Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 12:17 AM EDT

PDB ID	:	3BOW
Title	:	Structure of M-calpain in complex with Calpastatin
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Deposited on	:	2007-12-17
Resolution	:	2.40 Å(reported)

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

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

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

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

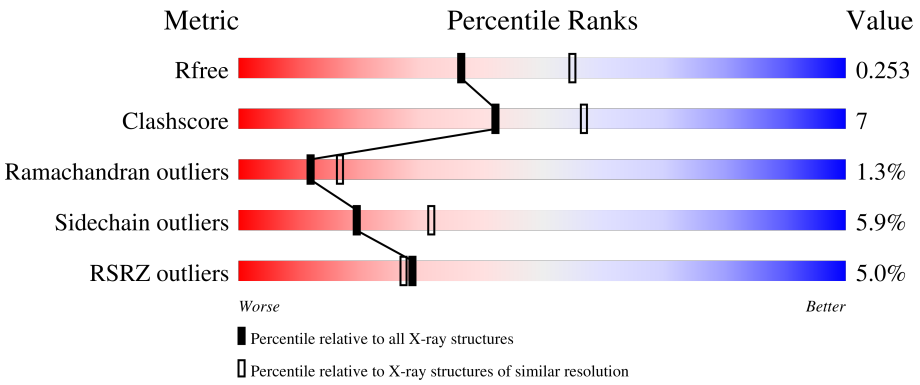
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	714	4% 77% 16% • 5%
2	B	184	7% 80% 14% • 5%
3	C	95	5% 55% 11% • 32%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7587 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 Calpain-2 catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	680	5470	3482	919	1045	24	0	1	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	engineered mutation	UNP Q07009
A	701	GLY	-	expression tag	UNP Q07009
A	702	LYS	-	expression tag	UNP Q07009
A	703	LEU	-	expression tag	UNP Q07009
A	704	ALA	-	expression tag	UNP Q07009
A	705	ALA	-	expression tag	UNP Q07009
A	706	ALA	-	expression tag	UNP Q07009
A	707	LEU	-	expression tag	UNP Q07009
A	708	GLU	-	expression tag	UNP Q07009
A	709	HIS	-	expression tag	UNP Q07009
A	710	HIS	-	expression tag	UNP Q07009
A	711	HIS	-	expression tag	UNP Q07009
A	712	HIS	-	expression tag	UNP Q07009
A	713	HIS	-	expression tag	UNP Q07009
A	714	HIS	-	expression tag	UNP Q07009

- Molecule 2 is a protein called Calpain small subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	174	1410	888	243	269	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	MET	-	expression tag	UNP Q64537

- Molecule 3 is a protein called Calpastatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	65	521	317	87	117	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	570	MET	-	expression tag	UNP P27321
C	646	PRO	LEU	SEE REMARK 999	UNP P27321

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	6	6	6	0	0
			Total	Ca		
4	B	4	4	4	0	0

- Molecule 5 is water.

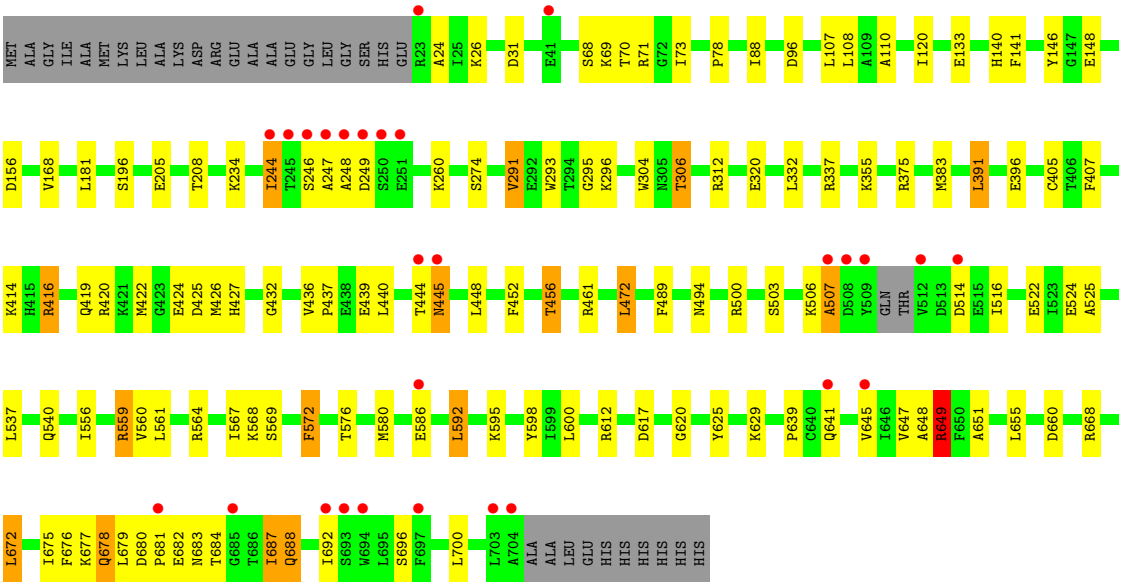
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	152	152	152	0	0
			Total	O		
5	B	15	15	15	0	0
			Total	O		
5	C	9	9	9	0	0

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.

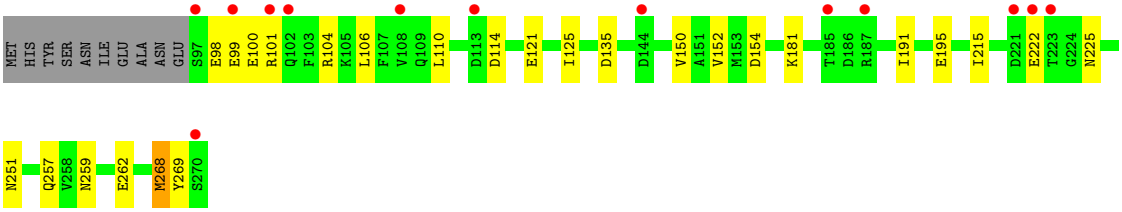
- Molecule 1: Calpain-2 catalytic subunit

Chain A:



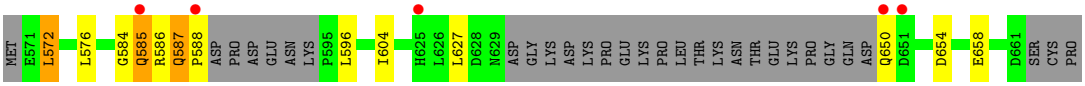
- Molecule 2: Calpain small subunit 1

Chain B:



- Molecule 3: Calpastatin

Chain C:


MET
E571
L572
L576
G584
Q585
R586
Q587
P588
ASP
PRO
ASP
GLU
ASN
LYS
P595
L596
I604
H625
L626
L627
D628
N629
ASP
GLY
LYS
ASP
LYS
PRO
GLU
LYS
PRO
LEU
THR
LYS
ASN
THR
GLU
LYS
PRO
GLY
GLN
ASP
Q650
D651
D654
E658
D661
SER
CYS
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.48Å 66.98Å 108.66Å 90.00° 100.76° 90.00°	Depositor
Resolution (Å)	66.23 – 2.40 66.29 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (66.23-2.40) 96.5 (66.29-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.258 0.198 , 0.253	Depositor DCC
R_{free} test set	1819 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7587	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.49	0/5595	0.63	2/7562 (0.0%)
2	B	0.45	0/1437	0.61	0/1932
3	C	0.36	0/526	0.61	0/707
All	All	0.47	0/7558	0.63	2/10201 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	472	LEU	CA-CB-CG	5.42	127.78	115.30

There are no chirality outliers.

There are no planarity outliers.

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	5470	0	5312	86	0
2	B	1410	0	1361	17	0
3	C	521	0	490	10	0
4	A	6	0	0	0	0
4	B	4	0	0	0	0
5	A	152	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	0	0	0
5	C	9	0	0	0	0
All	All	7587	0	7163	100	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 7.

All (100) 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:587:GLN:HB3	3:C:588:PRO:HA	1.09	1.07
1:A:524:GLU:O	1:A:524:GLU:HG3	1.48	1.05
3:C:587:GLN:HB3	3:C:588:PRO:CA	1.92	0.99
1:A:678:GLN:O	1:A:679:LEU:HB2	1.70	0.91
3:C:587:GLN:CB	3:C:588:PRO:HA	2.01	0.87
1:A:559:ARG:HG2	3:C:576:LEU:HD13	1.62	0.82
1:A:452:PHE:O	1:A:456:THR:HG23	1.83	0.79
1:A:312:ARG:CZ	5:A:850:HOH:O	2.35	0.73
1:A:524:GLU:O	1:A:524:GLU:CG	2.28	0.72
1:A:668:ARG:HG2	2:B:268:MET:CE	2.20	0.72
1:A:416:ARG:HG2	1:A:426:MET:HA	1.75	0.69
1:A:68:SER:HA	1:A:71:ARG:HD3	1.74	0.68
1:A:425:ASP:CG	1:A:426:MET:H	1.98	0.68
1:A:625:TYR:CZ	1:A:629:LYS:HD2	2.30	0.67
1:A:419:GLN:HB3	1:A:424:GLU:HB2	1.78	0.65
1:A:437:PRO:HG2	1:A:440:LEU:HD22	1.80	0.64
1:A:668:ARG:HG2	2:B:268:MET:HE3	1.79	0.64
1:A:687:ILE:O	2:B:257:GLN:HA	1.99	0.63
1:A:625:TYR:CE1	1:A:629:LYS:HD2	2.35	0.62
1:A:556:ILE:O	1:A:560:VAL:HG12	2.00	0.61
1:A:678:GLN:O	1:A:679:LEU:CB	2.50	0.59
1:A:355:LYS:NZ	1:A:507:ALA:HA	2.18	0.58
1:A:375:ARG:HB3	3:C:604:ILE:HD13	1.86	0.57
1:A:525:ALA:O	1:A:595:LYS:HD2	2.04	0.57
1:A:668:ARG:HG2	2:B:268:MET:HE1	1.86	0.57
1:A:274:SER:OG	1:A:306:THR:CG2	2.52	0.57
1:A:68:SER:HA	1:A:71:ARG:CD	2.33	0.56
1:A:500:ARG:HD3	5:A:857:HOH:O	2.04	0.56
1:A:645:VAL:O	1:A:648:ALA:O	2.23	0.56
1:A:422:MET:SD	2:B:114:ASP:HA	2.45	0.56
1:A:427:HIS:HE1	1:A:494:ASN:O	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:VAL:O	1:A:651:ALA:HB3	2.06	0.56
1:A:26:LYS:HE3	1:A:31:ASP:OD1	2.06	0.55
1:A:677:LYS:O	1:A:678:GLN:HB2	2.07	0.53
1:A:452:PHE:O	1:A:456:THR:CG2	2.56	0.53
1:A:564:ARG:NH2	3:C:584:GLY:O	2.41	0.53
2:B:121:GLU:O	2:B:125:ILE:HG12	2.09	0.53
1:A:676:PHE:O	1:A:687:ILE:HD11	2.09	0.52
1:A:274:SER:OG	1:A:306:THR:HG21	2.09	0.52
1:A:312:ARG:NH1	5:A:850:HOH:O	2.40	0.52
1:A:247:ALA:HB1	1:A:260:LYS:HD2	1.92	0.51
1:A:524:GLU:OE2	1:A:598:TYR:OH	2.22	0.51
1:A:592:LEU:HD21	1:A:600:LEU:HD13	1.91	0.51
1:A:69:LYS:HB3	3:C:627:LEU:HG	1.93	0.50
1:A:70:THR:HA	1:A:73:ILE:CD1	2.42	0.50
1:A:70:THR:HA	1:A:73:ILE:HD12	1.93	0.50
1:A:675:ILE:O	1:A:678:GLN:O	2.30	0.49
2:B:222:GLU:O	2:B:225:ASN:N	2.39	0.49
1:A:196:SER:O	1:A:420:ARG:NH2	2.21	0.49
1:A:500:ARG:CD	5:A:857:HOH:O	2.60	0.49
1:A:672:LEU:HD23	2:B:268:MET:HG2	1.95	0.48
1:A:444:THR:O	1:A:445:ASN:HB3	2.13	0.48
1:A:572:PHE:HE2	1:A:580:MET:HE1	1.78	0.48
1:A:78:PRO:HD3	1:A:156:ASP:O	2.14	0.48
1:A:439:GLU:HG2	1:A:440:LEU:HD12	1.95	0.48
1:A:648:ALA:O	1:A:649:ARG:CB	2.61	0.48
1:A:304:TRP:HB3	1:A:312:ARG:HE	1.77	0.48
1:A:576:THR:O	1:A:580:MET:HE2	2.14	0.47
1:A:205:GLU:CD	5:A:839:HOH:O	2.53	0.47
1:A:516:ILE:HG12	1:A:639:PRO:HD3	1.95	0.47
1:A:355:LYS:HZ3	1:A:507:ALA:HA	1.80	0.46
1:A:432:GLY:HA2	1:A:461:ARG:HG2	1.98	0.46
2:B:259:ASN:OD1	2:B:262:GLU:HG2	2.15	0.46
3:C:585:GLN:H	3:C:585:GLN:CD	2.19	0.46
1:A:425:ASP:CG	1:A:426:MET:N	2.67	0.45
2:B:150:VAL:O	2:B:154:ASP:HB2	2.16	0.45
1:A:682:GLU:O	1:A:684:THR:N	2.47	0.45
1:A:383[B]:MET:SD	1:A:617:ASP:HB3	2.56	0.45
1:A:688:GLN:HG3	2:B:257:GLN:HB3	1.98	0.45
2:B:152:VAL:HG12	2:B:269:TYR:HB3	1.98	0.44
1:A:568:LYS:HG3	1:A:620:GLY:HA3	1.99	0.43
1:A:677:LYS:O	1:A:678:GLN:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:MET:CE	2:B:268:MET:HA	2.49	0.43
1:A:146:TYR:CG	1:A:414:LYS:HG2	2.53	0.43
1:A:564:ARG:HD3	1:A:567:ILE:HD12	2.01	0.43
1:A:700:LEU:HD21	2:B:215:ILE:HD13	1.98	0.43
1:A:641:GLN:O	1:A:645:VAL:HG23	2.19	0.43
1:A:244:ILE:HG12	1:A:260:LYS:CB	2.48	0.43
2:B:135:ASP:OD2	2:B:181:LYS:HE2	2.18	0.43
1:A:291:VAL:N	1:A:320:GLU:OE2	2.46	0.42
1:A:489:PHE:HE2	3:C:604:ILE:HG22	1.84	0.42
1:A:205:GLU:CG	5:A:839:HOH:O	2.67	0.42
1:A:293:TRP:CZ2	1:A:295:GLY:HA3	2.54	0.42
1:A:391:LEU:HG	1:A:405:CYS:HB2	2.01	0.42
2:B:100:GLU:O	2:B:104:ARG:HG3	2.19	0.42
1:A:448:LEU:HD13	1:A:452:PHE:CE2	2.55	0.42
1:A:436:VAL:HA	1:A:437:PRO:HD2	1.78	0.42
2:B:191:ILE:HA	2:B:195:GLU:OE1	2.20	0.42
3:C:650:GLN:HB3	3:C:654:ASP:HB2	2.02	0.42
1:A:391:LEU:HD21	1:A:407:PHE:CE1	2.54	0.42
1:A:676:PHE:CD1	1:A:687:ILE:HD12	2.55	0.41
1:A:680:ASP:N	1:A:681:PRO:HD3	2.35	0.41
1:A:247:ALA:CB	1:A:260:LYS:HD2	2.50	0.41
1:A:444:THR:O	1:A:445:ASN:CB	2.69	0.41
1:A:355:LYS:HZ2	1:A:507:ALA:HA	1.86	0.41
1:A:141:PHE:CD1	1:A:181:LEU:HD13	2.56	0.41
1:A:569:SER:OG	1:A:660:ASP:HB2	2.22	0.41
1:A:120:ILE:HG21	1:A:208:THR:HG22	2.02	0.40
1:A:337:ARG:CZ	1:A:337:ARG:HB2	2.51	0.40
1:A:107:LEU:O	1:A:110:ALA:HB3	2.21	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	A	677/714 (95%)	642 (95%)	25 (4%)	10 (2%)	10	14
2	B	172/184 (94%)	164 (95%)	8 (5%)	0	100	100
3	C	59/95 (62%)	55 (93%)	2 (3%)	2 (3%)	3	3
All	All	908/993 (91%)	861 (95%)	35 (4%)	12 (1%)	12	17

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	SER
1	A	678	GLN
1	A	683	ASN
3	C	587	GLN
1	A	248	ALA
1	A	507	ALA
1	A	649	ARG
3	C	572	LEU
1	A	24	ALA
1	A	249	ASP
1	A	291	VAL
1	A	514	ASP

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	585/613 (95%)	550 (94%)	35 (6%)	19	31
2	B	153/162 (94%)	146 (95%)	7 (5%)	27	43
3	C	60/88 (68%)	55 (92%)	5 (8%)	11	17
All	All	798/863 (92%)	751 (94%)	47 (6%)	19	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ILE

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	133	GLU
1	A	140	HIS
1	A	148	GLU
1	A	168	VAL
1	A	234	LYS
1	A	244	ILE
1	A	296	LYS
1	A	306	THR
1	A	332	LEU
1	A	391	LEU
1	A	396	GLU
1	A	416	ARG
1	A	445	ASN
1	A	456	THR
1	A	472	LEU
1	A	503	SER
1	A	506	LYS
1	A	522	GLU
1	A	537	LEU
1	A	540	GLN
1	A	559	ARG
1	A	561	LEU
1	A	572	PHE
1	A	586	GLU
1	A	592	LEU
1	A	612	ARG
1	A	649	ARG
1	A	655	LEU
1	A	672	LEU
1	A	687	ILE
1	A	688	GLN
1	A	692	ILE
1	A	696	SER
2	B	98	GLU
2	B	99	GLU
2	B	101	ARG
2	B	106	LEU
2	B	110	LEU
2	B	251	ASN
2	B	268	MET
3	C	572	LEU

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Mol	Chain	Res	Type
3	C	585	GLN
3	C	586	ARG
3	C	596	LEU
3	C	658	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	256	GLN
1	A	379	ASN
1	A	415	HIS
1	A	427	HIS
1	A	445	ASN
1	A	540	GLN
1	A	688	GLN
2	B	109	GLN
2	B	225	ASN
2	B	251	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	680/714 (95%)	0.13	28 (4%)	37	36	2, 8, 28, 57	0
2	B	174/184 (94%)	0.50	13 (7%)	14	13	7, 15, 21, 29	0
3	C	65/95 (68%)	0.58	5 (7%)	13	12	2, 7, 16, 17	0
All	All	919/993 (92%)	0.23	46 (5%)	28	27	2, 10, 27, 57	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ALA	7.8
1	A	247	ALA	6.2
1	A	704	ALA	6.1
2	B	221	ASP	4.4
1	A	246	SER	4.1
1	A	694	TRP	3.8
3	C	650	GLN	3.7
1	A	509	TYR	3.7
1	A	250	SER	3.6
1	A	251	GLU	3.2
1	A	586	GLU	3.2
1	A	681	PRO	3.0
1	A	245	THR	3.0
3	C	588	PRO	2.9
2	B	187	ARG	2.9
2	B	113	ASP	2.8
1	A	249	ASP	2.8
1	A	445	ASN	2.8
1	A	507	ALA	2.8
1	A	508	ASP	2.8
2	B	102	GLN	2.7
2	B	101	ARG	2.7
1	A	685	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	270	SER	2.6
1	A	703	LEU	2.5
2	B	223	THR	2.5
3	C	651	ASP	2.5
1	A	645	VAL	2.4
2	B	97	SER	2.4
1	A	512	VAL	2.3
2	B	144	ASP	2.3
1	A	244	ILE	2.3
1	A	692	ILE	2.3
1	A	693	SER	2.3
1	A	41	GLU	2.2
2	B	222	GLU	2.2
1	A	641	GLN	2.2
1	A	697	PHE	2.1
3	C	585	GLN	2.1
1	A	23	ARG	2.1
1	A	444	THR	2.1
2	B	99	GLU	2.1
3	C	625	HIS	2.1
1	A	514	ASP	2.0
2	B	108	VAL	2.0
2	B	185	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	B	404	1/1	0.88	0.07	17,17,17,17	0
4	CA	B	403	1/1	0.96	0.13	20,20,20,20	0
4	CA	A	717	1/1	0.96	0.05	15,15,15,15	0
4	CA	A	720	1/1	0.97	0.11	33,33,33,33	0
4	CA	B	401	1/1	0.97	0.15	17,17,17,17	0
4	CA	B	402	1/1	0.98	0.06	15,15,15,15	0
4	CA	A	715	1/1	0.98	0.05	8,8,8,8	0
4	CA	A	719	1/1	0.98	0.04	11,11,11,11	0
4	CA	A	716	1/1	0.99	0.06	6,6,6,6	0
4	CA	A	718	1/1	0.99	0.04	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.