743:ILE:HD12	1:A:746:ARG:HH21	1.53	0.71
3:C:1526:MET:O	3:C:1528:LYS:NZ	2.22	0.71
1:A:734:ASP:HB3	1:A:737:LEU:HB2	1.73	0.71
1:A:134:GLN:OE1	1:A:212:ARG:NH1	2.24	0.71
1:A:354:ALA:O	1:A:358:LYS:NZ	2.24	0.70
1:A:619:GLU:HB3	1:A:623:ARG:HH22	1.54	0.70
1:A:695:LYS:HD3	1:A:698:ARG:HD2	1.72	0.70
1:A:1063:ASP:HA	1:A:1066:TYR:CD2	2.27	0.70
1:A:726:GLY:HA3	1:A:741:THR:HG21	1.74	0.69
1:A:329:LEU:HA	1:A:332:LYS:HD3	1.73	0.69
1:A:606:SER:HA	1:A:612:GLY:HA2	1.73	0.69
1:A:68:SER:HA	1:A:71:PHE:HB3	1.73	0.69
5:E:780:VAL:O	5:E:784:LYS:NZ	2.18	0.69
1:A:1121:PHE:O	1:A:1125:SER:N	2.26	0.69
1:A:134:GLN:NE2	1:A:209:LEU:O	2.26	0.69
1:A:948:LEU:O	3:C:1483:ARG:NH1	2.25	0.69
1:A:1033:ARG:O	1:A:1040:ARG:NH1	2.25	0.69
1:A:766:LEU:HB3	1:A:773:LEU:HD11	1.75	0.69
1:A:794:GLU:N	1:A:794:GLU:OE1	2.26	0.69
3:C:443:LEU:H	3:C:444:GLU:HB2	1.57	0.69
1:A:323:VAL:HA	1:A:326:GLN:HE22	1.57	0.68
3:C:314:VAL:O	3:C:317:SER:OG	2.11	0.68
1:A:114:ASP:O	1:A:116:GLN:NE2	2.26	0.68
1:A:46:LEU:O	1:A:49:SER:OG	2.10	0.68
1:A:819:THR:OG1	1:A:820:ARG:NH1	2.27	0.68
1:A:768:ASN:HA	1:A:773:LEU:HD22	1.76	0.68
1:A:462:LEU:HD21	1:A:466:GLU:OE2	1.94	0.67
1:A:1049:ASP:HB3	2:B:283:LEU:HD21	1.74	0.67
1:A:797:ILE:HA	1:A:800:ILE:HG12	1.76	0.67
1:A:380:ARG:HH11	2:B:241:SER:HB2	1.60	0.67
5:E:778:VAL:HG13	5:E:782:ARG:HH12	1.60	0.67
1:A:816:ARG:O	1:A:819:THR:OG1	2.11	0.67
1:A:523:ALA:HA	1:A:526:GLN:HE22	1.59	0.67
1:A:954:THR:O	1:A:1017:SER:OG	2.12	0.66
5:E:874:LEU:HD13	5:E:889:LYS:HD3	1.77	0.66
5:E:832:ASP:HB3	5:E:888:ARG:HD2	1.77	0.66
1:A:331:ALA:HA	1:A:334:LEU:HD23	1.76	0.66
3:C:404:LEU:O	3:C:408:ARG:N	2.28	0.66
3:C:312:SER:O	3:C:316:ASP:N	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:HD3	2:B:254:LEU:HB2	1.78	0.66
1:A:184:THR:OG1	1:A:185:MET:SD	2.54	0.65
1:A:739:LYS:HE3	1:A:795:GLN:HG3	1.77	0.65
1:A:1120:PHE:O	1:A:1124:LEU:N	2.29	0.65
1:A:322:LEU:HD12	1:A:323:VAL:N	2.10	0.65
1:A:458:TRP:HA	1:A:461:ARG:HD3	1.78	0.65
1:A:600:LEU:HB2	1:A:617:LEU:HD22	1.79	0.65
1:A:1046:ALA:O	1:A:1050:MET:HB2	1.96	0.65
1:A:10:GLU:HA	1:A:13:LYS:HD2	1.79	0.65
1:A:588:GLU:OE1	1:A:588:GLU:N	2.24	0.65
1:A:947:GLU:O	3:C:1483:ARG:NH2	2.29	0.65
1:A:720:GLU:O	1:A:724:ARG:NH1	2.30	0.65
1:A:380:ARG:HA	2:B:245:LEU:HD11	1.79	0.65
1:A:4:VAL:HG23	1:A:5:ASN:H	1.62	0.65
1:A:694:LYS:O	1:A:698:ARG:NH1	2.30	0.64
1:A:314:ARG:HD3	1:A:317:GLU:HB2	1.78	0.64
3:C:390:PHE:HA	3:C:394:LYS:O	1.96	0.64
1:A:724:ARG:HB2	1:A:725:ILE:HD12	1.79	0.64
1:A:600:LEU:HD12	1:A:617:LEU:HD13	1.80	0.64
1:A:729:ALA:HA	1:A:732:ARG:HH11	1.63	0.64
3:C:1434:MET:HB2	3:C:1440:TRP:CD2	2.32	0.64
3:C:303:VAL:HG22	3:C:1518:VAL:HB	1.80	0.64
1:A:133:LEU:O	1:A:137:LEU:HG	1.98	0.64
1:A:1021:GLU:N	1:A:1021:GLU:OE1	2.27	0.63
1:A:32:VAL:HG12	1:A:72:ASP:HB2	1.80	0.63
1:A:1015:VAL:HG13	1:A:1017:SER:H	1.63	0.63
1:A:723:LEU:O	1:A:775:LYS:NZ	2.31	0.63
1:A:698:ARG:HA	1:A:737:LEU:HD21	1.80	0.63
3:C:406:ARG:HA	3:C:410:VAL:HA	1.79	0.63
1:A:1122:THR:O	1:A:1126:THR:N	2.31	0.63
1:A:119:ILE:HA	1:A:122:HIS:CE1	2.33	0.63
3:C:406:ARG:HG3	3:C:410:VAL:HG23	1.81	0.63
5:E:874:LEU:HB3	5:E:887:ILE:HD11	1.80	0.63
1:A:262:GLU:HA	1:A:307:SER:HB3	1.81	0.63
1:A:212:ARG:HG3	1:A:213:PRO:HD3	1.80	0.62
1:A:334:LEU:HD22	1:A:345:LEU:HD13	1.80	0.62
5:E:888:ARG:NH1	5:E:889:LYS:O	2.32	0.62
1:A:618:ILE:O	1:A:622:LYS:HB3	2.00	0.62
1:A:723:LEU:HD23	1:A:727:LEU:HD13	1.80	0.62
1:A:402:LEU:HG	1:A:404:GLN:H	1.64	0.62
1:A:1118:ARG:HG3	1:A:1122:THR:HG23	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:VAL:HG21	2:B:268:LYS:HE3	1.82	0.61
1:A:78:LEU:HB3	1:A:135:TRP:CD1	2.36	0.61
1:A:347:GLU:OE1	1:A:351:ASN:ND2	2.33	0.61
1:A:576:MET:HA	1:A:597:MET:HE1	1.82	0.61
1:A:686:GLY:HA2	1:A:725:ILE:HD11	1.83	0.61
3:C:1486:SER:HB3	3:C:1509:ASN:HD21	1.66	0.61
1:A:306:LYS:O	1:A:309:SER:OG	2.19	0.61
1:A:595:ARG:NH2	1:A:656:GLU:OE2	2.30	0.61
1:A:883:ILE:O	1:A:1011:LYS:NZ	2.34	0.61
3:C:313:ASN:HA	3:C:316:ASP:HB2	1.83	0.61
1:A:1099:LEU:HG	1:A:1103:ALA:HB2	1.83	0.60
1:A:777:ALA:O	1:A:780:THR:OG1	2.19	0.60
1:A:179:GLU:O	1:A:232:HIS:NE2	2.33	0.60
1:A:326:GLN:OE1	1:A:326:GLN:N	2.33	0.60
3:C:360:LEU:HG	3:C:368:GLU:HB3	1.82	0.60
3:C:1472:VAL:HG12	3:C:1502:ILE:HB	1.82	0.60
1:A:312:MET:HA	1:A:315:LEU:HD12	1.83	0.60
1:A:348:VAL:O	1:A:352:MET:HG3	2.00	0.60
1:A:6:TRP:NE1	1:A:8:ILE:HG12	2.16	0.60
1:A:385:ASN:OD1	1:A:388:CYS:N	2.23	0.60
1:A:424:LYS:HA	2:B:254:LEU:HD22	1.84	0.60
1:A:427:HIS:O	1:A:431:ASN:ND2	2.34	0.60
1:A:718:GLU:O	1:A:721:THR:OG1	2.14	0.60
1:A:41:LEU:HD22	1:A:83:TYR:CB	2.32	0.60
1:A:743:ILE:HD11	1:A:795:GLN:HE21	1.65	0.60
1:A:1084:LEU:HD12	1:A:1085:THR:HG23	1.84	0.60
1:A:781:GLU:OE2	1:A:817:ARG:NH1	2.34	0.60
1:A:1013:MET:SD	1:A:1023:ASN:HB2	2.41	0.59
1:A:314:ARG:HD2	1:A:318:LEU:HD23	1.84	0.59
1:A:656:GLU:OE1	1:A:656:GLU:N	2.18	0.59
1:A:295:LYS:NZ	1:A:296:GLU:O	2.32	0.59
1:A:949:ASP:O	1:A:953:GLY:N	2.33	0.59
1:A:693:SER:OG	1:A:694:LYS:N	2.35	0.59
1:A:591:LYS:HA	1:A:594:ILE:HD12	1.84	0.59
3:C:1447:SER:OG	3:C:1450:GLU:OE1	2.18	0.59
1:A:354:ALA:O	1:A:357:SER:OG	2.14	0.59
5:E:838:THR:O	5:E:842:ASN:ND2	2.36	0.59
3:C:1492:ILE:O	3:C:1496:THR:OG1	2.20	0.59
5:E:848:TYR:HB3	5:E:852:VAL:HB	1.84	0.59
3:C:318:LEU:O	3:C:321:VAL:HB	2.02	0.59
1:A:1118:ARG:HA	1:A:1121:PHE:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ALA:HA	1:A:281:TYR:H	1.68	0.58
1:A:343:CYS:HB3	1:A:391:ARG:HD2	1.86	0.58
3:C:416:ARG:NH2	3:C:1466:LYS:O	2.32	0.58
4:D:8:UNK:O	4:D:10:UNK:N	2.36	0.58
3:C:1493:LYS:O	3:C:1497:ARG:NH1	2.36	0.58
3:C:306:PRO:O	3:C:309:SER:OG	2.20	0.58
3:C:416:ARG:NH2	3:C:1462:LEU:O	2.36	0.58
1:A:645:MET:SD	1:A:645:MET:N	2.77	0.58
3:C:1435:PRO:O	3:C:1437:LYS:N	2.37	0.58
3:C:1496:THR:O	3:C:1497:ARG:NH1	2.31	0.58
1:A:179:GLU:HG2	1:A:232:HIS:CD2	2.39	0.58
3:C:287:TYR:HB3	3:C:291:GLN:HG3	1.85	0.58
3:C:300:PHE:O	3:C:1515:SER:OG	2.22	0.57
1:A:247:GLY:HA2	1:A:284:LEU:HD11	1.86	0.57
1:A:748:ILE:HB	1:A:803:LEU:HD21	1.85	0.57
1:A:1029:THR:O	1:A:1033:ARG:NE	2.37	0.57
1:A:197:PHE:HB3	1:A:203:ARG:HG2	1.84	0.57
3:C:1491:TYR:HA	3:C:1495:ARG:HG2	1.87	0.57
1:A:517:ILE:O	1:A:521:ARG:HG2	2.04	0.57
1:A:93:PHE:O	1:A:97:THR:OG1	2.22	0.57
1:A:587:ILE:HG12	1:A:589:GLN:H	1.70	0.57
1:A:677:VAL:O	1:A:681:LEU:HG	2.04	0.57
3:C:1450:GLU:N	3:C:1450:GLU:OE1	2.38	0.57
3:C:276:ILE:HG13	3:C:356:PHE:CE2	2.40	0.57
1:A:119:ILE:HG22	1:A:196:ILE:HD13	1.86	0.57
1:A:200:THR:HA	1:A:203:ARG:HB2	1.85	0.57
1:A:668:MET:HB2	1:A:673:ILE:HD12	1.87	0.57
3:C:1434:MET:HA	3:C:1439:SER:O	2.05	0.57
1:A:1119:MET:HG2	2:B:262:ALA:H	1.70	0.57
1:A:427:HIS:CD2	1:A:427:HIS:H	2.22	0.56
3:C:278:HIS:CD2	3:C:355:HIS:HD2	2.23	0.56
1:A:530:SER:HA	1:A:533:ILE:HD12	1.85	0.56
1:A:1118:ARG:O	1:A:1122:THR:N	2.26	0.56
1:A:378:GLU:HA	1:A:381:PHE:CD1	2.40	0.56
1:A:411:GLN:HE22	1:A:549:PHE:HB2	1.69	0.56
3:C:459:ILE:HG23	3:C:1379:CYS:HB2	1.86	0.56
1:A:178:LEU:O	1:A:182:LEU:HG	2.04	0.56
1:A:7:ASP:O	1:A:10:GLU:N	2.37	0.56
1:A:174:SER:O	1:A:178:LEU:HG	2.04	0.56
2:B:289:ILE:HA	2:B:295:ILE:HG23	1.88	0.56
3:C:1408:ILE:HG13	3:C:1409:THR:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:273:ARG:NE	3:C:298:PRO:O	2.36	0.56
1:A:353:LEU:HD11	1:A:373:PHE:HB2	1.87	0.56
1:A:694:LYS:HA	1:A:697:ARG:CZ	2.35	0.56
1:A:1008:CYS:O	1:A:1012:LEU:HG	2.06	0.55
1:A:642:ALA:HB1	1:A:680:LYS:HE3	1.88	0.55
3:C:1508:ASN:HA	3:C:1511:PHE:CZ	2.40	0.55
3:C:418:LEU:HD23	3:C:418:LEU:H	1.71	0.55
1:A:1128:ASP:HA	1:A:1131:VAL:C	2.26	0.55
1:A:346:ILE:HG22	1:A:395:VAL:HG21	1.88	0.55
3:C:293:VAL:HG22	3:C:296:PHE:HE2	1.72	0.55
2:B:248:SER:OG	2:B:249:PHE:N	2.39	0.55
1:A:1110:ASP:O	1:A:1113:ILE:HG12	2.05	0.55
1:A:378:GLU:HA	1:A:381:PHE:HD1	1.71	0.55
3:C:1454:SER:O	3:C:1458:LEU:HG	2.05	0.55
5:E:781:ARG:HE	5:E:868:LEU:HG	1.70	0.55
2:B:287:LEU:HG	2:B:295:ILE:HG21	1.87	0.55
1:A:544:THR:O	1:A:548:LYS:HG3	2.06	0.55
1:A:1076:VAL:O	1:A:1080:CYS:N	2.30	0.55
1:A:743:ILE:HD11	1:A:795:GLN:HB3	1.88	0.55
3:C:1384:ARG:HA	3:C:1387:LEU:HD12	1.87	0.55
3:C:313:ASN:O	3:C:317:SER:N	2.40	0.55
1:A:308:VAL:O	1:A:312:MET:HG2	2.06	0.55
1:A:353:LEU:HD21	1:A:373:PHE:HB3	1.89	0.55
3:C:316:ASP:O	3:C:319:LEU:HB3	2.07	0.55
3:C:440:ASP:N	3:C:440:ASP:OD1	2.40	0.55
1:A:1041:SER:HB3	1:A:1079:THR:HG21	1.89	0.54
1:A:541:ARG:O	1:A:545:GLU:HG2	2.07	0.54
2:B:295:ILE:HB	2:B:297:PHE:CZ	2.42	0.54
1:A:720:GLU:N	1:A:720:GLU:OE1	2.38	0.54
3:C:355:HIS:CE1	3:C:376:VAL:HG13	2.42	0.54
3:C:306:PRO:HD3	5:E:866:LEU:HD21	1.89	0.54
5:E:846:ARG:NE	5:E:846:ARG:O	2.39	0.54
1:A:235:LYS:O	1:A:239:MET:HG2	2.07	0.54
1:A:412:ARG:HA	1:A:415:GLU:CD	2.27	0.54
3:C:412:LEU:HD12	3:C:416:ARG:HG2	1.90	0.54
1:A:266:GLU:OE1	1:A:314:ARG:NE	2.40	0.54
1:A:695:LYS:HA	1:A:698:ARG:HH11	1.72	0.54
1:A:196:ILE:HG23	1:A:197:PHE:HD2	1.72	0.54
1:A:667:MET:HG3	1:A:673:ILE:HD11	1.90	0.54
3:C:1462:LEU:H	3:C:1462:LEU:HD12	1.73	0.54
3:C:322:PHE:HB3	3:C:324:PHE:HE1	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1481:ASP:HB3	3:C:1484:ASN:ND2	2.23	0.53
1:A:946:ASN:O	1:A:948:LEU:HD12	2.08	0.53
3:C:1398:SER:O	3:C:1402:LYS:HG2	2.09	0.53
5:E:834:THR:HG21	5:E:836:ARG:HH11	1.74	0.53
1:A:316:SER:HB2	1:A:351:ASN:HD22	1.72	0.53
3:C:1447:SER:H	3:C:1451:LYS:HZ2	1.57	0.53
3:C:1494:GLU:HA	3:C:1497:ARG:NH2	2.19	0.53
1:A:571:GLU:N	1:A:571:GLU:OE1	2.36	0.53
1:A:656:GLU:O	1:A:660:LEU:HG	2.09	0.53
1:A:6:TRP:HA	1:A:6:TRP:CE3	2.42	0.53
1:A:723:LEU:HB2	1:A:724:ARG:NH1	2.23	0.53
3:C:447:GLU:HB2	3:C:452:THR:HG23	1.90	0.53
1:A:182:LEU:HA	1:A:185:MET:HG2	1.90	0.53
2:B:289:ILE:H	2:B:289:ILE:HD12	1.72	0.53
1:A:583:ASP:OD1	1:A:591:LYS:NZ	2.41	0.53
1:A:660:LEU:HA	1:A:663:LEU:HD12	1.90	0.53
1:A:122:HIS:O	1:A:126:LEU:HG	2.09	0.52
1:A:185:MET:SD	1:A:185:MET:N	2.82	0.52
1:A:221:GLU:O	1:A:225:LYS:NZ	2.30	0.52
5:E:837:PHE:HD2	5:E:884:GLU:HG2	1.73	0.52
1:A:806:HIS:HB3	1:A:809:VAL:HG13	1.91	0.52
3:C:358:GLU:HB2	3:C:373:SER:HB2	1.92	0.52
1:A:661:GLU:HA	1:A:706:MET:HB3	1.91	0.52
1:A:41:LEU:HD12	1:A:41:LEU:O	2.09	0.52
1:A:214:VAL:O	1:A:218:LEU:HG	2.09	0.52
1:A:772:VAL:O	1:A:776:LEU:HG	2.09	0.52
3:C:1446:LEU:H	3:C:1451:LYS:NZ	2.08	0.52
1:A:199:THR:O	1:A:203:ARG:N	2.42	0.52
1:A:313:ILE:O	1:A:316:SER:OG	2.26	0.52
1:A:369:GLN:HG2	1:A:373:PHE:CZ	2.45	0.52
1:A:134:GLN:NE2	1:A:213:PRO:HD3	2.25	0.52
1:A:768:ASN:ND2	1:A:806:HIS:O	2.43	0.52
1:A:1041:SER:HA	1:A:1076:VAL:HG13	1.91	0.51
1:A:587:ILE:HG23	1:A:590:ASN:HB3	1.92	0.51
3:C:1486:SER:HB3	3:C:1509:ASN:ND2	2.25	0.51
1:A:360:GLU:OE1	1:A:366:HIS:N	2.43	0.51
1:A:518:GLU:O	1:A:522:LYS:HG2	2.10	0.51
1:A:544:THR:HG22	1:A:548:LYS:HZ2	1.75	0.51
1:A:642:ALA:N	1:A:644:ASN:OD1	2.44	0.51
3:C:1405:TYR:CZ	3:C:1409:THR:HG21	2.45	0.51
3:C:380:LYS:HB2	3:C:390:PHE:HE1	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:443:LEU:N	3:C:444:GLU:HB2	2.24	0.51
1:A:109:HIS:O	1:A:113:SER:OG	2.19	0.51
1:A:583:ASP:HA	1:A:590:ASN:ND2	2.25	0.51
5:E:876:ILE:HG13	5:E:887:ILE:HD13	1.93	0.51
1:A:342:ARG:HB2	1:A:388:CYS:SG	2.50	0.51
1:A:622:LYS:HA	1:A:626:PHE:CD2	2.45	0.51
1:A:729:ALA:HA	1:A:732:ARG:HD2	1.91	0.51
1:A:736:GLN:HG2	1:A:788:GLU:OE2	2.09	0.51
2:B:260:GLU:HG3	2:B:261:PHE:CD1	2.45	0.51
3:C:455:TYR:CE1	3:C:1386:ARG:HB2	2.45	0.51
3:C:299:SER:O	3:C:1501:PHE:N	2.40	0.51
5:E:781:ARG:NH2	5:E:871:GLU:HB2	2.26	0.51
1:A:784:THR:HA	1:A:789:TRP:HZ3	1.76	0.51
3:C:362:LEU:N	3:C:366:GLY:O	2.44	0.51
3:C:1383:ARG:HB3	3:C:1386:ARG:HH21	1.76	0.51
1:A:1041:SER:O	1:A:1045:ILE:HG12	2.11	0.51
3:C:1441:LYS:NZ	3:C:1445:ASN:H	2.09	0.51
5:E:861:CYS:O	5:E:865:LEU:HG	2.10	0.51
1:A:815:ILE:O	1:A:819:THR:HG23	2.11	0.51
2:B:242:GLU:H	2:B:242:GLU:CD	2.15	0.51
1:A:107:VAL:O	1:A:111:LEU:HG	2.11	0.50
1:A:694:LYS:HG2	1:A:698:ARG:HH12	1.76	0.50
1:A:207:ILE:HD13	1:A:246:HIS:HB3	1.93	0.50
1:A:441:ARG:HA	1:A:585:TYR:CE2	2.46	0.50
1:A:656:GLU:H	1:A:656:GLU:CD	2.08	0.50
1:A:589:GLN:HB3	1:A:592:ILE:HD11	1.93	0.50
1:A:74:LEU:O	1:A:78:LEU:HG	2.11	0.50
1:A:1086:PHE:CE2	2:B:267:PHE:HA	2.47	0.50
3:C:273:ARG:NH2	3:C:299:SER:HB2	2.26	0.50
1:A:110:ASP:HB3	1:A:119:ILE:HG12	1.92	0.50
1:A:400:CYS:SG	1:A:442:THR:HB	2.52	0.50
1:A:653:THR:O	1:A:657:LEU:HD23	2.10	0.50
3:C:318:LEU:HD12	3:C:318:LEU:H	1.76	0.50
3:C:1383:ARG:HH11	3:C:1383:ARG:HA	1.75	0.50
1:A:182:LEU:HB2	1:A:232:HIS:NE2	2.26	0.50
1:A:609:GLU:OE1	1:A:611:LYS:NZ	2.35	0.50
1:A:765:ARG:HD3	1:A:804:SER:H	1.77	0.50
1:A:1013:MET:SD	1:A:1020:CYS:HA	2.51	0.50
1:A:1029:THR:HG22	1:A:1033:ARG:NE	2.26	0.50
1:A:181:ALA:O	1:A:184:THR:OG1	2.20	0.50
1:A:426:SER:HB2	1:A:430:ARG:NH2	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ASP:O	1:A:1040:ARG:HG3	2.12	0.50
1:A:213:PRO:O	1:A:217:ILE:HG12	2.12	0.50
3:C:416:ARG:NH2	3:C:1471:TYR:OH	2.37	0.50
1:A:266:GLU:CD	1:A:314:ARG:HB2	2.31	0.49
1:A:326:GLN:O	1:A:330:LEU:HG	2.12	0.49
1:A:446:THR:HB	1:A:450:GLY:HA3	1.94	0.49
3:C:299:SER:HA	3:C:1500:GLN:HA	1.94	0.49
3:C:322:PHE:HB3	3:C:324:PHE:CE1	2.47	0.49
3:C:357:HIS:HA	3:C:373:SER:O	2.12	0.49
1:A:564:LEU:HD22	1:A:596:LYS:HD3	1.95	0.49
1:A:685:TYR:OH	1:A:722:MET:HA	2.12	0.49
1:A:643:ARG:NH2	1:A:696:GLN:OE1	2.45	0.49
3:C:1461:ALA:O	3:C:1465:TYR:N	2.37	0.49
1:A:1029:THR:HG22	1:A:1033:ARG:HE	1.77	0.49
1:A:288:VAL:O	1:A:292:LEU:HG	2.12	0.49
3:C:306:PRO:HG3	5:E:870:ASN:CG	2.32	0.49
3:C:407:GLU:OE1	3:C:408:ARG:HG2	2.12	0.49
1:A:303:LYS:HA	1:A:306:LYS:HD3	1.94	0.49
1:A:70:ILE:HG12	1:A:74:LEU:HD23	1.94	0.49
3:C:1521:TYR:CE2	3:C:1528:LYS:HB2	2.48	0.49
1:A:212:ARG:HG3	1:A:213:PRO:CD	2.42	0.49
1:A:405:LYS:HB3	1:A:410:ARG:HD2	1.94	0.49
1:A:72:ASP:HA	1:A:75:GLN:CD	2.33	0.49
3:C:1517:LEU:HD23	3:C:1534:ASN:HB2	1.94	0.49
3:C:413:ASP:OD1	3:C:413:ASP:N	2.46	0.49
1:A:311:PHE:CE2	1:A:315:LEU:HD11	2.47	0.49
5:E:779:ASP:HA	5:E:782:ARG:HH11	1.78	0.49
1:A:182:LEU:HB2	1:A:232:HIS:CD2	2.48	0.49
1:A:308:VAL:HA	1:A:311:PHE:HB3	1.94	0.49
1:A:375:ASP:HA	1:A:378:GLU:HB2	1.95	0.49
1:A:660:LEU:O	1:A:664:LEU:HG	2.13	0.49
1:A:668:MET:HB2	1:A:707:LEU:HD11	1.95	0.49
1:A:712:PRO:O	1:A:716:VAL:HG13	2.13	0.49
1:A:526:GLN:OE1	1:A:526:GLN:N	2.32	0.49
1:A:746:ARG:HA	1:A:803:LEU:HD13	1.95	0.49
1:A:806:HIS:O	1:A:809:VAL:HG22	2.12	0.49
3:C:272:PRO:HB2	3:C:358:GLU:OE1	2.12	0.48
1:A:74:LEU:HD12	1:A:75:GLN:N	2.28	0.48
1:A:1045:ILE:HD11	1:A:1079:THR:HB	1.95	0.48
1:A:15:TYR:CE1	1:A:19:PRO:HB3	2.49	0.48
1:A:215:TYR:HA	1:A:218:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:CD1	2:B:245:LEU:HD12	2.44	0.48
1:A:461:ARG:HB3	1:A:543:TYR:CZ	2.49	0.48
3:C:443:LEU:HB2	3:C:444:GLU:HB2	1.96	0.48
3:C:1487:ILE:HG13	3:C:1491:TYR:CE2	2.48	0.48
3:C:312:SER:O	3:C:315:ILE:HB	2.14	0.48
3:C:397:ASN:O	3:C:400:THR:OG1	2.20	0.48
1:A:359:SER:OG	1:A:360:GLU:N	2.47	0.48
1:A:815:ILE:HA	1:A:818:LYS:HG3	1.96	0.48
3:C:1472:VAL:HA	3:C:1502:ILE:O	2.14	0.48
3:C:298:PRO:HB3	3:C:359:VAL:HG11	1.95	0.48
1:A:44:ASN:ND2	1:A:85:SER:OG	2.46	0.48
1:A:568:ASN:HB3	1:A:571:GLU:OE2	2.13	0.48
1:A:720:GLU:O	1:A:724:ARG:HG2	2.14	0.48
1:A:110:ASP:N	1:A:110:ASP:OD1	2.47	0.48
1:A:382:LEU:HD13	2:B:246:ALA:O	2.14	0.48
3:C:1477:ASP:N	3:C:1477:ASP:OD1	2.45	0.48
1:A:142:ALA:O	1:A:146:GLU:N	2.42	0.47
3:C:281:LEU:HD11	3:C:287:TYR:CB	2.44	0.47
1:A:257:ASN:HA	1:A:261:PHE:CD2	2.50	0.47
1:A:357:SER:HG	1:A:358:LYS:HZ3	1.55	0.47
1:A:554:HIS:O	1:A:558:PRO:HD3	2.15	0.47
3:C:1522:LYS:H	5:E:870:ASN:HD21	1.63	0.47
1:A:1082:MET:HA	1:A:1120:PHE:CE1	2.49	0.47
1:A:205:THR:O	1:A:209:LEU:HD23	2.14	0.47
1:A:429:ARG:O	1:A:433:ILE:HG13	2.14	0.47
1:A:453:LEU:HD12	1:A:585:TYR:HB3	1.95	0.47
1:A:572:VAL:O	1:A:576:MET:HG3	2.15	0.47
3:C:293:VAL:HG13	3:C:296:PHE:HZ	1.78	0.47
1:A:621:TYR:HA	1:A:624:LEU:HG	1.96	0.47
1:A:698:ARG:NE	1:A:734:ASP:OD2	2.43	0.47
3:C:1383:ARG:HB3	3:C:1386:ARG:NH2	2.30	0.47
3:C:422:GLY:O	3:C:426:SER:N	2.47	0.47
1:A:124:GLN:O	1:A:128:MET:HG2	2.15	0.47
1:A:383:ASP:O	1:A:389:ARG:NE	2.46	0.47
3:C:1434:MET:HB2	3:C:1440:TRP:CE2	2.50	0.47
1:A:200:THR:HG22	1:A:203:ARG:NH1	2.28	0.47
1:A:271:PHE:CE1	1:A:275:LEU:HD11	2.49	0.47
1:A:384:ILE:C	1:A:389:ARG:HH21	2.17	0.47
1:A:41:LEU:HD22	1:A:83:TYR:CG	2.49	0.47
1:A:595:ARG:NH2	1:A:652:ALA:O	2.48	0.47
1:A:41:LEU:HD22	1:A:83:TYR:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1411:GLY:C	3:C:1436:PRO:HA	2.34	0.47
3:C:1450:GLU:HG3	3:C:1453:LEU:HD22	1.96	0.47
3:C:279:LEU:HD12	3:C:353:ALA:O	2.15	0.47
1:A:314:ARG:HA	1:A:317:GLU:HB2	1.96	0.47
3:C:376:VAL:O	3:C:392:ASN:N	2.37	0.47
1:A:306:LYS:HD2	1:A:306:LYS:N	2.30	0.47
1:A:435:LEU:O	1:A:439:LEU:HG	2.14	0.47
1:A:574:GLU:HA	1:A:577:ASP:OD1	2.14	0.47
1:A:358:LYS:HE2	1:A:358:LYS:HB2	1.67	0.47
1:A:587:ILE:CG2	1:A:590:ASN:HB3	2.45	0.47
1:A:739:LYS:HB2	1:A:792:VAL:HG12	1.95	0.47
3:C:416:ARG:CZ	3:C:1462:LEU:HB3	2.45	0.47
3:C:1522:LYS:HA	3:C:1527:THR:HA	1.97	0.47
1:A:1085:THR:HB	1:A:1120:PHE:CD2	2.50	0.47
1:A:646:ILE:HG22	1:A:650:PHE:CZ	2.50	0.47
1:A:952:GLY:O	1:A:955:THR:OG1	2.20	0.47
2:B:289:ILE:HG13	2:B:295:ILE:HG23	1.96	0.47
3:C:282:THR:O	3:C:350:CYS:HA	2.14	0.47
1:A:394:GLN:HE22	1:A:431:ASN:HB3	1.79	0.46
1:A:397:ILE:HG22	1:A:435:LEU:HA	1.97	0.46
1:A:664:LEU:HB3	1:A:707:LEU:HD13	1.97	0.46
5:E:877:GLU:HG3	5:E:878:LYS:H	1.81	0.46
1:A:309:SER:O	1:A:313:ILE:HG13	2.14	0.46
1:A:311:PHE:O	1:A:315:LEU:HG	2.15	0.46
3:C:1468:THR:HG22	3:C:1470:LEU:H	1.79	0.46
1:A:549:PHE:HA	1:A:552:VAL:HG22	1.97	0.46
3:C:1442:ASN:OD1	3:C:1443:ILE:N	2.47	0.46
3:C:440:ASP:HA	3:C:441:GLY:HA3	1.54	0.46
3:C:449:ILE:H	3:C:449:ILE:HD12	1.80	0.46
1:A:182:LEU:HD12	1:A:232:HIS:HD2	1.81	0.46
1:A:293:SER:O	1:A:333:GLN:NE2	2.48	0.46
1:A:1049:ASP:OD1	1:A:1049:ASP:N	2.49	0.46
3:C:1535:LYS:HG3	3:C:1536:ASP:O	2.16	0.46
1:A:14:ASN:O	1:A:17:SER:OG	2.29	0.46
1:A:426:SER:HB2	1:A:430:ARG:HH21	1.80	0.46
5:E:835:LEU:HB2	5:E:887:ILE:O	2.16	0.46
1:A:1025:PRO:O	1:A:1029:THR:OG1	2.28	0.46
1:A:406:PHE:O	1:A:410:ARG:HG3	2.16	0.46
3:C:423:GLU:O	3:C:426:SER:OG	2.26	0.45
1:A:1111:LYS:HA	1:A:1114:ALA:HB3	1.98	0.45
1:A:339:TYR:HB2	1:A:385:ASN:ND2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ASP:HB2	1:A:594:ILE:HD11	1.98	0.45
1:A:681:LEU:O	1:A:684:VAL:HG22	2.16	0.45
1:A:393:ILE:O	1:A:397:ILE:HG23	2.16	0.45
3:C:302:SER:HA	3:C:1503:VAL:O	2.16	0.45
1:A:455:ARG:O	1:A:459:GLN:HB2	2.16	0.45
1:A:647:SER:HA	1:A:650:PHE:CD1	2.51	0.45
3:C:1509:ASN:HA	3:C:1512:GLU:OE2	2.17	0.45
5:E:841:MET:O	5:E:845:GLN:HG3	2.16	0.45
1:A:1036:ASP:OD2	1:A:1038:THR:OG1	2.22	0.45
1:A:39:GLU:OE1	1:A:39:GLU:N	2.50	0.45
1:A:723:LEU:HB3	1:A:775:LYS:HZ2	1.81	0.45
1:A:1119:MET:HE3	2:B:263:VAL:HA	1.99	0.45
1:A:796:ALA:O	1:A:799:ALA:HB3	2.16	0.45
1:A:87:HIS:O	1:A:91:LYS:HG2	2.17	0.45
2:B:287:LEU:HD12	2:B:287:LEU:HA	1.73	0.45
3:C:1536:ASP:OD1	3:C:1537:TYR:N	2.49	0.45
1:A:646:ILE:H	1:A:646:ILE:HD12	1.82	0.45
5:E:837:PHE:N	5:E:884:GLU:OE2	2.49	0.45
1:A:1020:CYS:O	1:A:1024:LEU:HG	2.17	0.45
1:A:255:VAL:O	1:A:258:LEU:HG	2.17	0.45
1:A:272:LEU:HA	1:A:275:LEU:HD12	1.98	0.45
1:A:273:HIS:ND1	1:A:318:LEU:HB3	2.32	0.45
1:A:622:LYS:HA	1:A:626:PHE:HD2	1.82	0.45
1:A:793:ALA:O	1:A:797:ILE:HG13	2.16	0.45
3:C:397:ASN:OD1	3:C:399:THR:HG22	2.17	0.45
1:A:452:GLN:O	1:A:458:TRP:NE1	2.49	0.45
1:A:6:TRP:CD1	1:A:8:ILE:HG12	2.51	0.45
1:A:419:ARG:HE	2:B:249:PHE:HD1	1.62	0.45
2:B:253:GLN:OE1	2:B:255:LYS:N	2.50	0.45
1:A:1031:MET:SD	1:A:1047:LEU:HD11	2.57	0.45
1:A:773:LEU:HA	1:A:776:LEU:HD12	1.98	0.45
1:A:420:SER:HA	2:B:249:PHE:CE1	2.52	0.44
1:A:540:LYS:HE3	1:A:540:LYS:HB3	1.85	0.44
3:C:443:LEU:CB	3:C:444:GLU:HB2	2.47	0.44
1:A:565:GLY:O	2:B:259:LEU:HB3	2.17	0.44
3:C:1480:LEU:O	3:C:1507:ARG:NH1	2.41	0.44
1:A:182:LEU:HD12	1:A:232:HIS:CD2	2.52	0.44
1:A:271:PHE:CZ	1:A:275:LEU:HD21	2.52	0.44
1:A:553:LEU:O	1:A:557:THR:OG1	2.29	0.44
1:A:815:ILE:HG22	1:A:818:LYS:HE2	1.98	0.44
1:A:655:ALA:HB2	2:B:298:ASP:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1445:ASN:OD1	3:C:1445:ASN:N	2.50	0.44
3:C:376:VAL:O	3:C:391:ILE:HD12	2.17	0.44
3:C:412:LEU:O	3:C:414:HIS:N	2.50	0.44
1:A:659:SER:O	1:A:663:LEU:HG	2.17	0.44
1:A:78:LEU:O	1:A:81:THR:OG1	2.36	0.44
1:A:380:ARG:HD3	2:B:245:LEU:HD21	1.99	0.44
1:A:1073:GLN:HA	1:A:1074:PRO:HA	1.82	0.44
1:A:179:GLU:HA	1:A:232:HIS:CD2	2.53	0.44
1:A:323:VAL:HA	1:A:326:GLN:NE2	2.29	0.44
3:C:421:GLN:O	3:C:425:GLU:HG2	2.17	0.44
5:E:842:ASN:HA	5:E:845:GLN:CD	2.38	0.44
1:A:590:ASN:N	1:A:590:ASN:OD1	2.49	0.44
1:A:723:LEU:HB2	1:A:724:ARG:HH12	1.82	0.44
1:A:382:LEU:HD12	2:B:245:LEU:HD12	2.00	0.44
3:C:1451:LYS:O	3:C:1454:SER:OG	2.28	0.44
1:A:377:LEU:HB2	1:A:396:TYR:OH	2.18	0.44
1:A:622:LYS:HD2	1:A:626:PHE:HB2	1.99	0.44
2:B:289:ILE:HG23	2:B:295:ILE:HG13	2.00	0.44
3:C:427:ILE:HB	3:C:1443:ILE:HD12	2.00	0.44
1:A:218:LEU:C	1:A:220:SER:H	2.22	0.43
1:A:222:GLN:HB3	1:A:223:ARG:CZ	2.48	0.43
1:A:6:TRP:CZ2	1:A:8:ILE:HG23	2.53	0.43
3:C:1449:GLY:O	3:C:1452:THR:OG1	2.22	0.43
3:C:424:VAL:HA	3:C:1455:SER:CB	2.48	0.43
1:A:1138:MET:SD	1:A:1141:LEU:HB2	2.58	0.43
1:A:426:SER:HA	1:A:429:ARG:CD	2.48	0.43
1:A:58:VAL:C	1:A:60:GLU:H	2.22	0.43
1:A:753:ARG:HA	1:A:754:GLN:CD	2.37	0.43
1:A:389:ARG:O	1:A:393:ILE:HG13	2.18	0.43
1:A:766:LEU:HD12	1:A:766:LEU:HA	1.83	0.43
1:A:776:LEU:O	1:A:780:THR:HG23	2.18	0.43
3:C:417:PHE:HB3	3:C:1468:THR:HG21	1.99	0.43
5:E:879:THR:HG21	5:E:885:LEU:HA	2.00	0.43
1:A:310:ALA:HA	1:A:313:ILE:HD12	2.00	0.43
1:A:956:GLU:OE1	1:A:956:GLU:N	2.50	0.43
2:B:282:LEU:O	2:B:283:LEU:HG	2.18	0.43
3:C:281:LEU:HB2	3:C:284:PHE:CD1	2.54	0.43
3:C:389:TYR:O	3:C:395:PRO:HA	2.18	0.43
1:A:115:GLU:O	1:A:119:ILE:HG13	2.18	0.43
1:A:473:LYS:HE3	1:A:473:LYS:HB3	1.57	0.43
1:A:737:LEU:O	1:A:741:THR:OG1	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1389:GLY:HA2	3:C:1392:GLU:HG2	2.00	0.43
3:C:1456:LEU:O	3:C:1459:VAL:HG22	2.18	0.43
5:E:832:ASP:HB3	5:E:888:ARG:NH1	2.34	0.43
1:A:47:ILE:HG22	1:A:51:LEU:HD23	2.00	0.43
1:A:794:GLU:HA	1:A:797:ILE:HD12	2.00	0.43
3:C:274:ILE:HA	3:C:358:GLU:HA	1.99	0.43
3:C:424:VAL:CG1	3:C:1452:THR:HA	2.48	0.43
1:A:1101:GLU:HA	1:A:1104:LYS:HE3	2.01	0.43
1:A:425:SER:O	1:A:429:ARG:HG3	2.19	0.43
1:A:540:LYS:O	1:A:544:THR:OG1	2.27	0.43
1:A:437:ALA:HB1	1:A:581:ILE:HD11	2.00	0.43
3:C:1447:SER:N	3:C:1451:LYS:HZ2	2.17	0.43
1:A:200:THR:HG22	1:A:203:ARG:CZ	2.49	0.43
1:A:78:LEU:O	1:A:135:TRP:NE1	2.52	0.43
1:A:815:ILE:HA	1:A:818:LYS:CG	2.48	0.43
1:A:820:ARG:H	1:A:820:ARG:HD2	1.83	0.43
3:C:1493:LYS:HG3	3:C:1494:GLU:HG2	1.99	0.43
1:A:273:HIS:CD2	1:A:321:ARG:HH22	2.37	0.43
1:A:271:PHE:O	1:A:275:LEU:HG	2.19	0.43
1:A:391:ARG:HA	1:A:394:GLN:HG2	2.01	0.43
1:A:51:LEU:HD13	1:A:54:ILE:HG13	2.00	0.43
1:A:569:LYS:HB2	1:A:569:LYS:HE3	1.75	0.43
3:C:391:ILE:HG23	3:C:394:LYS:HB3	2.01	0.43
3:C:420:LEU:O	3:C:424:VAL:HG23	2.19	0.43
1:A:18:ASP:OD1	1:A:20:SER:OG	2.24	0.43
1:A:221:GLU:HG3	1:A:263:HIS:CD2	2.54	0.43
3:C:1480:LEU:H	3:C:1480:LEU:HD23	1.84	0.43
1:A:215:TYR:CE2	1:A:253:SER:HB2	2.54	0.42
1:A:626:PHE:N	1:A:626:PHE:CD1	2.86	0.42
1:A:719:MET:O	1:A:723:LEU:HG	2.19	0.42
1:A:791:GLY:HA3	2:B:291:SER:HB3	2.00	0.42
1:A:725:ILE:HA	1:A:730:HIS:HB2	2.01	0.42
1:A:1075:MET:O	1:A:1079:THR:HG23	2.19	0.42
3:C:281:LEU:HG	3:C:291:GLN:HB2	1.99	0.42
3:C:359:VAL:HG23	3:C:368:GLU:O	2.19	0.42
1:A:52:ASN:N	1:A:53:PRO:HD2	2.34	0.42
1:A:800:ILE:O	1:A:807:PRO:HB3	2.19	0.42
1:A:84:LEU:HD11	1:A:88:ALA:HB3	2.02	0.42
1:A:1110:ASP:OD2	1:A:1113:ILE:HG23	2.20	0.42
3:C:275:VAL:HG11	3:C:298:PRO:HA	2.02	0.42
1:A:1023:ASN:O	1:A:1027:LEU:HD23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:MET:HA	1:A:1053:CYS:SG	2.59	0.42
1:A:557:THR:HA	1:A:560:ILE:HD12	2.01	0.42
1:A:767:PRO:HA	1:A:805:LYS:HB2	2.02	0.42
1:A:1000:ASN:O	1:A:1003:GLN:HB2	2.19	0.42
1:A:1071:ASP:N	1:A:1072:PRO:HD3	2.34	0.42
1:A:724:ARG:O	1:A:728:GLY:HA3	2.20	0.42
3:C:1523:VAL:HG22	5:E:870:ASN:HA	2.01	0.42
3:C:278:HIS:HA	3:C:296:PHE:CE1	2.55	0.42
3:C:405:LEU:CD2	3:C:413:ASP:HB3	2.50	0.42
1:A:313:ILE:O	1:A:317:GLU:HG3	2.20	0.42
1:A:426:SER:OG	1:A:429:ARG:NH1	2.52	0.42
1:A:583:ASP:HA	1:A:590:ASN:HD22	1.83	0.42
3:C:277:THR:N	3:C:355:HIS:O	2.51	0.42
1:A:134:GLN:HE22	1:A:212:ARG:HG3	1.84	0.42
1:A:257:ASN:HA	1:A:261:PHE:HD2	1.84	0.42
1:A:657:LEU:HD12	1:A:658:THR:N	2.35	0.42
3:C:378:SER:OG	3:C:390:PHE:HB2	2.20	0.42
1:A:1044:VAL:HG22	1:A:1047:LEU:HD12	2.02	0.42
1:A:222:GLN:O	1:A:225:LYS:HB2	2.19	0.42
1:A:123:LYS:HE3	1:A:197:PHE:CD1	2.55	0.41
1:A:581:ILE:O	1:A:585:TYR:HD2	2.03	0.41
1:A:77:LEU:H	1:A:77:LEU:HD12	1.85	0.41
5:E:781:ARG:HH21	5:E:868:LEU:HA	1.85	0.41
1:A:212:ARG:N	1:A:213:PRO:HD2	2.35	0.41
1:A:215:TYR:O	1:A:219:GLU:HG3	2.19	0.41
1:A:93:PHE:O	1:A:96:ILE:HG12	2.20	0.41
3:C:1435:PRO:HB2	3:C:1438:LYS:HE2	2.02	0.41
3:C:441:GLY:HA2	3:C:444:GLU:OE1	2.20	0.41
1:A:274:ILE:HG22	1:A:279:TYR:HE2	1.85	0.41
1:A:322:LEU:HD12	1:A:323:VAL:HG13	2.03	0.41
1:A:526:GLN:O	1:A:529:THR:OG1	2.25	0.41
1:A:579:PHE:CE1	1:A:593:GLY:HA3	2.55	0.41
1:A:680:LYS:HA	1:A:683:GLN:CD	2.40	0.41
1:A:1086:PHE:CZ	2:B:270:ALA:HB3	2.55	0.41
1:A:1085:THR:HA	1:A:1088:ILE:HD11	2.02	0.41
2:B:246:ALA:HB1	2:B:247:PRO:HD2	2.02	0.41
3:C:1431:PHE:CE2	3:C:1433:VAL:HB	2.55	0.41
3:C:361:ASP:OD1	3:C:361:ASP:N	2.51	0.41
1:A:75:GLN:HA	1:A:78:LEU:HD12	2.03	0.41
1:A:1084:LEU:HD12	1:A:1085:THR:N	2.35	0.41
1:A:224:VAL:O	1:A:230:ARG:NH2	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:HIS:ND1	1:A:772:VAL:HG23	2.36	0.41
3:C:424:VAL:HG13	3:C:1455:SER:HB2	2.03	0.41
5:E:778:VAL:HA	5:E:781:ARG:HB3	2.01	0.41
1:A:680:LYS:HA	1:A:683:GLN:OE1	2.21	0.41
1:A:54:ILE:CG2	1:A:70:ILE:HD12	2.51	0.41
1:A:796:ALA:O	1:A:800:ILE:HG23	2.21	0.41
1:A:44:ASN:HD21	1:A:85:SER:H	1.69	0.41
1:A:231:MET:O	1:A:234:PHE:HB2	2.20	0.41
1:A:214:VAL:HG21	1:A:237:LEU:HD11	2.02	0.41
1:A:370:MET:H	1:A:370:MET:HG2	1.71	0.41
1:A:444:PRO:O	1:A:446:THR:N	2.50	0.41
3:C:1533:ASP:OD1	5:E:882:LEU:HB3	2.21	0.41
3:C:277:THR:OG1	3:C:355:HIS:HB2	2.20	0.41
1:A:46:LEU:O	1:A:50:VAL:HG23	2.20	0.41
1:A:55:VAL:HA	1:A:58:VAL:HG12	2.01	0.41
1:A:723:LEU:HB3	1:A:775:LYS:NZ	2.36	0.41
3:C:359:VAL:HG23	3:C:368:GLU:H	1.86	0.41
1:A:122:HIS:HA	1:A:125:LEU:HD12	2.02	0.41
1:A:144:ALA:HA	1:A:147:LYS:HE3	2.02	0.41
1:A:264:LEU:C	1:A:267:PRO:HD2	2.41	0.41
1:A:349:PHE:HA	1:A:352:MET:HE2	2.03	0.41
1:A:425:SER:HB3	1:A:428:VAL:HG23	2.02	0.41
1:A:400:CYS:SG	1:A:439:LEU:HD23	2.61	0.41
1:A:773:LEU:HB3	1:A:810:LEU:HD11	2.02	0.41
1:A:43:ASP:OD2	1:A:46:LEU:N	2.32	0.40
1:A:745:LEU:HA	1:A:745:LEU:HD13	1.91	0.40
1:A:962:ALA:O	1:A:966:ILE:HG13	2.21	0.40
3:C:1477:ASP:O	3:C:1480:LEU:HD22	2.21	0.40
1:A:268:MET:O	1:A:272:LEU:HG	2.21	0.40
1:A:339:TYR:CG	1:A:340:THR:N	2.89	0.40
1:A:664:LEU:HD12	1:A:706:MET:HB2	2.04	0.40
1:A:768:ASN:CA	1:A:773:LEU:HD22	2.47	0.40
1:A:768:ASN:H	1:A:773:LEU:HD22	1.86	0.40
3:C:281:LEU:HD11	3:C:287:TYR:HB2	2.03	0.40
3:C:442:LEU:HA	3:C:445:TYR:HB2	2.01	0.40
1:A:1080:CYS:O	1:A:1083:THR:OG1	2.39	0.40
1:A:587:ILE:HG23	1:A:590:ASN:CB	2.51	0.40
3:C:1515:SER:O	3:C:1516:ARG:HD3	2.22	0.40
1:A:334:LEU:O	1:A:380:ARG:NH1	2.54	0.40
1:A:763:PHE:O	1:A:765:ARG:NH1	2.54	0.40
1:A:951:ILE:HD12	1:A:951:ILE:H	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1505:SER:HB2	3:C:1510:MET:HG3	2.02	0.40
3:C:281:LEU:HD11	3:C:287:TYR:HB3	2.03	0.40
1:A:231:MET:HA	1:A:234:PHE:CD1	2.56	0.40
1:A:701:ILE:O	1:A:704:LEU:HG	2.21	0.40
3:C:1480:LEU:HD23	3:C:1507:ARG:NH1	2.36	0.40
3:C:274:ILE:HB	3:C:358:GLU:HG2	2.02	0.40
3:C:351:GLU:OE1	3:C:378:SER:HB2	2.22	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:290:ARG:NH1	1:A:446:THR:O[2_745]	2.15	0.05

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	911/1155 (79%)	819 (90%)	91 (10%)	1 (0%)	51 85
2	B	46/197 (23%)	36 (78%)	10 (22%)	0	100 100
3	C	294/403 (73%)	266 (90%)	28 (10%)	0	100 100
5	E	67/135 (50%)	58 (87%)	9 (13%)	0	100 100
All	All	1318/1890 (70%)	1179 (90%)	138 (10%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1074	PRO

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	728/953 (76%)	710 (98%)	18 (2%)	47 68
2	B	43/166 (26%)	43 (100%)	0	100 100
3	C	274/345 (79%)	273 (100%)	1 (0%)	91 94
5	E	69/122 (57%)	67 (97%)	2 (3%)	42 64
All	All	1114/1586 (70%)	1093 (98%)	21 (2%)	57 75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	110	ASP
1	A	131	PHE
1	A	212	ARG
1	A	215	TYR
1	A	223	ARG
1	A	248	TYR
1	A	278	GLN
1	A	358	LYS
1	A	473	LYS
1	A	561	CYS
1	A	578	TYR
1	A	625	PHE
1	A	690	ARG
1	A	697	ARG
1	A	818	LYS
1	A	1080	CYS
1	A	1112	ARG
3	C	420	LEU
5	E	837	PHE
5	E	861	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	52	ASN
1	A	75	GLN
1	A	122	HIS
1	A	333	GLN
1	A	366	HIS
1	A	394	GLN
1	A	411	GLN
1	A	427	HIS
1	A	431	ASN
1	A	795	GLN
1	A	798	ASN
1	A	1061	ASN
1	A	1073	GLN
3	C	283	ASN
3	C	355	HIS
3	C	1463	HIS
3	C	1490	ASN
3	C	1509	ASN
5	E	845	GLN
5	E	867	HIS
5	E	870	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
4	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1180:UNK	C	1188:UNK	N	12.75
1	D	15:UNK	C	17:UNK	N	11.71
1	A	1165:GLU	C	1169:UNK	N	5.63
1	D	8:UNK	C	10:UNK	N	3.08

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, 95^{th} 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	935/1155 (80%)	-0.36	1 (0%) 95 95	128, 199, 242, 282	0
2	B	50/197 (25%)	-0.16	2 (4%) 38 34	147, 213, 247, 260	0
3	C	306/403 (75%)	-0.14	1 (0%) 94 90	186, 230, 288, 330	0
4	D	0/23	-	-	-	-
5	E	71/135 (52%)	-0.24	0 100 100	188, 234, 264, 272	0
All	All	1362/1913 (71%)	-0.30	4 (0%) 94 90	128, 210, 258, 330	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	298	ASP	3.1
1	A	1061	ASN	2.6
2	B	273	ASP	2.1
3	C	381	ALA	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.