wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 03:34 PM EDT

PDB ID	:	3O78
Title	:	The structure of Ca2+ Sensor (Case-12)
Authors	:	Leder, L.; Stark, W.; Freuler, F.; Marsh, M.; Meyerhofer, M.; Stettler, T.; Mayr, L.M.; Britanova, O.V.; Strukova, L.A.; Chudakov, D.M.
Deposited on	:	2010-07-30
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

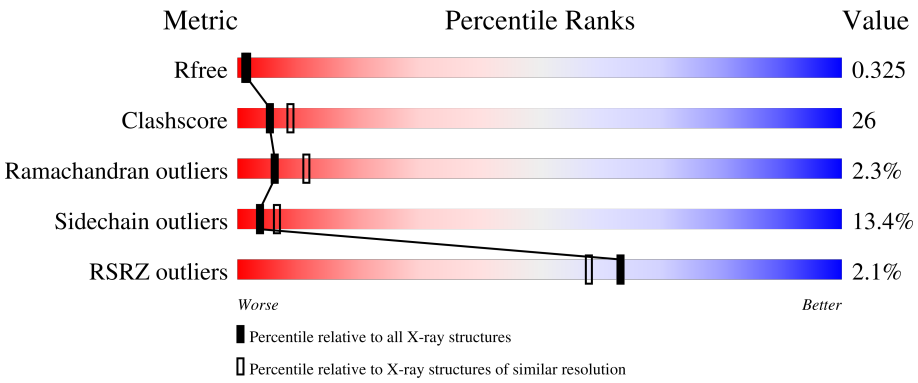
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	415	2% 55% 34% 7% • •
1	B	415	2% 56% 33% 7% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6423 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 Myosin light chain kinase, smooth muscle,Green fluorescent protein,Green fluorescent protein,Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	3168	1982	540	631	15	0	0	0
1	B	401	3170	1986	538	630	16	0	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11799
A	2	PRO	-	expression tag	UNP P11799
A	3	GLY	-	expression tag	UNP P11799
A	4	SER	-	expression tag	UNP P11799
A	5	SER	ALA	engineered mutation	UNP P11799
A	10	ASN	GLN	engineered mutation	UNP P11799
A	25	LEU	SER	engineered mutation	UNP P42212
A	26	GLU	HIS	engineered mutation	UNP P42212
A	41	ALA	VAL	engineered mutation	UNP P42212
A	49	VAL	ILE	engineered mutation	UNP P42212
A	81	PHE	THR	engineered mutation	UNP P42212
A	84	VAL	ALA	engineered mutation	UNP P42212
A	109	LEU	HIS	engineered mutation	UNP P42212
A	116	ASN	LYS	engineered mutation	UNP P42212
A	117	VAL	-	linker	UNP P42212
A	118	ASP	-	linker	UNP P42212
A	119	GLY	-	linker	UNP P42212
A	120	GLY	-	linker	UNP P42212
A	121	SER	-	linker	UNP P42212
A	122	GLY	-	linker	UNP P42212
A	123	GLY	-	linker	UNP P42212
A	124	THR	-	linker	UNP P42212
A	125	GLY	-	linker	UNP P42212
A	170	LEU	PHE	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	PHE	engineered mutation	UNP P42212
A	190	CR2	SER	chromophore	UNP P42212
A	190	CR2	TYR	chromophore	UNP P42212
A	190	CR2	GLY	chromophore	UNP P42212
A	192	LEU	VAL	engineered mutation	UNP P42212
A	193	LYS	GLN	engineered mutation	UNP P42212
A	196	ALA	SER	see sequence details	UNP P42212
A	253	GLY	ASP	engineered mutation	UNP P42212
A	269	THR	TYR	engineered mutation	UNP P42212
A	270	ARG	ASN	engineered mutation	UNP P42212
B	1	GLY	-	expression tag	UNP P11799
B	2	PRO	-	expression tag	UNP P11799
B	3	GLY	-	expression tag	UNP P11799
B	4	SER	-	expression tag	UNP P11799
B	5	SER	ALA	engineered mutation	UNP P11799
B	10	ASN	GLN	engineered mutation	UNP P11799
B	25	LEU	SER	engineered mutation	UNP P42212
B	26	GLU	HIS	engineered mutation	UNP P42212
B	41	ALA	VAL	engineered mutation	UNP P42212
B	49	VAL	ILE	engineered mutation	UNP P42212
B	81	PHE	THR	engineered mutation	UNP P42212
B	84	VAL	ALA	engineered mutation	UNP P42212
B	109	LEU	HIS	engineered mutation	UNP P42212
B	116	ASN	LYS	engineered mutation	UNP P42212
B	117	VAL	-	linker	UNP P42212
B	118	ASP	-	linker	UNP P42212
B	119	GLY	-	linker	UNP P42212
B	120	GLY	-	linker	UNP P42212
B	121	SER	-	linker	UNP P42212
B	122	GLY	-	linker	UNP P42212
B	123	GLY	-	linker	UNP P42212
B	124	THR	-	linker	UNP P42212
B	125	GLY	-	linker	UNP P42212
B	170	LEU	PHE	engineered mutation	UNP P42212
B	188	LEU	PHE	engineered mutation	UNP P42212
B	190	CR2	SER	chromophore	UNP P42212
B	190	CR2	TYR	chromophore	UNP P42212
B	190	CR2	GLY	chromophore	UNP P42212
B	192	LEU	VAL	engineered mutation	UNP P42212
B	193	LYS	GLN	engineered mutation	UNP P42212
B	196	ALA	SER	see sequence details	UNP P42212
B	253	GLY	ASP	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	269	THR	TYR	engineered mutation	UNP P42212
B	270	ARG	ASN	engineered mutation	UNP P42212

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

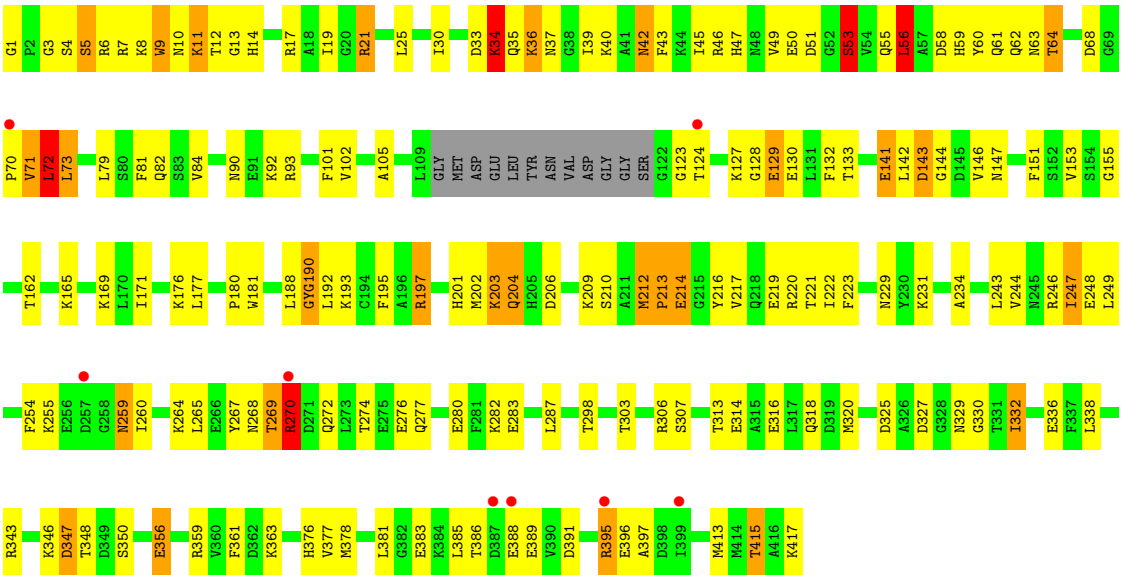
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	41	41	41	0	0
			Total	O		
3	B	36	36	36	0	0

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.

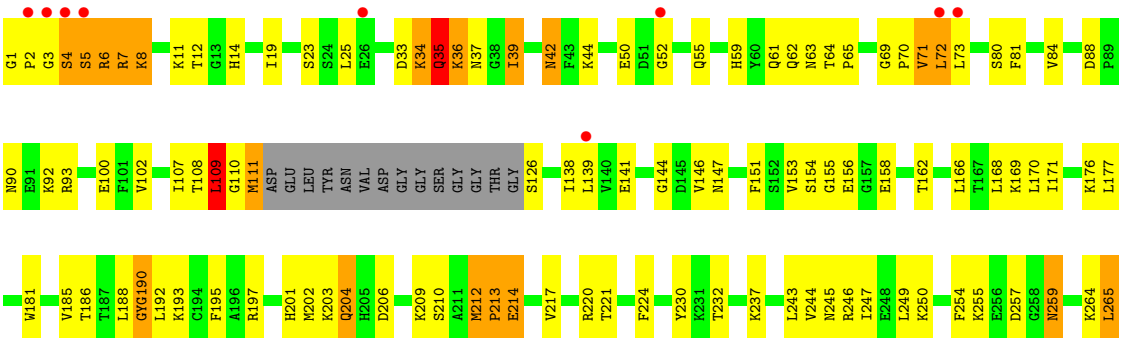
• Molecule 1: Myosin light chain kinase, smooth muscle,Green fluorescent protein,Green fluorescent protein,Calmodulin-1

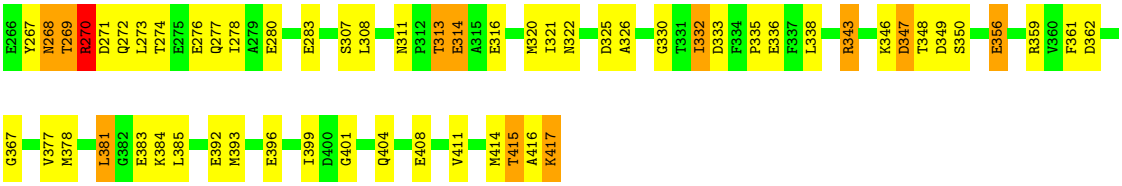
Chain A:



• Molecule 1: Myosin light chain kinase, smooth muscle,Green fluorescent protein,Green fluorescent protein,Calmodulin-1

Chain B:




E266 Y267 N268 T269 R270 D271 Q272 L273 T274 E275 E276 Q277 I278 A279 E280
E283
S307 L308
N311 P312 T313 E314 A315 E316
M320 I321 N322
D325 A326
G330 T331 I332 D333 F334 P335 E336 F337 L338
R343
K346 D347 T348 D349 S350
E356
R359 V360 F361 D362
G367
V377 M378
L381 G382 E383 K384 L385
E392 M393
E396
I399 D400 G401
Q404
E408
V411
M414 T415 A416 K417

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.37Å 101.64Å 82.21Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	50.83 – 2.60 50.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.83-2.60) 99.8 (50.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.316 0.261 , 0.325	Depositor DCC
R_{free} test set	1174 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 20.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.052 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6423	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: CR2, 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	1.14	5/3203 (0.2%)	0.93	7/4311 (0.2%)
1	B	0.82	0/3205	0.86	3/4312 (0.1%)
All	All	0.99	5/6408 (0.1%)	0.89	10/8623 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	TRP	CB-CG	-6.14	1.39	1.50
1	A	219	GLU	CG-CD	-5.18	1.44	1.51
1	A	219	GLU	CD-OE2	-5.16	1.20	1.25
1	A	21	ARG	CZ-NH2	-5.04	1.26	1.33
1	A	132	PHE	CD1-CE1	-5.03	1.29	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	ARG	NE-CZ-NH1	-11.03	114.79	120.30
1	A	270	ARG	NE-CZ-NH2	10.21	125.41	120.30
1	A	395	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	B	270	ARG	NE-CZ-NH1	6.63	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	395	ARG	NE-CZ-NH1	6.20	123.40	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	MET	Peptide
1	A	415	THR	Peptide
1	B	212	MET	Peptide
1	B	268	ASN	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	3168	0	3061	169	0
1	B	3170	0	3080	192	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	41	0	0	23	0
3	B	36	0	0	21	0
All	All	6423	0	6141	328	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 26.

The worst 5 of 328 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:A:6:ARG:NH1	1:B:396:GLU:OE2	1.80	1.14
1:B:1:GLY:N	1:B:2:PRO:HD2	1.63	1.13
1:B:35:GLN:HB2	3:B:448:HOH:O	1.51	1.10
1:B:6:ARG:HG2	1:B:7:ARG:H	1.13	1.07
1:B:108:THR:O	1:B:109:LEU:HB3	1.54	1.05

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ASN:OD1	1:B:50:GLU:OE1[1_455]	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	396/415 (95%)	364 (92%)	23 (6%)	9 (2%)	6 11
1	B	394/415 (95%)	357 (91%)	28 (7%)	9 (2%)	6 11
All	All	790/830 (95%)	721 (91%)	51 (6%)	18 (2%)	6 11

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
1	A	124	THR
1	A	213	PRO
1	B	4	SER
1	B	6	ARG

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	339/351 (97%)	295 (87%)	44 (13%)	4 7
1	B	342/351 (97%)	295 (86%)	47 (14%)	3 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	681/702 (97%)	590 (87%)	91 (13%)	4 6

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	259	ASN
1	B	93	ARG
1	B	197	ARG
1	B	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	277	GLN
1	B	48	ASN
1	B	263	HIS
1	B	42	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CR2	A	190	1	20,20,21	3.69	6 (30%)	25,27,29	3.24	7 (28%)
1	CR2	B	190	1	20,20,21	3.59	4 (20%)	25,27,29	4.46	7 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	A	190	1	-	1/6/25/26	0/2/2/2
1	CR2	B	190	1	-	1/6/25/26	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	CR2	CB2-CA2	14.56	1.47	1.35
1	B	190	CR2	CB2-CA2	14.34	1.47	1.35
1	A	190	CR2	CA2-C2	-4.22	1.44	1.48
1	B	190	CR2	CA2-C2	-4.08	1.44	1.48
1	B	190	CR2	C1-N2	3.82	1.39	1.32

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	CR2	CA2-C2-N3	16.62	111.23	103.37
1	B	190	CR2	O2-C2-CA2	-10.74	124.93	130.96
1	A	190	CR2	O2-C2-CA2	-9.71	125.51	130.96
1	A	190	CR2	CA2-C2-N3	9.68	107.95	103.37
1	B	190	CR2	C2-N3-C1	-7.32	104.41	107.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	190	CR2	C3-CA3-N3-C2
1	B	190	CR2	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	190	CR2	2	0
1	B	190	CR2	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	188:LEU	C	190:CR2	N1	1.20

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	402/415 (96%)	-0.03	8 (1%)	65	60	2, 19, 35, 51	0
1	B	400/415 (96%)	0.02	9 (2%)	60	54	6, 24, 43, 55	0
All	All	802/830 (96%)	-0.00	17 (2%)	63	58	2, 22, 40, 55	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	SER	4.5
1	A	270	ARG	4.0
1	A	399	ILE	3.3
1	B	5	SER	3.2
1	B	72	LEU	3.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CR2	B	190	19/20	0.91	0.20	19,28,32,32	0
1	CR2	A	190	19/20	0.93	0.14	2,2,2,5	0

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	A	502	1/1	0.76	0.06	47,47,47,47	0
2	CA	A	503	1/1	0.83	0.13	32,32,32,32	0
2	CA	A	504	1/1	0.89	0.06	39,39,39,39	0
2	CA	B	504	1/1	0.92	0.09	30,30,30,30	0
2	CA	B	502	1/1	0.95	0.08	18,18,18,18	0
2	CA	A	501	1/1	0.97	0.09	20,20,20,20	0
2	CA	B	501	1/1	0.97	0.12	18,18,18,18	0
2	CA	B	503	1/1	0.99	0.07	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.