



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:53 PM GMT

PDB ID : 4N0A
Title : Crystal structure of Lsm2-3-Pat1C complex from *Saccharomyces cerevisiae*
Authors : Wu, D.H.
Deposited on : 2013-10-01
Resolution : 3.15 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

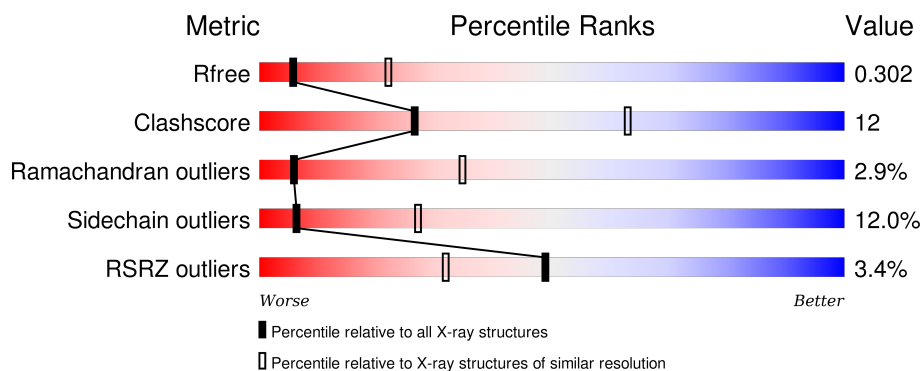
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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. 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	89	<div> <div>2%</div> <div>61% 25% 10%</div> </div>
1	B	89	<div> <div>2%</div> <div>43% 40% 7% 10%</div> </div>
1	E	89	<div> <div>6%</div> <div>69% 8% 24%</div> </div>
1	F	89	<div> <div>3%</div> <div>61% 20% 16%</div> </div>
2	C	109	<div> <div>5%</div> <div>53% 20% 6% 21%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	109	<div><div></div><div>45%25%7%23%</div></div>
2	G	109	<div><div>6%</div><div></div><div>52%22%5%21%</div></div>
3	H	380	<div><div>3%</div><div></div><div>58%19%5%16%</div></div>
3	I	380	<div><div>%</div><div></div><div>58%23%17%</div></div>
3	J	380	<div><div>3%</div><div></div><div>62%18%16%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12345 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 U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			633	395	108	126	4			
1	B	80	Total	C	N	O	S	0	0	0
			634	395	108	127	4			
1	E	68	Total	C	N	O	S	0	0	0
			534	334	93	103	4			
1	F	75	Total	C	N	O	S	0	0	0
			594	372	102	116	4			

- Molecule 2 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	86	Total	C	N	O	S	0	0	0
			704	446	117	137	4			
2	D	84	Total	C	N	O	S	0	0	0
			689	438	113	134	4			
2	G	86	Total	C	N	O	S	0	0	0
			704	446	117	137	4			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	MET	-	EXPRESSION TAG	UNP P38203
C	-12	GLY	-	EXPRESSION TAG	UNP P38203
C	-11	SER	-	EXPRESSION TAG	UNP P38203
C	-10	SER	-	EXPRESSION TAG	UNP P38203
C	-9	HIS	-	EXPRESSION TAG	UNP P38203
C	-8	HIS	-	EXPRESSION TAG	UNP P38203
C	-7	HIS	-	EXPRESSION TAG	UNP P38203
C	-6	HIS	-	EXPRESSION TAG	UNP P38203
C	-5	HIS	-	EXPRESSION TAG	UNP P38203
C	-4	HIS	-	EXPRESSION TAG	UNP P38203

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	SER	-	EXPRESSION TAG	UNP P38203
C	-2	GLN	-	EXPRESSION TAG	UNP P38203
C	-1	ASP	-	EXPRESSION TAG	UNP P38203
C	0	PRO	-	EXPRESSION TAG	UNP P38203
D	-13	MET	-	EXPRESSION TAG	UNP P38203
D	-12	GLY	-	EXPRESSION TAG	UNP P38203
D	-11	SER	-	EXPRESSION TAG	UNP P38203
D	-10	SER	-	EXPRESSION TAG	UNP P38203
D	-9	HIS	-	EXPRESSION TAG	UNP P38203
D	-8	HIS	-	EXPRESSION TAG	UNP P38203
D	-7	HIS	-	EXPRESSION TAG	UNP P38203
D	-6	HIS	-	EXPRESSION TAG	UNP P38203
D	-5	HIS	-	EXPRESSION TAG	UNP P38203
D	-4	HIS	-	EXPRESSION TAG	UNP P38203
D	-3	SER	-	EXPRESSION TAG	UNP P38203
D	-2	GLN	-	EXPRESSION TAG	UNP P38203
D	-1	ASP	-	EXPRESSION TAG	UNP P38203
D	0	PRO	-	EXPRESSION TAG	UNP P38203
G	-13	MET	-	EXPRESSION TAG	UNP P38203
G	-12	GLY	-	EXPRESSION TAG	UNP P38203
G	-11	SER	-	EXPRESSION TAG	UNP P38203
G	-10	SER	-	EXPRESSION TAG	UNP P38203
G	-9	HIS	-	EXPRESSION TAG	UNP P38203
G	-8	HIS	-	EXPRESSION TAG	UNP P38203
G	-7	HIS	-	EXPRESSION TAG	UNP P38203
G	-6	HIS	-	EXPRESSION TAG	UNP P38203
G	-5	HIS	-	EXPRESSION TAG	UNP P38203
G	-4	HIS	-	EXPRESSION TAG	UNP P38203
G	-3	SER	-	EXPRESSION TAG	UNP P38203
G	-2	GLN	-	EXPRESSION TAG	UNP P38203
G	-1	ASP	-	EXPRESSION TAG	UNP P38203
G	0	PRO	-	EXPRESSION TAG	UNP P38203

- Molecule 3 is a protein called DNA topoisomerase 2-associated protein PAT1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	318	Total	C	N	O	S	0	0	0
			2595	1676	423	488	8			
3	I	317	Total	C	N	O	S	0	0	0
			2586	1671	422	485	8			
3	J	318	Total	C	N	O	S	0	0	0
			2595	1676	423	488	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	417	GLY	-	EXPRESSION TAG	UNP P25644
H	418	PRO	-	EXPRESSION TAG	UNP P25644
H	419	LEU	-	EXPRESSION TAG	UNP P25644
H	420	GLY	-	EXPRESSION TAG	UNP P25644
H	421	SER	-	EXPRESSION TAG	UNP P25644
H	688	VAL	ASP	ENGINEERED MUTATION	UNP P25644
I	417	GLY	-	EXPRESSION TAG	UNP P25644
I	418	PRO	-	EXPRESSION TAG	UNP P25644
I	419	LEU	-	EXPRESSION TAG	UNP P25644
I	420	GLY	-	EXPRESSION TAG	UNP P25644
I	421	SER	-	EXPRESSION TAG	UNP P25644
I	688	VAL	ASP	ENGINEERED MUTATION	UNP P25644
J	417	GLY	-	EXPRESSION TAG	UNP P25644
J	418	PRO	-	EXPRESSION TAG	UNP P25644
J	419	LEU	-	EXPRESSION TAG	UNP P25644
J	420	GLY	-	EXPRESSION TAG	UNP P25644
J	421	SER	-	EXPRESSION TAG	UNP P25644
J	688	VAL	ASP	ENGINEERED MUTATION	UNP P25644

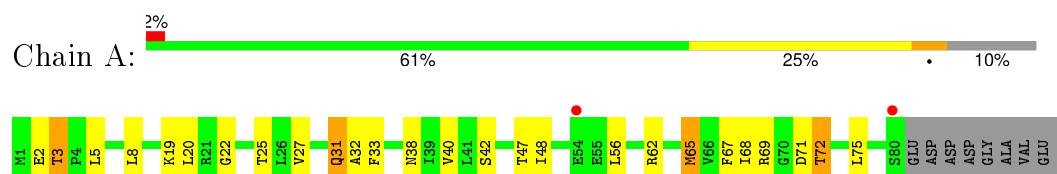
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	3	Total O 3 3	0	0
4	C	11	Total O 11 11	0	0
4	D	13	Total O 13 13	0	0
4	E	2	Total O 2 2	0	0
4	F	3	Total O 3 3	0	0
4	G	3	Total O 3 3	0	0
4	H	13	Total O 13 13	0	0
4	I	13	Total O 13 13	0	0
4	J	9	Total O 9 9	0	0

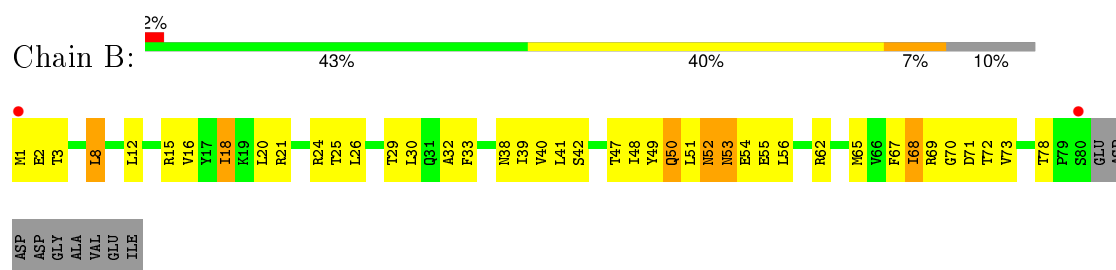
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

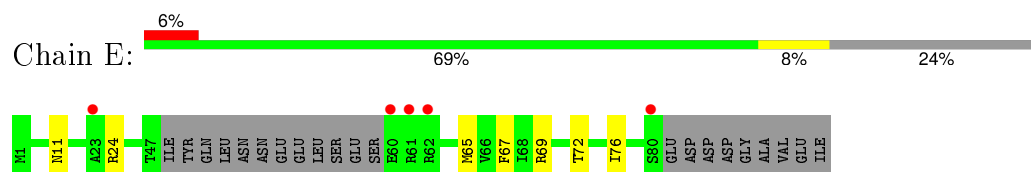
- Molecule 1: U6 snRNA-associated Sm-like protein LSm3



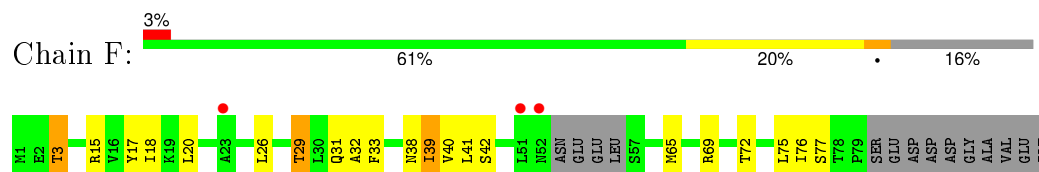
- Molecule 1: U6 snRNA-associated Sm-like protein LSm3



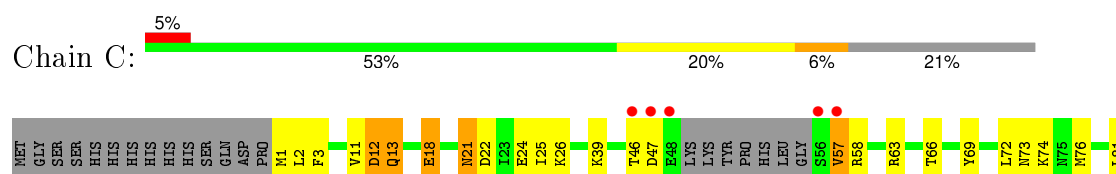
- Molecule 1: U6 snRNA-associated Sm-like protein LSm3



- Molecule 1: U6 snRNA-associated Sm-like protein LSm3



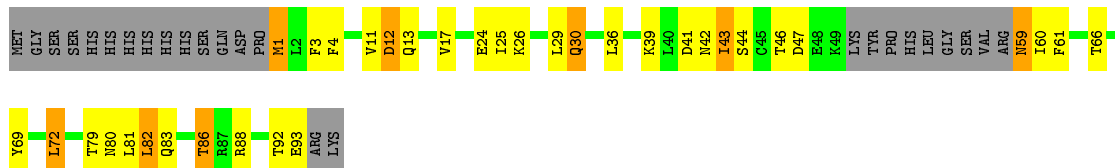
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2





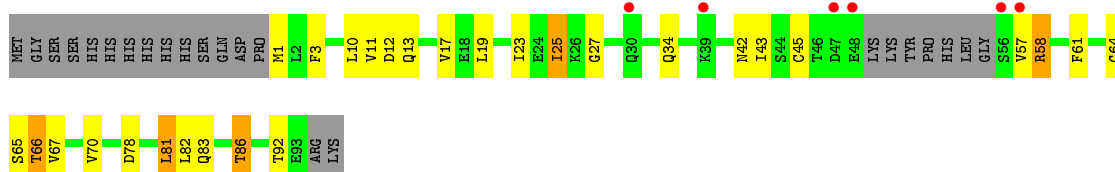
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2

Chain D:



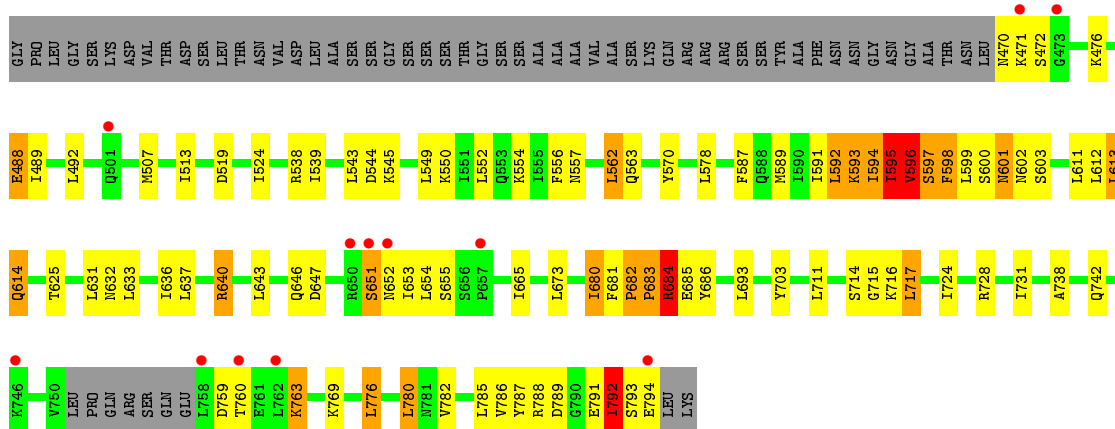
- Molecule 2: U6 snRNA-associated Sm-like protein LSm2

Chain G:



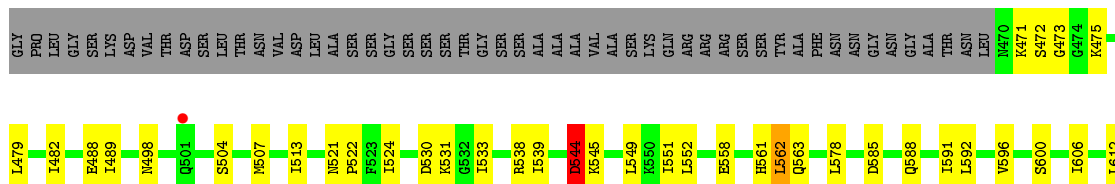
- Molecule 3: DNA topoisomerase 2-associated protein PAT1

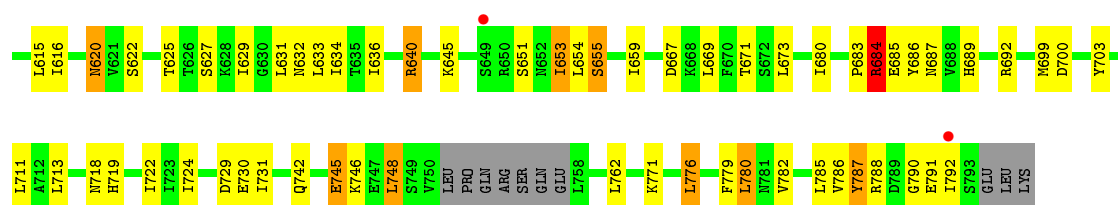
Chain H:



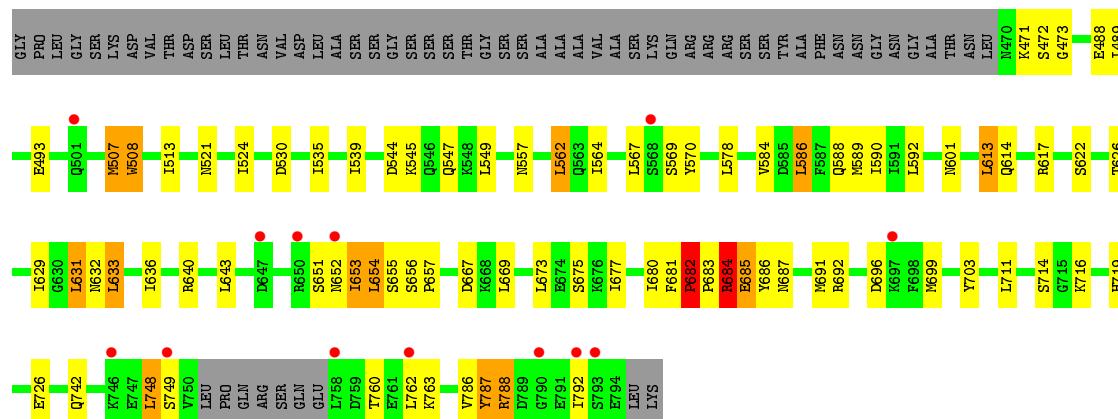
- Molecule 3: DNA topoisomerase 2-associated protein PAT1

Chain I:





• Molecule 3: DNA topoisomerase 2-associated protein PAT1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.45Å 251.51Å 120.31Å 90.00° 112.09° 90.00°	Depositor
Resolution (Å)	19.88 – 3.15 19.88 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.88-3.15) 99.0 (19.88-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.15Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.272 , 0.300 0.266 , 0.302	Depositor DCC
R_{free} test set	3283 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	115.8	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 35.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 64738 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12345	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/639	0.60	0/865
1	B	0.53	0/640	0.66	0/866
1	E	0.34	0/538	0.51	0/726
1	F	0.33	0/599	0.57	0/809
2	C	0.47	0/710	0.61	0/955
2	D	0.40	0/695	0.63	0/934
2	G	0.36	0/710	0.60	0/955
3	H	0.38	0/2635	0.56	0/3552
3	I	0.35	0/2626	0.56	0/3540
3	J	0.33	0/2635	0.53	0/3552
All	All	0.38	0/12427	0.57	0/16754

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
3	H	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	682	PRO	Peptide
3	J	682	PRO	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	633	0	643	17	1
1	B	634	0	643	32	1
1	E	534	0	552	3	0
1	F	594	0	608	15	0
2	C	704	0	713	27	0
2	D	689	0	699	27	0
2	G	704	0	713	19	0
3	H	2595	0	2683	74	0
3	I	2586	0	2677	57	0
3	J	2595	0	2683	52	0
4	A	7	0	0	1	0
4	B	3	0	0	1	0
4	C	11	0	0	3	0
4	D	13	0	0	2	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	1	0
4	H	13	0	0	6	0
4	I	13	0	0	2	0
4	J	9	0	0	6	0
All	All	12345	0	12614	303	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 12.

All (303) 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:H:594:ILE:HG22	3:H:595:ILE:N	1.55	1.15
3:H:595:ILE:HG12	3:H:596:VAL:N	1.40	1.15
2:C:57:VAL:HB	2:C:58:ARG:HA	1.29	1.14
2:D:43:ILE:HB	2:D:44:SER:HA	1.23	1.09
1:B:78:THR:HB	4:B:103:HOH:O	1.51	1.06
3:J:471:LYS:HB2	3:J:472:SER:HB3	1.13	1.06
3:H:471:LYS:HB2	3:H:472:SER:HB3	1.34	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:640:ARG:HG2	3:I:640:ARG:HH11	1.21	1.02
1:B:54:GLU:HG3	1:B:54:GLU:O	1.61	1.01
3:J:471:LYS:CB	3:J:472:SER:HB3	1.91	1.00
2:D:43:ILE:HB	2:D:44:SER:CA	1.93	0.98
3:H:653:ILE:HA	3:H:654:LEU:HB2	1.50	0.94
1:B:1:MET:HB2	1:B:2:GLU:HA	1.51	0.93
3:H:594:ILE:HG22	3:H:595:ILE:H	1.24	0.92
2:C:57:VAL:CB	2:C:58:ARG:HA	1.98	0.92
1:B:51:LEU:O	1:B:52:ASN:HB2	1.67	0.91
3:H:595:ILE:HG12	3:H:596:VAL:H	1.09	0.90
3:I:653:ILE:HA	3:I:654:LEU:HB3	1.54	0.89
2:D:43:ILE:CB	2:D:44:SER:HA	2.00	0.89
3:H:595:ILE:CG1	3:H:596:VAL:N	2.30	0.88
3:H:592:LEU:N	3:H:592:LEU:HD23	1.87	0.87
3:H:471:LYS:CB	3:H:472:SER:HB3	2.05	0.86
3:J:547:GLN:HB2	4:J:803:HOH:O	1.75	0.85
3:J:787:TYR:CG	3:J:788:ARG:HA	2.12	0.84
3:J:691:MET:SD	4:J:804:HOH:O	2.37	0.83
1:F:18:ILE:HD11	1:F:41:LEU:HD11	1.59	0.82
1:A:32:ALA:HA	2:D:86:THR:HG21	1.61	0.81
3:H:597:SER:HB2	4:H:802:HOH:O	1.83	0.79
3:I:471:LYS:CB	3:I:472:SER:HB2	2.12	0.78
1:A:31:GLN:HE21	1:A:31:GLN:HA	1.48	0.77
2:C:57:VAL:HB	2:C:58:ARG:CA	2.13	0.77
1:B:18:ILE:HD11	1:B:20:LEU:HD23	1.65	0.77
3:H:632:ASN:HD21	3:H:703:TYR:HB2	1.51	0.76
1:E:67:PHE:HB3	1:F:76:ILE:HB	1.68	0.76
1:A:25:THR:HG23	1:A:47:THR:HG23	1.69	0.74
3:I:632:ASN:HD21	3:I:703:TYR:HB2	1.53	0.73
1:A:31:GLN:NE2	1:A:31:GLN:HA	2.04	0.73
3:I:471:LYS:HB2	3:I:472:SER:HB2	1.71	0.73
3:H:631:LEU:HD21	3:H:680:ILE:HD11	1.69	0.72
3:H:647:ASP:HA	4:H:801:HOH:O	1.89	0.72
3:J:786:VAL:HG12	3:J:787:TYR:H	1.54	0.72
1:B:53:ASN:O	1:B:54:GLU:HB3	1.89	0.72
3:I:640:ARG:CG	3:I:640:ARG:HH11	2.00	0.72
1:A:31:GLN:HE22	2:D:83:GLN:HE21	1.36	0.71
3:J:632:ASN:HD21	3:J:703:TYR:HB2	1.54	0.71
3:H:643:LEU:HD13	4:H:813:HOH:O	1.90	0.70
3:H:597:SER:O	3:H:598:PHE:C	2.29	0.70
2:D:17:VAL:O	2:D:24:GLU:O	2.09	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:625:THR:HB	3:H:680:ILE:HD12	1.74	0.70
2:G:57:VAL:HB	2:G:58:ARG:HA	1.74	0.70
3:H:598:PHE:HD1	3:H:599:LEU:HD23	1.56	0.69
3:H:594:ILE:O	3:H:595:ILE:C	2.30	0.69
3:I:504:SER:HA	4:I:813:HOH:O	1.93	0.69
2:D:11:VAL:O	2:D:12:ASP:HB2	1.91	0.69
3:I:787:TYR:HB3	3:I:788:ARG:HA	1.75	0.68
3:H:594:ILE:CG2	3:H:595:ILE:H	1.88	0.67
3:H:597:SER:O	3:H:600:SER:N	2.27	0.67
1:B:49:TYR:C	1:B:50:GLN:HG2	2.13	0.67
3:I:653:ILE:HA	3:I:654:LEU:CB	2.23	0.67
3:I:651:SER:HB3	3:I:654:LEU:HB2	1.76	0.67
3:I:472:SER:N	3:I:473:GLY:HA2	2.10	0.66
3:H:595:ILE:O	3:H:596:VAL:C	2.30	0.66
3:J:613:LEU:HD22	3:J:617:ARG:HD2	1.77	0.66
3:H:594:ILE:O	3:H:596:VAL:N	2.30	0.65
1:A:31:GLN:CA	1:A:31:GLN:HE21	2.08	0.64
3:H:594:ILE:CG2	3:H:595:ILE:N	2.29	0.64
3:H:592:LEU:O	3:H:594:ILE:N	2.30	0.64
3:H:595:ILE:O	3:H:597:SER:N	2.30	0.64
1:B:40:VAL:HG23	2:G:3:PHE:HE2	1.62	0.64
3:H:632:ASN:O	3:H:636:ILE:HG12	1.97	0.64
3:I:482:ILE:HG21	3:I:531:LYS:HG3	1.80	0.64
2:G:17:VAL:HG12	2:G:70:VAL:HG22	1.80	0.63
3:I:513:ILE:HD13	3:I:551:ILE:HD13	1.81	0.63
1:B:51:LEU:O	1:B:52:ASN:CB	2.43	0.63
1:B:51:LEU:HA	1:B:55:GLU:O	1.99	0.63
2:D:41:ASP:O	2:D:42:ASN:HB2	1.99	0.63
3:H:742:GLN:HE22	3:H:788:ARG:HD2	1.64	0.62
3:H:552:LEU:O	3:H:556:PHE:HD2	1.82	0.62
1:E:76:ILE:HB	2:G:61:PHE:HB2	1.81	0.62
3:J:471:LYS:HB2	3:J:472:SER:CB	2.09	0.62
3:H:592:LEU:HD23	3:H:592:LEU:H	1.65	0.62
3:H:786:VAL:O	3:H:791:GLU:HA	1.99	0.62
3:H:613:LEU:HG	3:H:665:ILE:HD11	1.82	0.61
1:B:1:MET:HB2	1:B:2:GLU:CA	2.27	0.61
3:J:653:ILE:HA	3:J:654:LEU:CB	2.29	0.61
1:B:33:PHE:HB3	1:B:39:ILE:HG22	1.82	0.61
3:I:588:GLN:HG3	3:I:592:LEU:HD12	1.82	0.61
3:I:632:ASN:O	3:I:636:ILE:HG12	2.00	0.61
1:E:69:ARG:O	1:E:72:THR:HG22	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:731:ILE:HG13	3:I:776:LEU:HD21	1.83	0.60
3:H:787:TYR:CG	3:H:788:ARG:HA	2.36	0.60
3:H:470:ASN:HB3	4:H:806:HOH:O	2.01	0.60
2:C:73:ASN:HB2	2:C:76:MET:CE	2.31	0.60
2:C:2:LEU:HB3	4:C:103:HOH:O	2.00	0.60
3:J:524:ILE:HG23	3:J:562:LEU:HD22	1.84	0.60
1:B:12:LEU:HD22	2:G:83:GLN:HB2	1.83	0.59
2:G:27:GLY:HA3	2:G:43:ILE:HG22	1.83	0.59
3:J:787:TYR:CB	3:J:788:ARG:HA	2.32	0.59
3:I:612:LEU:O	3:I:616:ILE:HG12	2.03	0.58
3:H:592:LEU:O	3:H:593:LYS:C	2.37	0.58
3:H:596:VAL:HG12	3:H:597:SER:N	2.18	0.58
3:H:625:THR:HB	3:H:680:ILE:CD1	2.32	0.58
3:H:601:ASN:HA	4:H:811:HOH:O	2.03	0.58
2:C:57:VAL:CB	2:C:58:ARG:CA	2.79	0.57
2:C:11:VAL:O	2:C:12:ASP:HB2	2.05	0.57
3:H:557:ASN:HB3	3:H:614:GLN:HG2	1.87	0.57
2:C:3:PHE:HE2	1:F:40:VAL:HG23	1.70	0.57
3:J:651:SER:HA	3:J:652:ASN:HB2	1.86	0.57
2:C:57:VAL:CG1	2:C:58:ARG:HA	2.35	0.56
3:J:544:ASP:C	4:J:803:HOH:O	2.43	0.56
3:H:625:THR:HG21	3:H:673:LEU:HD21	1.87	0.56
3:H:594:ILE:O	3:H:597:SER:N	2.30	0.56
1:A:33:PHE:HA	1:A:38:ASN:O	2.05	0.56
3:H:613:LEU:HG	3:H:665:ILE:CD1	2.36	0.56
1:B:33:PHE:HA	1:B:38:ASN:O	2.05	0.56
3:H:742:GLN:HG3	3:H:769:LYS:HD2	1.88	0.56
2:C:2:LEU:N	4:C:103:HOH:O	2.39	0.56
2:D:43:ILE:HD13	2:D:44:SER:HB3	1.88	0.55
2:C:73:ASN:HB2	2:C:76:MET:SD	2.47	0.55
3:I:718:ASN:O	3:I:722:ILE:HG12	2.07	0.55
3:H:489:ILE:HD11	3:H:539:ILE:HG12	1.88	0.55
3:I:620:ASN:HD22	3:I:620:ASN:C	2.11	0.55
1:B:8:LEU:HD22	1:B:30:LEU:HD21	1.89	0.55
1:A:42:SER:HB3	1:A:65:MET:CE	2.37	0.55
2:C:83:GLN:HA	2:C:86:THR:CG2	2.38	0.54
2:G:19:LEU:HD21	2:G:25:ILE:HD12	1.90	0.54
1:A:20:LEU:HD22	1:A:72:THR:HG23	1.90	0.54
1:B:40:VAL:CG2	2:G:3:PHE:HE2	2.20	0.54
1:B:49:TYR:C	1:B:50:GLN:CG	2.76	0.53
1:B:32:ALA:HA	2:G:86:THR:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:779:PHE:O	3:I:782:VAL:HG22	2.07	0.53
1:F:69:ARG:O	1:F:72:THR:HG22	2.08	0.53
2:C:86:THR:HG21	1:F:32:ALA:HA	1.91	0.53
2:G:19:LEU:HD23	2:G:23:ILE:HB	1.91	0.53
2:C:18:GLU:HB2	2:C:69:TYR:HB2	1.91	0.53
3:I:748:LEU:HB3	3:I:762:LEU:HD21	1.91	0.53
3:H:681:PHE:C	3:H:683:PRO:HD3	2.30	0.52
3:J:544:ASP:CA	4:J:803:HOH:O	2.56	0.52
1:F:33:PHE:HA	1:F:38:ASN:O	2.09	0.52
2:C:21:ASN:O	2:C:22:ASP:HB2	2.09	0.52
3:H:780:LEU:HB3	3:H:785:LEU:O	2.09	0.52
3:J:762:LEU:HD12	3:J:763:LYS:HG3	1.91	0.52
3:H:524:ILE:HG23	3:H:562:LEU:HD22	1.91	0.52
3:H:682:PRO:N	3:H:683:PRO:HD3	2.25	0.52
3:I:787:TYR:CB	3:I:788:ARG:HA	2.40	0.52
3:H:598:PHE:CD1	3:H:599:LEU:HD23	2.41	0.51
3:I:640:ARG:NH1	3:I:640:ARG:HG2	2.02	0.51
3:I:654:LEU:HG	3:I:655:SER:H	1.74	0.51
3:I:684:ARG:O	3:I:684:ARG:HG2	2.11	0.51
3:H:599:LEU:HD22	3:H:603:SER:HB3	1.92	0.51
2:G:42:ASN:ND2	4:G:103:HOH:O	2.42	0.51
3:J:544:ASP:N	4:J:803:HOH:O	2.43	0.51
2:G:57:VAL:HB	2:G:58:ARG:CA	2.40	0.51
3:I:788:ARG:HB3	3:I:792:ILE:HD12	1.91	0.51
2:C:83:GLN:HE21	1:F:31:GLN:HE22	1.58	0.51
3:I:653:ILE:CA	3:I:654:LEU:CB	2.89	0.51
3:I:700:ASP:O	4:I:803:HOH:O	2.19	0.51
3:J:569:SER:HA	3:J:626:THR:O	2.11	0.50
3:J:488:GLU:HG2	3:J:507:MET:HB3	1.94	0.50
1:F:18:ILE:HG22	1:F:76:ILE:HG12	1.93	0.50
3:J:716:LYS:H	3:J:719:HIS:CD2	2.29	0.50
3:H:556:PHE:CE1	3:H:637:LEU:HD11	2.47	0.49
2:D:43:ILE:HG22	4:D:110:HOH:O	2.11	0.49
3:J:632:ASN:O	3:J:636:ILE:HG12	2.12	0.49
3:I:683:PRO:HB3	3:I:684:ARG:C	2.32	0.49
3:J:684:ARG:H	3:J:687:ASN:HB2	1.77	0.49
3:H:593:LYS:O	3:H:594:ILE:O	2.30	0.49
3:J:592:LEU:HD21	3:J:633:LEU:HD22	1.94	0.49
3:J:687:ASN:O	3:J:691:MET:HB2	2.11	0.49
3:H:597:SER:O	3:H:599:LEU:N	2.46	0.49
3:H:731:ILE:HG23	3:H:776:LEU:HD21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:GLN:HG2	2:C:76:MET:HG2	1.96	0.48
3:J:675:SER:HA	3:J:726:GLU:OE1	2.14	0.48
2:G:19:LEU:HD12	2:G:66:THR:HB	1.95	0.48
3:I:631:LEU:HD11	3:I:680:ILE:HG23	1.96	0.48
3:I:471:LYS:HB3	3:I:472:SER:HB2	1.96	0.48
3:J:631:LEU:HD21	3:J:680:ILE:HG23	1.95	0.48
3:H:556:PHE:CD2	3:H:611:LEU:HD12	2.49	0.47
1:A:32:ALA:HB2	2:D:82:LEU:HD13	1.94	0.47
3:J:682:PRO:N	3:J:683:PRO:HD3	2.29	0.47
3:J:716:LYS:H	3:J:719:HIS:HD2	1.61	0.47
3:J:557:ASN:HB3	3:J:614:GLN:HG2	1.96	0.47
3:I:533:ILE:HG23	3:I:591:ILE:CD1	2.44	0.47
3:H:595:ILE:C	3:H:597:SER:N	2.65	0.47
3:J:787:TYR:CD2	3:J:788:ARG:HA	2.50	0.47
2:D:11:VAL:O	2:D:12:ASP:CB	2.61	0.47
3:J:521:ASN:HB3	3:J:524:ILE:HD13	1.96	0.47
1:A:19:LYS:HD3	1:A:75:LEU:HD12	1.97	0.47
3:I:689:HIS:CD2	3:I:692:ARG:HH21	2.33	0.47
1:B:40:VAL:HG23	2:G:3:PHE:CE2	2.48	0.47
3:H:738:ALA:O	3:H:742:GLN:HB2	2.15	0.47
3:H:488:GLU:O	3:H:492:LEU:HD13	2.15	0.47
3:J:508:TRP:CZ3	3:J:513:ILE:HB	2.50	0.47
2:C:73:ASN:HB2	2:C:76:MET:HG3	1.97	0.47
1:B:70:GLY:O	1:B:72:THR:N	2.48	0.47
3:I:625:THR:HG21	3:I:673:LEU:HD21	1.97	0.46
3:I:684:ARG:H	3:I:687:ASN:HB2	1.81	0.46
3:J:622:SER:HA	4:J:801:HOH:O	2.15	0.46
3:I:524:ILE:HG23	3:I:562:LEU:HD22	1.97	0.46
3:J:748:LEU:HB3	3:J:749:SER:H	1.60	0.46
3:J:656:SER:HB2	3:J:657:PRO:HD3	1.98	0.46
3:H:513:ILE:HG23	3:H:554:LYS:HG3	1.97	0.46
3:I:745:GLU:HG3	3:I:746:LYS:N	2.29	0.46
2:D:82:LEU:O	2:D:86:THR:HG22	2.16	0.46
1:B:18:ILE:HD13	1:B:73:VAL:HG13	1.98	0.46
3:J:570:TYR:CD1	3:J:682:PRO:HB3	2.51	0.46
2:C:46:THR:HA	2:C:47:ASP:HA	1.58	0.46
3:J:562:LEU:HD12	3:J:564:ILE:HG22	1.97	0.46
3:H:715:GLY:C	3:H:716:LYS:HG3	2.37	0.46
3:H:640:ARG:NH1	4:H:813:HOH:O	2.49	0.46
1:A:65:MET:HG2	2:D:72:LEU:HB2	1.97	0.46
2:D:43:ILE:HB	2:D:44:SER:CB	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:586:LEU:HD23	3:J:590:ILE:HD13	1.98	0.46
3:I:742:GLN:HA	3:I:745:GLU:HG2	1.99	0.45
3:I:667:ASP:OD2	3:I:719:HIS:HE1	1.99	0.45
3:I:521:ASN:HA	3:I:522:PRO:HD2	1.75	0.45
3:I:640:ARG:CG	3:I:640:ARG:NH1	2.68	0.45
1:B:1:MET:CB	1:B:2:GLU:HA	2.24	0.45
4:A:104:HOH:O	2:C:63:ARG:CD	2.64	0.45
3:H:570:TYR:CD2	3:H:682:PRO:HB3	2.51	0.45
3:J:677:ILE:HD12	3:J:726:GLU:HG3	1.99	0.45
3:H:760:THR:HG23	3:H:763:LYS:HE2	1.98	0.45
3:J:589:MET:HB3	3:J:590:ILE:HD12	1.98	0.45
2:G:64:GLY:O	2:G:67:VAL:HG22	2.16	0.45
3:I:544:ASP:HA	3:I:545:LYS:HA	1.81	0.45
3:H:728:ARG:HA	3:H:731:ILE:HD12	1.99	0.45
2:C:26:LYS:HG2	4:C:108:HOH:O	2.16	0.44
1:F:33:PHE:HB3	1:F:39:ILE:HG22	1.99	0.44
1:A:31:GLN:NE2	2:D:83:GLN:HE21	2.11	0.44
1:F:20:LEU:HD22	1:F:72:THR:HG23	1.98	0.44
1:B:20:LEU:HB2	1:B:24:ARG:HG3	1.99	0.44
2:C:73:ASN:O	2:C:74:LYS:C	2.53	0.44
3:H:684:ARG:HA	3:H:685:GLU:C	2.38	0.44
1:B:20:LEU:HD21	1:B:68:ILE:HG21	1.99	0.44
3:I:645:LYS:HD2	3:I:659:ILE:HG23	1.98	0.44
3:I:475:LYS:HE2	3:I:479:LEU:HD11	2.00	0.44
1:B:16:VAL:HG22	1:B:78:THR:HG22	1.99	0.44
2:G:83:GLN:HA	2:G:86:THR:CG2	2.47	0.44
3:J:653:ILE:HA	3:J:654:LEU:HB3	1.98	0.44
3:J:651:SER:HA	3:J:652:ASN:CB	2.47	0.44
1:F:29:THR:HB	1:F:42:SER:HB2	2.00	0.44
3:J:544:ASP:HA	3:J:545:LYS:HA	1.82	0.44
3:J:471:LYS:CB	3:J:472:SER:CB	2.82	0.43
1:F:17:TYR:HB2	1:F:77:SER:HB3	2.00	0.43
1:B:26:LEU:CD1	1:B:41:LEU:HD12	2.48	0.43
1:B:69:ARG:O	1:B:72:THR:HG22	2.18	0.43
3:I:488:GLU:HG2	3:I:507:MET:HB3	1.99	0.43
3:I:606:ILE:HD12	3:I:606:ILE:H	1.82	0.43
3:I:596:VAL:O	3:I:600:SER:HB2	2.18	0.43
1:B:38:ASN:HB3	1:B:67:PHE:HE1	1.84	0.43
2:C:83:GLN:HB3	1:F:31:GLN:O	2.19	0.43
3:H:595:ILE:O	3:H:597:SER:C	2.56	0.43
2:C:83:GLN:HA	2:C:86:THR:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:785:LEU:H	3:H:785:LEU:HD12	1.84	0.43
2:D:46:THR:HA	2:D:47:ASP:HA	1.60	0.43
2:C:73:ASN:CB	2:C:76:MET:HG3	2.48	0.43
3:J:570:TYR:CG	3:J:682:PRO:HB3	2.54	0.43
2:D:1:MET:HA	2:D:1:MET:CE	2.49	0.43
3:I:683:PRO:HB3	3:I:685:GLU:N	2.33	0.42
1:B:8:LEU:HD13	1:B:33:PHE:CD1	2.54	0.42
3:H:552:LEU:HD11	3:H:595:ILE:HB	2.01	0.42
2:D:30:GLN:NE2	2:D:41:ASP:OD2	2.52	0.42
3:J:535:ILE:HG23	3:J:539:ILE:HD11	2.02	0.42
3:H:587:PHE:CE1	3:H:591:ILE:HG13	2.54	0.42
2:G:11:VAL:O	2:G:12:ASP:HB2	2.20	0.42
1:A:67:PHE:O	2:D:69:TYR:HA	2.19	0.42
3:H:651:SER:HA	3:H:652:ASN:HB2	2.00	0.42
3:I:615:LEU:HD21	3:I:634:ILE:HG12	2.01	0.42
3:H:598:PHE:HD1	3:H:599:LEU:CD2	2.30	0.42
1:A:31:GLN:NE2	2:D:83:GLN:HG3	2.35	0.42
1:B:8:LEU:HD22	1:B:30:LEU:CD2	2.50	0.42
2:G:78:ASP:OD1	2:G:81:LEU:HB2	2.19	0.42
3:J:681:PHE:C	3:J:683:PRO:HD3	2.39	0.42
3:H:544:ASP:HA	3:H:545:LYS:HA	1.79	0.42
3:J:654:LEU:CD2	3:J:655:SER:H	2.32	0.42
3:J:584:VAL:HG13	3:J:629:ILE:HD11	2.01	0.42
1:B:18:ILE:HD11	1:B:20:LEU:CD2	2.43	0.42
3:J:489:ILE:HG13	3:J:535:ILE:HD11	2.02	0.42
1:A:69:ARG:O	1:A:72:THR:HG22	2.19	0.41
2:D:4:PHE:HB2	4:D:103:HOH:O	2.20	0.41
2:C:73:ASN:O	2:C:76:MET:N	2.50	0.41
3:I:689:HIS:HD2	3:I:692:ARG:HH21	1.68	0.41
3:I:489:ILE:HD11	3:I:539:ILE:HG12	2.01	0.41
1:B:29:THR:HB	1:B:42:SER:OG	2.20	0.41
2:D:59:ASN:N	2:D:59:ASN:OD1	2.53	0.41
1:A:40:VAL:HG23	2:D:3:PHE:CE2	2.55	0.41
2:C:83:GLN:HE21	1:F:31:GLN:NE2	2.19	0.41
3:H:792:ILE:H	3:H:792:ILE:HG13	1.72	0.41
2:D:80:ASN:HD22	2:D:80:ASN:HA	1.68	0.41
3:H:716:LYS:HA	3:H:717:LEU:HA	1.92	0.41
1:F:18:ILE:HD13	1:F:39:ILE:HD12	2.03	0.41
3:I:620:ASN:HD21	3:I:622:SER:HB3	1.86	0.41
2:D:1:MET:HE2	2:D:1:MET:HA	2.02	0.41
3:I:471:LYS:CB	3:I:472:SER:CB	2.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:786:VAL:O	3:I:787:TYR:C	2.60	0.40
3:I:558:GLU:OE1	3:I:561:HIS:HD2	2.03	0.40
3:H:592:LEU:C	3:H:594:ILE:N	2.72	0.40
2:G:83:GLN:HA	2:G:86:THR:HG23	2.03	0.40
3:I:780:LEU:HD12	3:I:785:LEU:HB2	2.03	0.40
2:D:61:PHE:CD1	2:D:61:PHE:C	2.94	0.40
3:I:684:ARG:NH1	3:I:730:GLU:OE1	2.50	0.40
3:J:472:SER:HA	3:J:473:GLY:HA2	1.83	0.40
3:J:685:GLU:O	3:J:687:ASN:N	2.54	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:22:GLY:O	1:B:54:GLU:OE1[2_657]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/89 (88%)	66 (85%)	10 (13%)	2 (3%)	7	38
1	B	78/89 (88%)	66 (85%)	10 (13%)	2 (3%)	7	38
1	E	64/89 (72%)	56 (88%)	8 (12%)	0	100	100
1	F	71/89 (80%)	67 (94%)	3 (4%)	1 (1%)	14	55
2	C	82/109 (75%)	71 (87%)	8 (10%)	3 (4%)	4	27
2	D	80/109 (73%)	70 (88%)	7 (9%)	3 (4%)	4	26
2	G	82/109 (75%)	74 (90%)	5 (6%)	3 (4%)	4	27
3	H	314/380 (83%)	279 (89%)	20 (6%)	15 (5%)	3	20
3	I	313/380 (82%)	285 (91%)	19 (6%)	9 (3%)	6	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	314/380 (83%)	287 (91%)	22 (7%)	5 (2%)	12	52
All	All	1476/1823 (81%)	1321 (90%)	112 (8%)	43 (3%)	6	35

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	B	52	ASN
1	B	71	ASP
2	C	57	VAL
2	G	25	ILE
3	H	594	ILE
3	H	595	ILE
3	H	792	ILE
3	I	653	ILE
3	I	686	TYR
3	J	653	ILE
3	J	684	ARG
2	C	25	ILE
2	D	12	ASP
3	H	593	LYS
3	H	596	VAL
3	H	598	PHE
3	H	793	SER
3	J	686	TYR
2	D	43	ILE
2	G	45	CYS
3	H	597	SER
3	H	651	SER
3	H	684	ARG
3	I	655	SER
3	I	713	LEU
2	G	65	SER
3	H	602	ASN
3	H	686	TYR
3	H	789	ASP
3	I	544	ASP
3	I	787	TYR
3	I	791	GLU
3	J	748	LEU
2	C	12	ASP
2	D	25	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	3	THR
3	H	683	PRO
3	I	790	GLY
1	A	71	ASP
3	H	655	SER
3	I	684	ARG
3	J	682	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	74/81 (91%)	62 (84%)	12 (16%)	3	13
1	B	74/81 (91%)	60 (81%)	14 (19%)	2	10
1	E	62/81 (76%)	59 (95%)	3 (5%)	31	71
1	F	69/81 (85%)	62 (90%)	7 (10%)	9	35
2	C	83/104 (80%)	72 (87%)	11 (13%)	5	22
2	D	81/104 (78%)	63 (78%)	18 (22%)	1	5
2	G	83/104 (80%)	73 (88%)	10 (12%)	6	27
3	H	299/348 (86%)	263 (88%)	36 (12%)	6	27
3	I	298/348 (86%)	271 (91%)	27 (9%)	12	41
3	J	299/348 (86%)	267 (89%)	32 (11%)	8	32
All	All	1422/1680 (85%)	1252 (88%)	170 (12%)	6	27

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	THR
1	A	5	LEU
1	A	8	LEU
1	A	27	VAL
1	A	31	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	48	ILE
1	A	56	LEU
1	A	62	ARG
1	A	65	MET
1	A	68	ILE
1	A	72	THR
1	B	3	THR
1	B	8	LEU
1	B	15	ARG
1	B	18	ILE
1	B	21	ARG
1	B	25	THR
1	B	47	THR
1	B	48	ILE
1	B	50	GLN
1	B	53	ASN
1	B	56	LEU
1	B	62	ARG
1	B	65	MET
1	B	68	ILE
2	C	1	MET
2	C	13	GLN
2	C	18	GLU
2	C	21	ASN
2	C	24	GLU
2	C	39	LYS
2	C	66	THR
2	C	72	LEU
2	C	81	LEU
2	C	82	LEU
2	C	86	THR
2	D	1	MET
2	D	13	GLN
2	D	26	LYS
2	D	29	LEU
2	D	30	GLN
2	D	36	LEU
2	D	39	LYS
2	D	59	ASN
2	D	60	ILE
2	D	66	THR
2	D	72	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	79	THR
2	D	81	LEU
2	D	82	LEU
2	D	86	THR
2	D	88	ARG
2	D	92	THR
2	D	93	GLU
1	E	11	ASN
1	E	24	ARG
1	E	65	MET
1	F	3	THR
1	F	15	ARG
1	F	26	LEU
1	F	29	THR
1	F	39	ILE
1	F	65	MET
1	F	75	LEU
2	G	1	MET
2	G	10	LEU
2	G	13	GLN
2	G	34	GLN
2	G	58	ARG
2	G	66	THR
2	G	81	LEU
2	G	82	LEU
2	G	86	THR
2	G	92	THR
3	H	476	LYS
3	H	488	GLU
3	H	507	MET
3	H	519	ASP
3	H	538	ARG
3	H	543	LEU
3	H	549	LEU
3	H	550	LYS
3	H	562	LEU
3	H	563	GLN
3	H	578	LEU
3	H	589	MET
3	H	592	LEU
3	H	595	ILE
3	H	596	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	601	ASN
3	H	612	LEU
3	H	613	LEU
3	H	614	GLN
3	H	633	LEU
3	H	640	ARG
3	H	646	GLN
3	H	680	ILE
3	H	684	ARG
3	H	693	LEU
3	H	711	LEU
3	H	714	SER
3	H	717	LEU
3	H	724	ILE
3	H	759	ASP
3	H	763	LYS
3	H	776	LEU
3	H	780	LEU
3	H	782	VAL
3	H	792	ILE
3	H	794	GLU
3	I	498	ASN
3	I	530	ASP
3	I	538	ARG
3	I	544	ASP
3	I	549	LEU
3	I	552	LEU
3	I	562	LEU
3	I	563	GLN
3	I	578	LEU
3	I	585	ASP
3	I	620	ASN
3	I	627	SER
3	I	629	ILE
3	I	633	LEU
3	I	640	ARG
3	I	669	LEU
3	I	671	THR
3	I	684	ARG
3	I	699	MET
3	I	711	LEU
3	I	724	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	729	ASP
3	I	745	GLU
3	I	748	LEU
3	I	771	LYS
3	I	776	LEU
3	I	780	LEU
3	J	493	GLU
3	J	507	MET
3	J	508	TRP
3	J	530	ASP
3	J	549	LEU
3	J	562	LEU
3	J	567	LEU
3	J	578	LEU
3	J	586	LEU
3	J	588	GLN
3	J	601	ASN
3	J	613	LEU
3	J	631	LEU
3	J	633	LEU
3	J	640	ARG
3	J	643	LEU
3	J	654	LEU
3	J	667	ASP
3	J	669	LEU
3	J	673	LEU
3	J	684	ARG
3	J	685	GLU
3	J	692	ARG
3	J	696	ASP
3	J	699	MET
3	J	711	LEU
3	J	714	SER
3	J	742	GLN
3	J	760	THR
3	J	787	TYR
3	J	788	ARG
3	J	792	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
2	C	21	ASN
2	C	80	ASN
2	D	59	ASN
2	D	80	ASN
1	F	11	ASN
1	F	31	GLN
2	G	13	GLN
2	G	83	GLN
3	H	495	ASN
3	H	602	ASN
3	H	620	ASN
3	H	632	ASN
3	H	742	GLN
3	I	495	ASN
3	I	501	GLN
3	I	546	GLN
3	I	561	HIS
3	I	563	GLN
3	I	614	GLN
3	I	620	ASN
3	I	632	ASN
3	I	689	HIS
3	I	719	HIS
3	J	632	ASN
3	J	689	HIS
3	J	719	HIS
3	J	777	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	80/89 (89%)	-0.08	2 (2%) 61 45	46, 62, 73, 77	0
1	B	80/89 (89%)	-0.08	2 (2%) 61 45	59, 72, 83, 86	0
1	E	68/89 (76%)	0.18	5 (7%) 17 9	108, 111, 117, 118	0
1	F	75/89 (84%)	0.22	3 (4%) 42 26	84, 90, 98, 98	0
2	C	86/109 (78%)	0.09	5 (5%) 26 13	51, 83, 96, 106	0
2	D	84/109 (77%)	-0.18	0 100 100	47, 73, 87, 90	0
2	G	86/109 (78%)	0.07	6 (6%) 19 10	54, 94, 120, 126	0
3	H	318/380 (83%)	-0.02	12 (3%) 44 27	61, 90, 135, 151	0
3	I	317/380 (83%)	-0.11	3 (0%) 85 77	64, 87, 124, 143	0
3	J	318/380 (83%)	0.02	13 (4%) 41 25	72, 101, 135, 143	0
All	All	1512/1823 (82%)	-0.02	51 (3%) 49 32	46, 91, 128, 151	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	47	ASP	5.1
3	J	652	ASN	4.9
2	G	56	SER	4.7
3	J	762	LEU	4.3
3	H	651	SER	4.2
3	H	652	ASN	4.1
1	E	80	SER	4.0
3	H	794	GLU	3.6
2	C	56	SER	3.6
1	F	51	LEU	3.5
1	F	52	ASN	3.5
3	H	762	LEU	3.4
3	J	746	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	48	GLU	3.1
1	F	23	ALA	3.0
2	G	47	ASP	2.9
2	C	48	GLU	2.8
3	I	649	SER	2.8
3	J	790	GLY	2.7
2	G	39	LYS	2.7
1	A	80	SER	2.7
3	H	650	ARG	2.6
3	H	471	LYS	2.6
1	E	23	ALA	2.6
3	J	749	SER	2.6
1	A	54	GLU	2.5
3	H	473	GLY	2.5
3	I	792	ILE	2.5
2	G	57	VAL	2.5
1	E	60	GLU	2.4
1	E	62	ARG	2.4
3	J	501	GLN	2.4
2	C	57	VAL	2.4
3	I	501	GLN	2.4
3	J	647	ASP	2.3
3	H	746	LYS	2.3
3	J	758	LEU	2.3
3	H	501	GLN	2.3
1	B	1	MET	2.3
3	H	657	PRO	2.2
3	J	697	LYS	2.2
1	B	80	SER	2.2
3	J	793	SER	2.2
2	G	30	GLN	2.1
3	J	792	ILE	2.1
1	E	61	ARG	2.1
3	H	758	LEU	2.1
3	J	568	SER	2.1
3	J	650	ARG	2.1
3	H	760	THR	2.1
2	C	46	THR	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 [i](#)

There are no carbohydrates 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.