Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 09:42 AM EST

PDB ID	:	3UO8
Title	:	Crystal structure of the MALT1 paracaspase (P1 form)
Authors	:	Jeffrey, P.D.; Yu, J.W.; Shi, Y.
Deposited on	:	2011-11-16
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

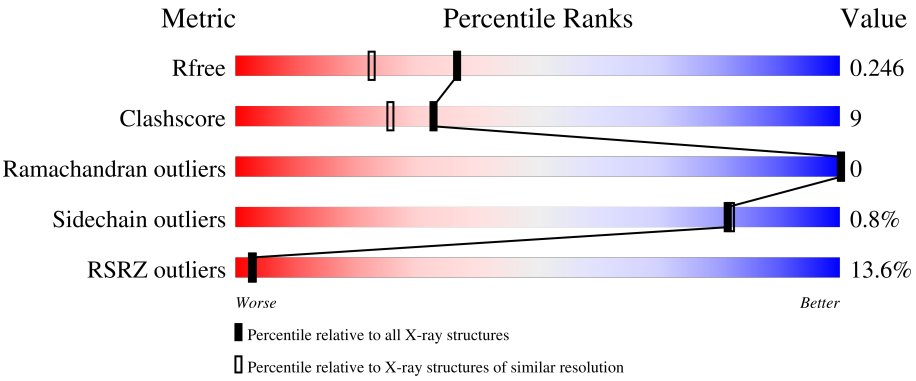
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	B	390	13% 75% 19% 7%
1	C	390	13% 78% 15% 7%
2	L	6	17% 33% 33% 33%
2	M	6	33% 17% 17% 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11804 atoms, of which 5800 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 Mucosa-associated lymphoid tissue lymphoma translocation protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	364	Total	C	H	N	O	S	0	0	0
			5728	1835	2869	463	540	21			
1	C	363	Total	C	H	N	O	S	0	0	0
			5698	1831	2847	464	535	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	338	MET	-	expression tag	UNP Q9UDY8
B	720	LEU	-	expression tag	UNP Q9UDY8
B	721	GLU	-	expression tag	UNP Q9UDY8
B	722	HIS	-	expression tag	UNP Q9UDY8
B	723	HIS	-	expression tag	UNP Q9UDY8
B	724	HIS	-	expression tag	UNP Q9UDY8
B	725	HIS	-	expression tag	UNP Q9UDY8
B	726	HIS	-	expression tag	UNP Q9UDY8
B	727	HIS	-	expression tag	UNP Q9UDY8
C	338	MET	-	expression tag	UNP Q9UDY8
C	720	LEU	-	expression tag	UNP Q9UDY8
C	721	GLU	-	expression tag	UNP Q9UDY8
C	722	HIS	-	expression tag	UNP Q9UDY8
C	723	HIS	-	expression tag	UNP Q9UDY8
C	724	HIS	-	expression tag	UNP Q9UDY8
C	725	HIS	-	expression tag	UNP Q9UDY8
C	726	HIS	-	expression tag	UNP Q9UDY8
C	727	HIS	-	expression tag	UNP Q9UDY8

- Molecule 2 is a protein called Z-Val-Arg-Pro-DL-Arg-fluoromethylketone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	4	Total	C	H	N	O	0	0	0
			78	22	42	10	4			
2	M	4	Total	C	H	N	O	0	0	0
			78	22	42	10	4			

- Molecule 3 is water.

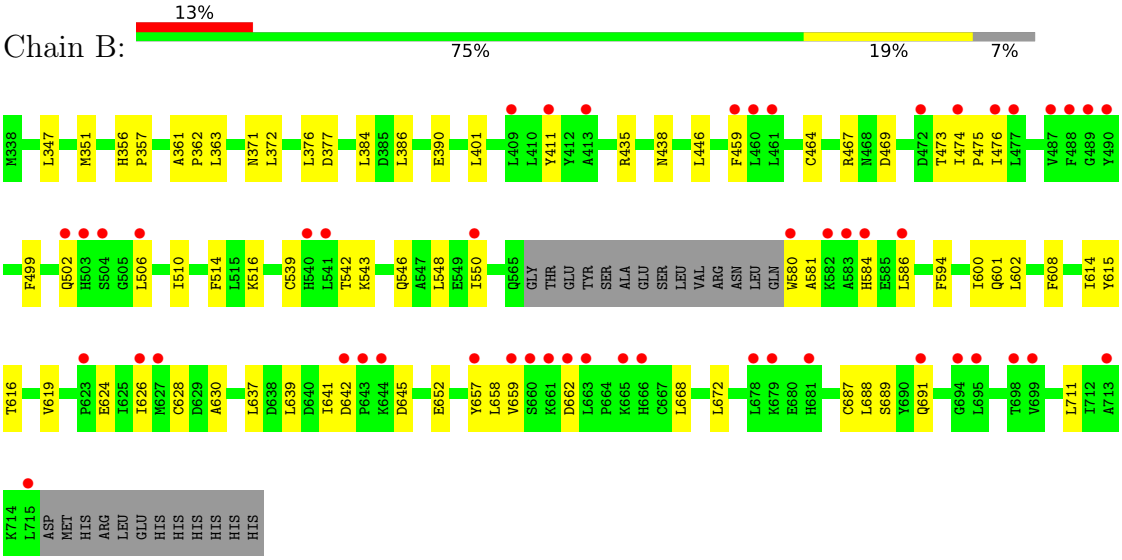
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	105	Total	O	0	0
			105	105		
3	C	112	Total	O	0	0
			112	112		
3	L	2	Total	O	0	0
			2	2		
3	M	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

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

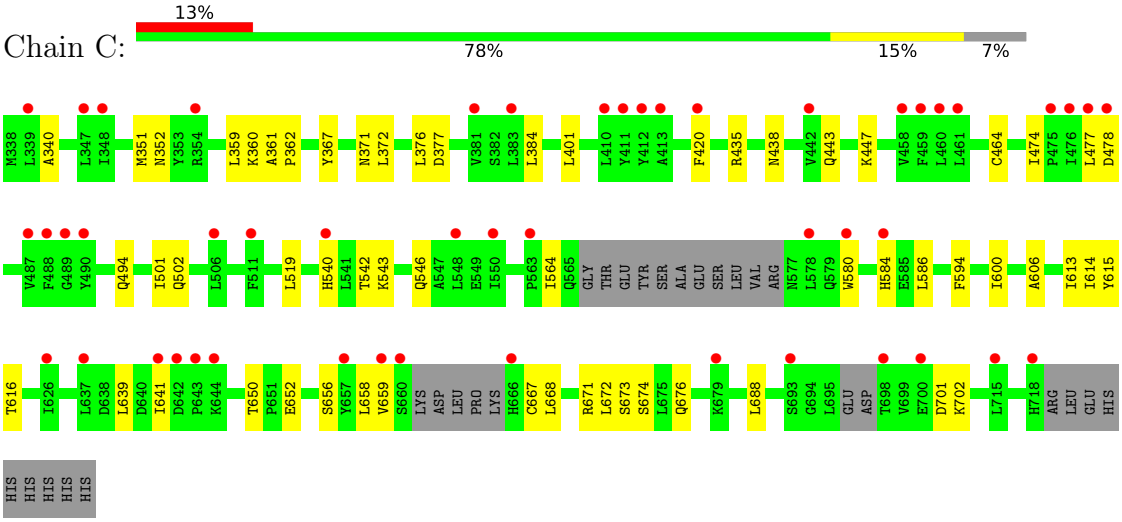
• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

Chain B:



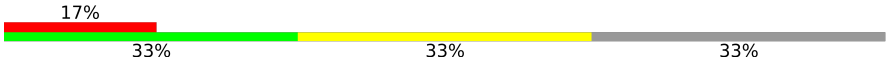
• Molecule 1: Mucosa-associated lymphoid tissue lymphoma translocation protein 1

Chain C:



• Molecule 2: Z-Val-Arg-Pro-DL-Arg-fluoromethylketone

Chain L:



• Molecule 2: Z-Val-Arg-Pro-DL-Arg-fluoromethylketone

Chain M:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.23Å 61.16Å 71.13Å 108.59° 97.23° 117.23°	Depositor
Resolution (Å)	34.26 – 1.90 34.26 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (34.26-1.90) 92.4 (34.26-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.207 , 0.250 0.201 , 0.246	Depositor DCC
R_{free} test set	3197 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-h-k-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11804	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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	B	0.32	0/2910	0.49	0/3936
1	C	0.33	0/2901	0.49	0/3920
2	L	0.43	0/36	0.66	0/47
2	M	0.44	0/36	0.72	0/47
All	All	0.33	0/5883	0.49	0/7950

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	2859	2869	2876	55	0
1	C	2851	2847	2854	46	0
2	L	36	42	44	4	0
2	M	36	42	44	5	0
3	B	105	0	0	8	0
3	C	112	0	0	4	0
3	L	2	0	0	1	0
3	M	3	0	0	2	0
All	All	6004	5800	5818	101	0

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 9.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:ASP:HB2	3:B:903:HOH:O	1.87	0.73
1:C:594:PHE:CE1	1:C:600:ILE:HD12	2.24	0.73
2:L:1:VAL:HA	3:L:101:HOH:O	1.92	0.69
1:B:502:GLN:H	2:L:1:VAL:HG23	1.57	0.68
1:B:499:PHE:HB2	1:B:510:ILE:HD13	1.77	0.67
1:C:600:ILE:HD11	1:C:688:LEU:HD13	1.76	0.66
1:B:351:MET:HE1	3:B:840:HOH:O	1.95	0.66
1:B:600:ILE:HD11	1:B:688:LEU:HD13	1.79	0.65
1:C:464:CYS:SG	2:M:4:ARG:C	2.76	0.64
1:B:363:LEU:HD21	1:B:657:TYR:HB2	1.79	0.63
1:B:601:GLN:HB2	1:B:619:VAL:HG11	1.80	0.63
1:B:594:PHE:CE1	1:B:600:ILE:HD12	2.35	0.62
1:C:401:LEU:HD22	1:C:580:TRP:CD2	2.35	0.61
1:B:464:CYS:SG	2:L:4:ARG:C	2.79	0.61
1:C:352:ASN:HB3	3:C:883:HOH:O	1.98	0.61
1:B:658:LEU:HB3	3:B:903:HOH:O	1.99	0.61
1:C:435:ARG:H	1:C:438:ASN:HD22	1.49	0.60
1:B:539:CYS:O	1:B:543:LYS:HG3	2.02	0.59
1:B:624:GLU:HB2	3:B:863:HOH:O	2.05	0.56
1:B:435:ARG:H	1:B:438:ASN:HD22	1.53	0.56
1:B:347:LEU:HG	1:B:411:TYR:HB3	1.87	0.56
2:M:1:VAL:HA	3:M:101:HOH:O	2.06	0.55
1:C:650:THR:HG22	1:C:652:GLU:HG2	1.87	0.55
1:B:602:LEU:HD13	1:B:616:THR:HG22	1.89	0.55
1:B:659:VAL:N	3:B:903:HOH:O	2.40	0.55
1:B:473:THR:HG22	1:B:475:PRO:HD3	1.89	0.53
1:C:447:LYS:HE3	1:C:478:ASP:HB2	1.90	0.53
1:B:642:ASP:HB3	1:B:645:ASP:OD1	2.09	0.53
1:B:506:LEU:HD23	1:B:506:LEU:O	2.09	0.52
1:C:501:ILE:HA	2:M:1:VAL:HG23	1.92	0.51
1:B:628:CYS:HA	1:B:689:SER:O	2.10	0.51
1:C:376:LEU:O	1:C:377:ASP:HB2	2.11	0.51
1:B:506:LEU:HD21	1:B:657:TYR:CE1	2.46	0.50
1:B:363:LEU:C	1:B:363:LEU:HD23	2.33	0.50
1:C:401:LEU:CD2	1:C:580:TRP:CG	2.95	0.49
1:C:502:GLN:HG3	2:M:1:VAL:HB	1.94	0.49
1:B:361:ALA:N	1:B:362:PRO:CD	2.76	0.49
1:B:474:ILE:HD13	1:C:474:ILE:HG21	1.93	0.49
1:C:650:THR:CG2	1:C:652:GLU:HG2	2.42	0.49
1:B:601:GLN:HB2	1:B:619:VAL:CG1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:ILE:CD1	1:B:672:LEU:HD11	2.43	0.48
1:B:499:PHE:HB2	1:B:510:ILE:CD1	2.44	0.48
1:C:351:MET:HE3	1:C:360:LYS:HA	1.95	0.48
1:C:656:SER:OG	1:C:671:ARG:HD2	2.14	0.48
1:B:372:LEU:HD11	1:B:516:LYS:HG3	1.94	0.48
1:B:371:ASN:HB3	3:B:827:HOH:O	2.14	0.48
1:B:386:LEU:HD22	1:B:390:GLU:HB3	1.96	0.47
1:C:616:THR:O	1:C:667:CYS:HB3	2.14	0.47
1:C:401:LEU:HD21	1:C:580:TRP:CG	2.49	0.47
1:C:367:TYR:CG	1:C:658:LEU:HD13	2.50	0.47
1:B:548:LEU:HD22	1:B:550:ILE:HG13	1.97	0.46
1:C:639:LEU:HB3	1:C:641:ILE:HD12	1.97	0.46
1:B:467:ARG:HH12	1:B:469:ASP:HA	1.81	0.46
1:C:701:ASP:O	1:C:702:LYS:HB3	2.14	0.46
1:B:474:ILE:HG22	1:C:420:PHE:CZ	2.51	0.46
1:B:639:LEU:CB	1:B:641:ILE:HD12	2.46	0.46
1:C:656:SER:HB3	1:C:659:VAL:HG23	1.97	0.46
2:M:1:VAL:CA	3:M:101:HOH:O	2.64	0.46
1:C:613:ILE:HG13	1:C:659:VAL:HG22	1.96	0.45
1:B:376:LEU:O	1:B:377:ASP:HB2	2.16	0.45
1:B:473:THR:C	1:B:475:PRO:HD3	2.37	0.45
1:C:351:MET:HB3	1:C:359:LEU:O	2.15	0.45
1:C:361:ALA:N	1:C:362:PRO:CD	2.80	0.45
1:B:384:LEU:HD11	1:B:608:PHE:CE2	2.52	0.44
1:B:639:LEU:HB2	1:B:641:ILE:HD12	2.00	0.44
1:C:340:ALA:O	1:C:564:ILE:HA	2.18	0.44
1:B:474:ILE:CG2	1:C:420:PHE:CZ	3.01	0.44
1:B:600:ILE:HD13	1:B:630:ALA:CB	2.48	0.44
1:C:615:TYR:HA	1:C:668:LEU:O	2.18	0.44
1:C:673:SER:O	1:C:674:SER:HB2	2.18	0.43
1:B:514:PHE:CZ	1:B:539:CYS:HB2	2.53	0.43
1:B:614:ILE:HD12	1:B:672:LEU:HD11	2.01	0.43
1:B:502:GLN:N	2:L:1:VAL:HG23	2.29	0.43
1:C:584:HIS:HB2	3:C:828:HOH:O	2.17	0.43
1:C:542:THR:HB	1:C:546:GLN:HB3	1.99	0.43
1:C:586:LEU:HD11	1:C:606:ALA:N	2.34	0.43
1:B:467:ARG:NH1	1:B:469:ASP:HA	2.34	0.42
1:B:586:LEU:HD13	1:B:711:LEU:HD21	2.00	0.42
1:B:542:THR:HB	1:B:546:GLN:HB3	2.01	0.42
1:C:372:LEU:HB3	1:C:519:LEU:HD23	2.01	0.42
1:C:477:LEU:HD12	1:C:477:LEU:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:TYR:HA	1:B:668:LEU:O	2.19	0.42
1:C:586:LEU:HD21	1:C:606:ALA:HB2	2.01	0.42
1:C:674:SER:HA	1:C:676:GLN:OE1	2.20	0.42
1:B:580:TRP:HA	3:B:894:HOH:O	2.20	0.42
1:B:630:ALA:HA	1:B:687:CYS:O	2.20	0.42
1:C:351:MET:SD	1:C:384:LEU:HD11	2.60	0.42
1:C:494:GLN:NE2	3:C:866:HOH:O	2.52	0.42
1:C:614:ILE:HD11	1:C:672:LEU:HD11	2.02	0.42
1:B:476:ILE:HG13	1:B:476:ILE:O	2.19	0.41
1:C:401:LEU:HD22	1:C:580:TRP:CE2	2.55	0.41
1:C:639:LEU:CB	1:C:641:ILE:HD12	2.50	0.41
1:B:626:ILE:HG12	1:B:691:GLN:O	2.20	0.41
1:B:356:HIS:HB3	1:B:357:PRO:HD2	2.02	0.41
1:C:371:ASN:ND2	3:C:863:HOH:O	2.54	0.41
1:C:443:GLN:HB3	1:C:477:LEU:CD2	2.51	0.41
1:C:540:HIS:ND1	1:C:543:LYS:HE2	2.36	0.41
1:B:600:ILE:HD13	1:B:630:ALA:HB1	2.02	0.40
1:C:401:LEU:HD22	1:C:580:TRP:CG	2.56	0.40
1:B:446:LEU:HD13	1:B:459:PHE:CE2	2.57	0.40
1:B:581:ALA:HB3	3:B:824:HOH:O	2.22	0.40

There are no symmetry-related clashes.

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	B	360/390 (92%)	338 (94%)	22 (6%)	0	100	100
1	C	355/390 (91%)	342 (96%)	13 (4%)	0	100	100
2	L	2/6 (33%)	2 (100%)	0	0	100	100
2	M	2/6 (33%)	2 (100%)	0	0	100	100
All	All	719/792 (91%)	684 (95%)	35 (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	Percentiles
1	B	316/347 (91%)	312 (99%)	4 (1%)	69 68
1	C	312/347 (90%)	312 (100%)	0	100 100
2	L	4/4 (100%)	4 (100%)	0	100 100
2	M	4/4 (100%)	3 (75%)	1 (25%)	0 0
All	All	636/702 (91%)	631 (99%)	5 (1%)	81 82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	401	LEU
1	B	584	HIS
1	B	637	LEU
1	B	652	GLU
2	M	1	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	371	ASN
1	B	438	ASN
1	B	508	ASN
1	B	666	HIS
1	C	371	ASN
1	C	422	ASN
1	C	438	ASN
1	C	502	GLN
1	C	508	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 monosaccharides 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

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, 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	B	364/390 (93%)	0.63	50 (13%) 3 3	20, 41, 80, 158	0
1	C	363/390 (93%)	0.68	49 (13%) 3 3	19, 38, 76, 111	0
2	L	4/6 (66%)	0.54	1 (25%) 0 0	29, 36, 50, 67	0
2	M	4/6 (66%)	0.41	0 100 100	31, 36, 47, 57	0
All	All	735/792 (92%)	0.65	100 (13%) 3 3	19, 39, 79, 158	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	474	ILE	7.3
1	C	659	VAL	6.6
1	C	476	ILE	5.9
1	C	641	ILE	5.5
1	B	476	ILE	5.5
1	B	659	VAL	5.2
1	B	626	ILE	5.1
1	B	661	LYS	5.0
1	B	715	LEU	4.6
1	C	637	LEU	4.5
1	C	477	LEU	4.4
1	C	644	LYS	4.3
1	C	460	LEU	4.3
1	C	693	SER	4.0
1	B	657	TYR	3.7
1	B	694	GLY	3.7
1	B	663	LEU	3.7
1	C	578	LEU	3.6
1	B	666	HIS	3.5
1	B	580	TRP	3.5
1	C	411	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	506	LEU	3.4
1	B	679	LYS	3.4
1	B	691	GLN	3.4
1	B	586	LEU	3.4
1	C	666	HIS	3.4
1	C	459	PHE	3.3
1	B	660	SER	3.2
1	B	488	PHE	3.2
1	C	550	ILE	3.2
1	B	541	LEU	3.2
1	C	461	LEU	3.2
1	C	475	PRO	3.2
1	B	540	HIS	3.1
1	C	718	HIS	3.1
1	C	490	TYR	3.1
1	C	488	PHE	3.1
1	C	626	ILE	3.1
1	B	644	LYS	3.1
1	B	583	ALA	3.1
1	C	580	TRP	3.0
1	B	487	VAL	3.0
1	C	339	LEU	2.9
1	B	461	LEU	2.9
1	C	489	GLY	2.9
1	B	623	PRO	2.8
1	B	642	ASP	2.8
1	C	700	GLU	2.8
1	B	698	THR	2.8
1	B	550	ILE	2.8
1	C	506	LEU	2.7
1	B	504	SER	2.7
1	B	627	MET	2.7
1	B	665	LYS	2.7
1	B	503	HIS	2.7
1	C	548	LEU	2.7
1	C	420	PHE	2.7
1	C	584	HIS	2.7
1	B	490	TYR	2.7
1	C	348	ILE	2.6
1	B	409	LEU	2.6
1	B	460	LEU	2.6
1	B	584	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	662	ASP	2.5
1	C	643	PRO	2.5
1	B	713	ALA	2.5
1	C	642	ASP	2.4
1	B	411	TYR	2.4
1	C	410	LEU	2.4
1	C	563	PRO	2.4
1	C	660	SER	2.4
1	C	354	ARG	2.3
1	C	478	ASP	2.3
1	C	412	TYR	2.3
1	C	511	PHE	2.3
1	B	477	LEU	2.3
1	B	472	ASP	2.3
1	C	347	LEU	2.3
1	C	540	HIS	2.3
1	C	657	TYR	2.2
1	B	489	GLY	2.2
1	C	698	THR	2.2
1	B	681	HIS	2.2
2	L	1	VAL	2.2
1	B	695	LEU	2.2
1	C	715	LEU	2.2
1	B	643	PRO	2.1
1	B	678	LEU	2.1
1	B	582	LYS	2.1
1	C	442	VAL	2.1
1	B	413	ALA	2.1
1	C	679	LYS	2.1
1	B	502	GLN	2.1
1	C	381	VAL	2.1
1	C	458	VAL	2.0
1	C	487	VAL	2.0
1	C	413	ALA	2.0
1	C	383	LEU	2.0
1	B	699	VAL	2.0
1	B	459	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.