



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 08:25 PM UTC

PDB ID : 5DJ4 / pdb_00005dj4
Title : Leucine-bound Sestrin2 from Homo sapiens
Authors : Saxton, R.A.; Knockenhauer, K.E.; Schwartz, T.U.
Deposited on : 2015-09-01
Resolution : 2.70 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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

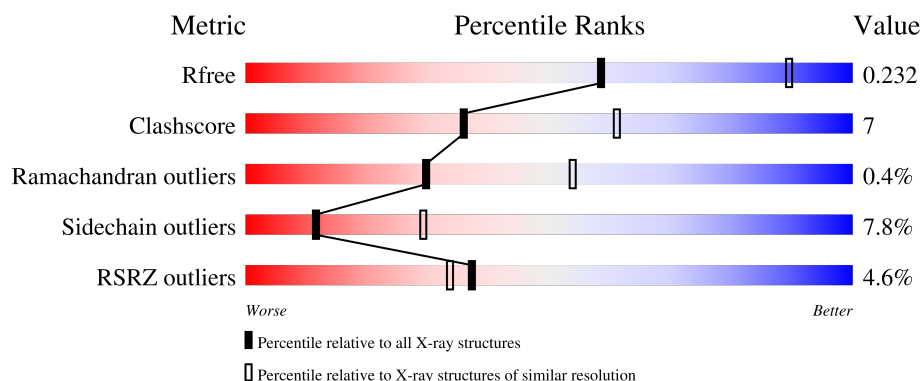
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. 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	480	3% 62% 12% • 24%
1	B	480	3% 62% 13% • 24%
1	C	480	3% 58% 16% • 24%
1	D	480	4% 58% 16% • 24%
1	E	480	4% 60% 15% • 24%

2 Entry composition [i](#)

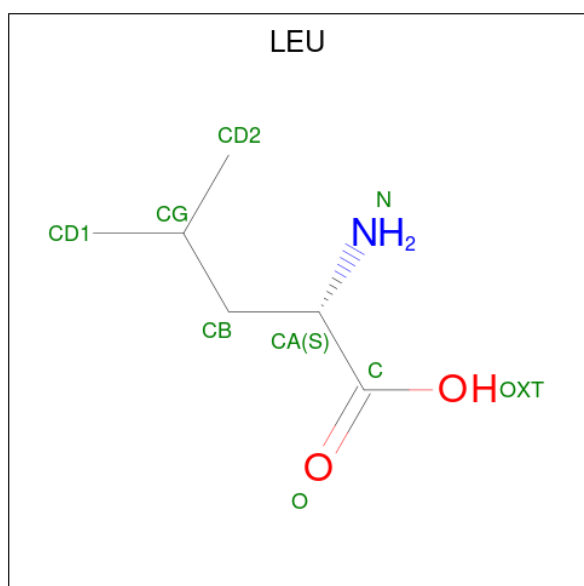
There are 3 unique types of molecules in this entry. The entry contains 14911 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sestrin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2962	1897	513	534	18			
1	B	365	Total	C	N	O	S	0	0	0
			2936	1883	507	528	18			
1	C	364	Total	C	N	O	S	0	0	0
			2952	1892	511	531	18			
1	D	364	Total	C	N	O	S	0	0	0
			2945	1888	508	531	18			
1	E	365	Total	C	N	O	S	0	0	0
			2956	1894	512	532	18			

- Molecule 2 is LEUCINE (CCD ID: LEU) (formula: C₆H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			9	6	1	2		
2	C	1	Total	C	N	O	0	0
			9	6	1	2		
2	D	1	Total	C	N	O	0	0
			9	6	1	2		
2	E	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	24	Total	O	0	0
			24	24		
3	C	16	Total	O	0	0
			16	16		
3	D	17	Total	O	0	0
			17	17		
3	E	21	Total	O	0	0
			21	21		

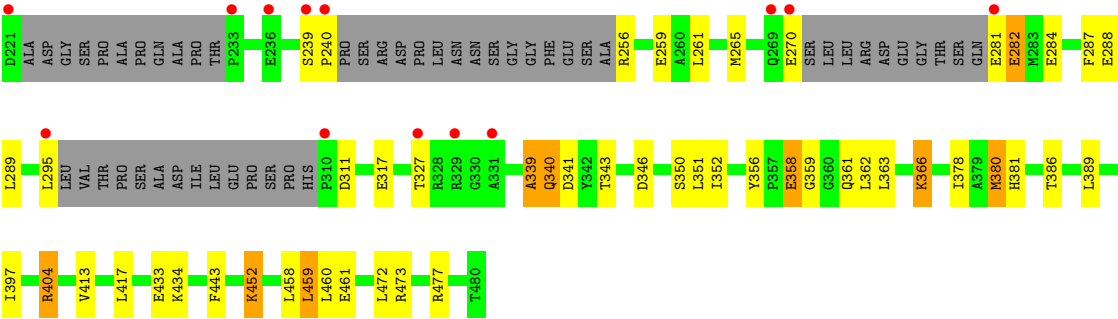
Chain C:

Chain D:

Residue	Category
A379	Green
M390	Green
D385	Green
T386	Green
S387	Orange
I393	Green
I397	Green
D409	Green
L417	Green
V428	Green
A429	Green
C430	Green
Y431	Green
P432	Green
E433	Green
F443	Green
R448	Green
K452	Green
M456	Green
L457	Green
L458	Green
L459	Green
L460	Green
L472	Green
T480	Green
Q266	Green
Q267	Green
L268	Green
Q269	Green
GLU	Green
SER	Green
LEU	Green
LEU	Green
ARG	Green
ASP	Green
GLY	Green
THR	Green
SER	Green
GLN	Green
E281	Green
E282	Green
M283	Orange
E284	Green
S285	Green
R286	Green
L295	Green
LEU	Green
VAL	Green
THR	Green
PRO	Green
SER	Green
ALA	Green
ASP	Green
ILE	Green
LEU	Green
GLU	Green
PRO	Green
SER	Green
GLY	Green
LEU	Green
PRO	Green
E236	Green
Q237	Green
S238	Green
S239	Green
P240	Green
PRO	Green
P310	Green
D311	Green
D318	Green
P319	Green
T320	Green
E324	Orange
T327	Green
R328	Green
R329	Green
R338	Green
A339	Green
Q340	Green
L351	Green
L362	Green
K366	Orange
K183	Green
T184	Green
G185	Green
E186	Green
L191	Green
L194	Green
I195	Green
L201	Green
L207	Green
L216	Green
L217	Green
G220	Green
D221	Green
ALA	Green
ASP	Green
GLY	Green
SER	Green
PRO	Green
ALA	Green
PRO	Green
ALA	Green
THR	Green
P233	Green
E236	Green
Q237	Green
S238	Green
S239	Green
P240	Green
PRO	Green
P310	Green
D311	Green
D318	Green
P319	Green
T320	Green
E324	Orange
T327	Green
R328	Green
R329	Green
R338	Green
A339	Green
Q340	Green
L351	Green
L362	Green
K366	Orange
K183	Green
T184	Green
G185	Green
E186	Green
L191	Green
L194	Green
I195	Green
L201	Green
L207	Green
L216	Green
L217	Green
G220	Green
D221	Green
ALA	Green
ASP	Green
GLY	Green
SER	Green
PRO	Green
ALA	Green
PRO	Green
ALA	Green
THR	Green
P233	Green
E236	Green
Q237	Green
S238	Green
S239	Green
P240	Green
PRO	Green
P310	Green
D311	Green
D318	Green
P319	Green
T320	Green
E324	Orange
T327	Green
R328	Green
R329	Green
R338	Green
A339	Green
Q340	Green
L351	Green
L362	Green
K366	Orange
K183	Green
T184	Green
G185	Green
E186	Green
L191	Green
L194	Green
I195	Green
L201	Green
L207	Green
L216	Green
L217	Green
G220	Green
D221	Green
ALA	Green
ASP	Green
GLY	Green
SER	Green
PRO	Green
ALA	Green
PRO	Green
ALA	Green
THR	Green
P233	Green
E236	Green
Q237	Green
S238	Green
S239	Green
P240	Green
PRO	Green
P310	Green
D311	Green
D318	Green
P319	Green
T320	Green
E324	Orange
T327	Green
R328	Green
R329	Green
R338	Green
A339	Green
Q340	Green
L351	Green
L362	Green
K366	Orange
K183	Green
T184	Green
G185	Green
E186	Green
L191	Green
L194	Green
I195	Green
L201	Green
L207	Green
L216	Green
L217	Green
G220	Green
D221	Green
ALA	

Chain E:

Residue Type	Count
MET	1
ILE	1
VAL	1
ALA	1
ASP	1
SER	1
GLU	1
CYS	1
ARG	1
ALA	1
LEU	1
LYS	1
ASP	1
TYR	1
LEU	1
ARG	1
PHE	1
ALA	1
PRO	1
GLY	1
VAL	1
GLY	1
ASP	1
SER	1
GLY	1
PRO	1
GLY	1
GLU	1
GLN	1
ARG	1
GLU	1
SER	1
ARG	1
ALA	1
ARG	1
GLY	1
PRO	1
ARG	1
GLY	1
PRO	1
SER	1
PHE	1
THR	1
LEU	1
VAL	1
GLU	1
GLY	1
VAL	1
LEU	1
ARG	1
GLU	1
GLY	1
ALA	1
GLY	1
SER	1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	293.03Å 293.03Å 293.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.66 – 2.70 92.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.66-2.70) 92.4 (92.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.196 , 0.223 0.209 , 0.232	Depositor DCC
R_{free} test set	2001 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14911	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.75	0/3039	0.83	2/4115 (0.0%)
1	B	0.77	0/3013	0.85	2/4083 (0.0%)
1	C	0.62	0/3029	0.78	2/4101 (0.0%)
1	D	0.62	0/3022	0.79	4/4093 (0.1%)
1	E	0.66	0/3033	0.81	3/4107 (0.1%)
All	All	0.69	0/15136	0.81	13/20499 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	282	GLU	N-CA-C	-6.62	105.20	113.28
1	D	86	HIS	CA-C-N	6.31	126.79	119.47
1	D	86	HIS	C-N-CA	6.31	126.79	119.47
1	E	86	HIS	CA-C-N	6.24	126.14	119.28
1	E	86	HIS	C-N-CA	6.24	126.14	119.28

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	2962	0	2875	38	0
1	B	2936	0	2839	33	0
1	C	2952	0	2870	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2945	0	2857	60	0
1	E	2956	0	2870	40	0
2	A	9	0	10	0	0
2	B	9	0	10	0	0
2	C	9	0	10	0	0
2	D	9	0	10	0	0
2	E	9	0	10	0	0
3	A	37	0	0	5	0
3	B	24	0	0	4	0
3	C	16	0	0	2	0
3	D	17	0	0	3	0
3	E	21	0	0	3	0
All	All	14911	0	14361	214	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.

The worst 5 of 214 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:D:338:ARG:HG2	1:D:340:GLN:NE2	1.32	1.39
1:D:338:ARG:CD	1:D:340:GLN:HE22	1.46	1.28
1:D:338:ARG:CG	1:D:340:GLN:NE2	1.99	1.26
1:D:179:GLN:NE2	1:D:183:LYS:HG3	1.59	1.15
1:D:97:HIS:ND1	3:D:601:HOH:O	1.93	1.02

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	356/480 (74%)	346 (97%)	9 (2%)	1 (0%)	36	60
1	B	355/480 (74%)	346 (98%)	9 (2%)	0	100	100
1	C	354/480 (74%)	342 (97%)	10 (3%)	2 (1%)	21	44
1	D	354/480 (74%)	344 (97%)	8 (2%)	2 (1%)	21	44
1	E	355/480 (74%)	343 (97%)	10 (3%)	2 (1%)	21	44
All	All	1774/2400 (74%)	1721 (97%)	46 (3%)	7 (0%)	30	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	339	ALA
1	E	340	GLN
1	A	379	ALA
1	C	268	LEU
1	D	184	THR

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	313/410 (76%)	291 (93%)	22 (7%)	14	34
1	B	308/410 (75%)	289 (94%)	19 (6%)	16	39
1	C	312/410 (76%)	290 (93%)	22 (7%)	13	33
1	D	311/410 (76%)	286 (92%)	25 (8%)	11	28
1	E	312/410 (76%)	283 (91%)	29 (9%)	8	21
All	All	1556/2050 (76%)	1439 (92%)	117 (8%)	11	31

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	434	LYS
1	E	404	ARG
1	D	237	GLN

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Mol	Chain	Res	Type
1	E	389	LEU
1	E	311	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	381	HIS
1	D	179	GLN
1	E	441	ASN
1	E	97	HIS
1	E	124	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands 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	$\# Z > 2$
2	LEU	D	501	-	6,8,8	1.15	1 (16%)	5,10,10	1.23	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LEU	E	501	-	6,8,8	1.08	1 (16%)	5,10,10	1.69	1 (20%)
2	LEU	A	501	-	6,8,8	1.17	1 (16%)	5,10,10	1.46	1 (20%)
2	LEU	C	501	-	6,8,8	1.05	1 (16%)	5,10,10	1.45	1 (20%)
2	LEU	B	501	-	6,8,8	1.03	1 (16%)	5,10,10	1.43	1 (20%)

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
2	LEU	D	501	-	-	3/8/8/8	-
2	LEU	E	501	-	-	2/8/8/8	-
2	LEU	A	501	-	-	3/8/8/8	-
2	LEU	C	501	-	-	3/8/8/8	-
2	LEU	B	501	-	-	2/8/8/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	LEU	OXT-C	-2.83	1.21	1.30
2	D	501	LEU	OXT-C	-2.76	1.21	1.30
2	E	501	LEU	OXT-C	-2.57	1.22	1.30
2	C	501	LEU	OXT-C	-2.44	1.22	1.30
2	B	501	LEU	OXT-C	-2.42	1.22	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	LEU	OXT-C-O	-3.73	115.63	124.08
2	A	501	LEU	OXT-C-O	-3.26	116.68	124.08
2	B	501	LEU	OXT-C-O	-3.17	116.89	124.08
2	C	501	LEU	OXT-C-O	-3.17	116.89	124.08
2	D	501	LEU	OXT-C-O	-2.68	118.00	124.08

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LEU	N-CA-CB-CG
2	B	501	LEU	N-CA-CB-CG
2	B	501	LEU	C-CA-CB-CG
2	D	501	LEU	N-CA-CB-CG
2	D	501	LEU	C-CA-CB-CG

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	366/480 (76%)	-0.02	14 (3%) 44 40	36, 48, 84, 105	0
1	B	365/480 (76%)	-0.08	16 (4%) 39 35	34, 46, 82, 101	0
1	C	364/480 (75%)	0.08	16 (4%) 39 35	42, 59, 91, 110	0
1	D	364/480 (75%)	0.07	20 (5%) 30 27	38, 57, 94, 109	0
1	E	365/480 (76%)	0.06	17 (4%) 36 33	41, 57, 89, 102	0
All	All	1824/2400 (76%)	0.02	83 (4%) 37 34	34, 54, 90, 110	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	240	PRO	7.6
1	C	240	PRO	6.4
1	E	310	PRO	6.2
1	D	310	PRO	6.1
1	C	281	GLU	5.9

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 oligosaccharides 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	LEU	E	501	9/9	0.94	0.12	46,50,51,51	0
2	LEU	C	501	9/9	0.97	0.08	50,53,56,56	0
2	LEU	D	501	9/9	0.97	0.09	47,51,52,54	0
2	LEU	B	501	9/9	0.97	0.10	43,46,48,52	0
2	LEU	A	501	9/9	0.98	0.08	46,50,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.