



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:26 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 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	:	4-5-2 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

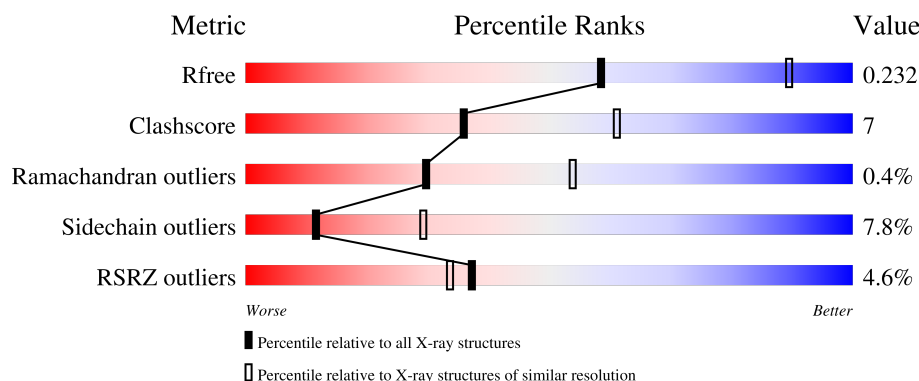
1 Overall quality at a glance

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](#)

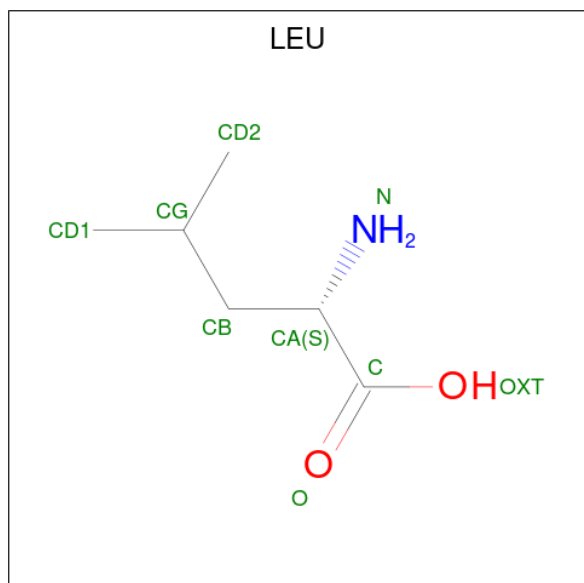
There are 3 unique types of molecules in this entry. The entry contains 14911 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

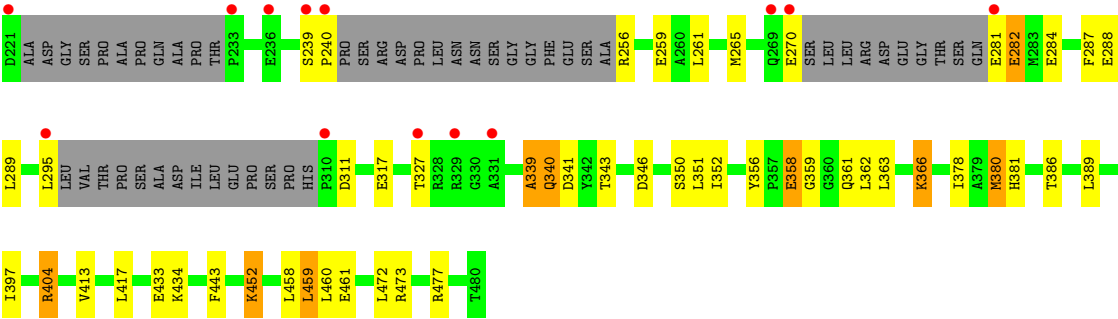
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	24	Total	O	0	0
			24	24		
3	C	16	Total	O	0	0
			16	16		
3	D	17	Total	O	0	0
			17	17		
3	E	21	Total	O	0	0
			21	21		

- Molecule 1: Sestrin-2



Chain E:

LEU
GLU
GLN
HIS
HIS
G66
S72
H86
S92
L99
S109
I117
R122
S126
V129
A134
Q138
E144
R151
E154
K155
L156
R157
I162
L166
I173
T174
K175
E176
H177
L181
L182
K183
T184
G185
E186
L191
L194
I195



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.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	C	86	HIS	CA-C-N	6.20	126.39	119.32
1	C	86	HIS	C-N-CA	6.20	126.39	119.32
1	B	318	ASP	CA-C-N	5.89	125.51	119.56
1	B	318	ASP	C-N-CA	5.89	125.51	119.56
1	A	86	HIS	CA-C-N	5.54	125.89	119.47
1	A	86	HIS	C-N-CA	5.54	125.89	119.47
1	D	318	ASP	CA-C-N	5.24	124.93	119.64
1	D	318	ASP	C-N-CA	5.24	124.93	119.64

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
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.

All (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
1:D:179:GLN:HE21	1:D:183:LYS:HG3	1.28	0.96
1:D:338:ARG:CG	1:D:340:GLN:HE22	1.64	0.96
1:D:179:GLN:NE2	1:D:183:LYS:CG	2.31	0.94
1:A:99:LEU:HD22	1:A:362:LEU:HD12	1.52	0.91
1:E:339:ALA:O	1:E:341:ASP:N	2.05	0.89
1:D:338:ARG:CD	1:D:340:GLN:NE2	2.28	0.88
1:D:338:ARG:HD2	1:D:340:GLN:HE22	1.34	0.88
1:D:338:ARG:HG2	1:D:340:GLN:HE21	1.02	0.84
1:E:99:LEU:HD22	1:E:362:LEU:HD12	1.60	0.82
1:B:97:HIS:ND1	3:B:602:HOH:O	2.13	0.81
1:D:179:GLN:HE22	1:D:183:LYS:HG3	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LEU:HD22	1:B:362:LEU:HD12	1.66	0.77
1:D:179:GLN:HE21	1:D:183:LYS:CG	1.94	0.76
1:A:162:ILE:O	1:A:166:LEU:HG	1.85	0.76
1:D:174:THR:HG22	1:D:176:GLU:H	1.51	0.74
1:C:338:ARG:NH2	1:C:406:ASP:OD2	2.21	0.74
1:B:92:SER:HB3	1:B:366:LYS:HG2	1.69	0.74
1:B:338:ARG:HH11	1:B:340:GLN:HB2	1.52	0.74
1:E:144:GLU:OE2	1:E:151:ARG:NH2	2.22	0.73
1:B:343:THR:OG1	1:B:346:ASP:OD1	2.05	0.73
1:E:162:ILE:O	1:E:166:LEU:HG	1.90	0.72
1:E:265:MET:HE1	1:E:386:THR:HA	1.70	0.72
1:A:181:LEU:HD13	1:A:194:LEU:HD11	1.72	0.72
1:A:323:TYR:O	1:A:332:GLN:NE2	2.23	0.70
1:A:66:GLY:N	3:A:602:HOH:O	2.23	0.70
1:E:181:LEU:HD13	1:E:194:LEU:HD11	1.74	0.70
1:A:412:GLU:OE2	3:A:601:HOH:O	2.09	0.69
1:E:351:LEU:HD23	1:E:472:LEU:HD22	1.75	0.69
1:D:338:ARG:CG	1:D:340:GLN:HE21	1.83	0.68
1:D:379:ALA:O	1:D:448:ARG:NH1	2.26	0.68
1:E:240:PRO:O	3:E:601:HOH:O	2.12	0.67
1:E:181:LEU:HD13	1:E:194:LEU:CD1	2.24	0.67
1:A:134:ALA:O	1:A:138:GLN:HG2	1.95	0.66
1:B:217:LEU:HD21	1:B:236:GLU:HB3	1.77	0.66
1:C:66:GLY:N	3:C:603:HOH:O	2.27	0.66
1:C:162:ILE:O	1:C:166:LEU:HG	1.95	0.66
1:C:134:ALA:O	1:C:138:GLN:HG2	1.96	0.65
1:D:92:SER:HB3	1:D:366:LYS:HG2	1.80	0.64
1:A:388:VAL:HG12	1:A:416:LEU:CD1	2.28	0.64
1:A:351:LEU:HD23	1:A:472:LEU:HD22	1.80	0.64
1:A:413:VAL:HG13	1:A:417:LEU:HD22	1.80	0.63
1:B:162:ILE:O	1:B:166:LEU:HG	1.98	0.63
1:C:99:LEU:HD22	1:C:362:LEU:HD12	1.81	0.63
1:E:443:PHE:O	1:E:452:LYS:NZ	2.32	0.63
1:A:388:VAL:HG12	1:A:416:LEU:HD11	1.80	0.63
1:D:99:LEU:HD22	1:D:362:LEU:HD12	1.80	0.62
1:B:134:ALA:O	1:B:138:GLN:HG2	2.00	0.62
1:D:265:MET:HE1	1:D:386:THR:HA	1.82	0.62
1:E:134:ALA:O	1:E:138:GLN:HG2	1.99	0.61
1:B:338:ARG:HG3	1:B:404:ARG:HH21	1.65	0.61
1:D:286:ARG:NH1	1:D:409:ASP:OD1	2.34	0.61
1:D:162:ILE:O	1:D:166:LEU:HG	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:THR:OG1	1:E:346:ASP:OD1	2.19	0.60
1:E:117:ILE:HG23	1:E:129:VAL:HG13	1.84	0.60
1:E:413:VAL:HG13	1:E:417:LEU:HD22	1.84	0.60
1:E:281:GLU:OE1	1:E:281:GLU:N	2.35	0.59
1:C:388:VAL:HG12	1:C:391:ARG:HH21	1.68	0.59
1:B:89:TYR:CD2	1:B:457:LEU:HD22	2.37	0.59
1:A:217:LEU:HD21	1:A:236:GLU:HB3	1.83	0.59
1:A:92:SER:HB3	1:A:366:LYS:HG2	1.83	0.59
1:D:134:ALA:O	1:D:138:GLN:HG2	2.03	0.59
1:D:351:LEU:HD23	1:D:472:LEU:HB3	1.83	0.58
1:B:351:LEU:HD23	1:B:472:LEU:HD22	1.85	0.58
1:E:287:PHE:CG	1:E:404:ARG:HG3	2.39	0.57
1:D:181:LEU:HD13	1:D:194:LEU:HD11	1.86	0.57
1:E:359:GLY:O	1:E:363:LEU:HG	2.04	0.57
1:D:181:LEU:HD13	1:D:194:LEU:CD1	2.35	0.57
1:D:338:ARG:NE	1:D:340:GLN:HE22	1.98	0.57
1:E:366:LYS:HD2	1:E:461:GLU:OE2	2.05	0.57
1:D:338:ARG:HD2	1:D:340:GLN:NE2	2.11	0.56
1:B:89:TYR:CE2	1:B:457:LEU:HD22	2.39	0.56
1:A:281:GLU:N	3:A:606:HOH:O	2.38	0.56
1:C:265:MET:HE1	1:C:386:THR:HA	1.87	0.56
1:B:186:GLU:N	3:B:601:HOH:O	2.39	0.55
1:C:324:GLU:OE1	1:C:332:GLN:N	2.38	0.55
1:E:166:LEU:HD23	1:E:173:ILE:HD11	1.88	0.55
1:C:284:GLU:O	1:C:288:GLU:HG2	2.07	0.55
1:B:325:ASP:O	3:B:603:HOH:O	2.18	0.55
1:D:351:LEU:HD23	1:D:472:LEU:HD22	1.89	0.55
1:E:99:LEU:HD13	1:E:358:GLU:HG2	1.90	0.54
1:C:166:LEU:HD23	1:C:173:ILE:CD1	2.38	0.54
1:C:351:LEU:HD23	1:C:472:LEU:HD22	1.88	0.54
1:D:87:PRO:O	1:D:91:THR:HG23	2.07	0.54
1:D:324:GLU:HB2	1:D:431:TYR:OH	2.08	0.54
1:E:284:GLU:O	1:E:288:GLU:HG2	2.07	0.54
1:D:149:LEU:HD22	1:D:157:ARG:HG2	1.89	0.54
1:C:166:LEU:HD23	1:C:173:ILE:HD11	1.89	0.54
1:B:413:VAL:HG13	1:B:417:LEU:HD22	1.88	0.53
1:A:99:LEU:HD22	1:A:362:LEU:CD1	2.32	0.53
1:C:325:ASP:OD1	1:C:327:THR:HG22	2.10	0.52
1:B:119:ALA:HB2	1:B:201:LEU:HD23	1.91	0.52
1:A:181:LEU:HD13	1:A:194:LEU:CD1	2.38	0.51
1:C:267:GLN:O	1:C:270:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:HIS:ND1	3:C:601:HOH:O	1.99	0.51
1:C:380:MET:HE2	1:C:381:HIS:CE1	2.47	0.50
1:D:166:LEU:HD23	1:D:173:ILE:CD1	2.41	0.50
1:D:179:GLN:NE2	1:D:183:LYS:HG2	2.25	0.50
1:A:166:LEU:HD23	1:A:173:ILE:CD1	2.42	0.50
1:A:476:THR:O	1:A:480:THR:HG23	2.11	0.50
1:C:443:PHE:O	1:C:452:LYS:NZ	2.45	0.49
1:B:233:PRO:HB2	1:B:234:PRO:HD3	1.93	0.49
1:E:174:THR:HG23	1:E:176:GLU:H	1.77	0.49
1:B:181:LEU:HD13	1:B:194:LEU:HD11	1.95	0.49
1:B:428:VAL:O	1:B:432:PRO:HG3	2.13	0.49
1:A:166:LEU:HD23	1:A:173:ILE:HD11	1.95	0.49
1:D:79:LEU:HA	1:D:216:ILE:HD13	1.94	0.49
1:A:325:ASP:OD1	1:A:327:THR:HG22	2.13	0.49
1:A:454:HIS:HE1	3:A:605:HOH:O	1.95	0.48
1:E:287:PHE:CD1	1:E:404:ARG:HG3	2.48	0.48
1:B:476:THR:O	1:B:480:THR:HG23	2.14	0.48
1:C:444:TRP:HB3	1:C:447:PHE:HB2	1.96	0.48
1:D:393:ILE:O	1:D:397:ILE:HD12	2.13	0.48
1:E:154:GLU:HA	1:E:157:ARG:HE	1.77	0.48
1:E:380:MET:HE2	1:E:381:HIS:CE1	2.49	0.48
1:E:92:SER:HB3	1:E:366:LYS:HG3	1.95	0.47
1:A:174:THR:HG23	1:A:176:GLU:H	1.78	0.47
1:E:281:GLU:HG2	1:E:282:GLU:H	1.79	0.47
1:A:388:VAL:CG1	1:A:416:LEU:HD11	2.43	0.47
1:E:122:ARG:NH1	3:E:602:HOH:O	2.24	0.47
1:B:284:GLU:O	1:B:288:GLU:HG2	2.15	0.47
1:D:92:SER:HB3	1:D:366:LYS:CG	2.45	0.47
1:D:385:ASP:OD1	1:D:387:SER:OG	2.31	0.47
1:C:397:ILE:HD13	1:C:459:LEU:HA	1.96	0.47
1:A:174:THR:CG2	1:A:176:GLU:H	2.28	0.47
1:B:433:GLU:H	1:B:433:GLU:CD	2.22	0.46
1:D:117:ILE:HG23	1:D:129:VAL:HG13	1.97	0.46
1:A:284:GLU:O	1:A:288:GLU:HG2	2.14	0.46
1:C:124:GLN:HE22	1:C:313:LEU:HD23	1.81	0.46
1:E:151:ARG:NH1	3:E:606:HOH:O	2.47	0.46
1:E:166:LEU:HD23	1:E:173:ILE:CD1	2.45	0.46
1:B:184:THR:HG22	1:B:185:GLY:N	2.30	0.46
1:D:179:GLN:HE22	1:D:183:LYS:CG	2.16	0.46
1:E:256:ARG:CZ	1:E:380:MET:HE3	2.45	0.46
1:C:480:THR:OXT	1:C:480:THR:OG1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.75	0.45
1:A:378:ILE:HG22	1:A:381:HIS:HB2	1.99	0.45
1:E:397:ILE:HD13	1:E:459:LEU:HA	1.98	0.45
1:B:379:ALA:O	1:B:448:ARG:NH1	2.49	0.45
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.81	0.45
1:D:133:MET:HG2	1:D:146:LEU:HD22	1.99	0.45
1:C:261:LEU:O	1:C:265:MET:HG3	2.16	0.45
1:C:133:MET:HG2	1:C:146:LEU:HD22	1.99	0.45
1:D:119:ALA:HB2	1:D:201:LEU:HD23	1.99	0.45
1:E:181:LEU:HD13	1:E:194:LEU:HD13	1.99	0.45
1:C:211:VAL:HG13	1:C:216:ILE:HB	1.97	0.45
1:D:429:ALA:HB2	1:D:459:LEU:HD13	1.98	0.45
1:A:186:GLU:N	3:A:603:HOH:O	2.49	0.45
1:B:397:ILE:HD13	1:B:459:LEU:HA	1.99	0.45
1:D:166:LEU:HD23	1:D:173:ILE:HD11	1.99	0.45
1:B:174:THR:CG2	1:B:176:GLU:H	2.30	0.44
1:A:443:PHE:CZ	1:A:452:LYS:HG3	2.52	0.44
1:C:92:SER:HB3	1:C:366:LYS:HG2	1.99	0.44
1:D:269:GLN:N	3:D:608:HOH:O	2.51	0.44
1:A:69:ALA:O	1:A:73:SER:HB3	2.18	0.44
1:C:285:SER:O	1:C:289:LEU:HG	2.18	0.44
1:D:456:ASN:OD1	3:D:602:HOH:O	2.21	0.44
1:B:325:ASP:OD1	1:B:327:THR:HB	2.18	0.44
1:C:183:LYS:HB3	1:C:183:LYS:HE2	1.72	0.44
1:D:99:LEU:CD2	1:D:362:LEU:HD12	2.48	0.43
1:C:170:PRO:HB2	1:C:470:TYR:CD2	2.53	0.43
1:D:397:ILE:HD13	1:D:459:LEU:HA	1.99	0.43
1:A:479:MET:HA	1:A:479:MET:HE2	2.00	0.43
1:B:79:LEU:HA	1:B:216:ILE:HD13	1.99	0.43
1:E:174:THR:HG22	1:E:177:HIS:ND1	2.33	0.43
1:A:85:LEU:HD12	1:A:453:VAL:HG21	1.99	0.43
1:C:89:TYR:CE2	1:C:457:LEU:HD22	2.53	0.43
1:D:283:MET:HE3	1:D:283:MET:HB3	1.86	0.43
1:D:221:ASP:N	1:D:221:ASP:OD1	2.51	0.43
1:B:187:HIS:N	3:B:601:HOH:O	1.81	0.43
1:A:85:LEU:CD1	1:A:453:VAL:HG21	2.49	0.42
1:A:265:MET:O	1:A:269:GLN:HG3	2.18	0.42
1:C:267:GLN:O	1:C:269:GLN:N	2.52	0.42
1:C:475:ILE:O	1:C:479:MET:HG3	2.19	0.42
1:D:174:THR:HG22	1:D:176:GLU:HB2	2.01	0.42
1:B:429:ALA:HB2	1:B:459:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:LEU:O	1:C:195:ILE:HG12	2.20	0.42
1:D:257:ASP:N	1:D:257:ASP:OD1	2.52	0.42
1:C:413:VAL:O	1:C:417:LEU:HB2	2.20	0.42
1:A:380:MET:HE2	1:A:380:MET:HB2	1.74	0.42
1:C:149:LEU:HD22	1:C:157:ARG:HG3	2.01	0.42
1:D:443:PHE:CZ	1:D:452:LYS:HG2	2.55	0.42
1:E:473:ARG:HD2	1:E:477:ARG:NH2	2.35	0.42
1:B:291:LYS:HB3	1:B:291:LYS:HE3	1.94	0.41
1:D:428:VAL:O	1:D:432:PRO:HG3	2.20	0.41
1:E:443:PHE:CZ	1:E:452:LYS:HG2	2.55	0.41
1:A:397:ILE:HD13	1:A:459:LEU:HA	2.02	0.41
1:D:191:LEU:HD23	1:D:191:LEU:HA	1.86	0.41
1:E:352:ILE:O	1:E:356:TYR:N	2.52	0.41
1:B:69:ALA:O	1:B:73:SER:HB3	2.21	0.41
1:B:133:MET:HG2	1:B:146:LEU:HD22	2.02	0.41
1:C:286:ARG:NH1	1:C:409:ASP:OD1	2.52	0.41
1:A:411:GLY:O	1:A:415:GLN:HG3	2.21	0.41
1:D:263:GLU:O	1:D:267:GLN:HG3	2.21	0.41
1:D:154:GLU:HA	1:D:157:ARG:HE	1.86	0.41
1:D:217:LEU:HD21	1:D:236:GLU:HB2	2.03	0.41
1:C:156:LEU:HD12	1:C:156:LEU:HA	1.79	0.41
1:E:195:ILE:HD12	1:E:195:ILE:HG23	1.83	0.41
1:C:127:TYR:OH	1:C:219:GLU:OE2	2.37	0.40
1:C:207:LEU:HD12	1:C:207:LEU:HA	1.86	0.40
1:C:215:GLY:O	1:C:236:GLU:HG2	2.21	0.40
1:D:174:THR:CG2	1:D:176:GLU:H	2.27	0.40
1:C:217:LEU:HD21	1:C:236:GLU:HB3	2.03	0.40
1:C:380:MET:SD	1:C:380:MET:N	2.85	0.40
1:D:191:LEU:O	1:D:195:ILE:HG12	2.21	0.40
1:D:261:LEU:O	1:D:265:MET:HG3	2.20	0.40
1:C:174:THR:HG23	1:C:176:GLU:H	1.85	0.40
1:E:380:MET:HE2	1:E:381:HIS:ND1	2.36	0.40
1:A:154:GLU:O	1:A:158:LYS:HG3	2.21	0.40
1:E:261:LEU:O	1:E:265:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

All (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
1	D	220	GLY
1	C	267	GLN

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LEU
1	A	133	MET
1	A	156	LEU
1	A	159	LEU
1	A	174	THR
1	A	207	LEU
1	A	239	SER
1	A	256	ARG
1	A	264	ARG
1	A	281	GLU
1	A	289	LEU
1	A	317	GLU
1	A	327	THR
1	A	358	GLU
1	A	361	GLN
1	A	366	LYS
1	A	378	ILE
1	A	380	MET
1	A	433	GLU
1	A	452	LYS
1	A	459	LEU
1	A	460	LEU
1	B	124	GLN
1	B	156	LEU
1	B	159	LEU
1	B	174	THR
1	B	207	LEU
1	B	233	PRO
1	B	239	SER
1	B	295	LEU
1	B	311	ASP
1	B	327	THR
1	B	366	LYS

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Mol	Chain	Res	Type
1	B	378	ILE
1	B	380	MET
1	B	433	GLU
1	B	434	LYS
1	B	452	LYS
1	B	458	LEU
1	B	459	LEU
1	B	460	LEU
1	C	126	SER
1	C	138	GLN
1	C	149	LEU
1	C	154	GLU
1	C	156	LEU
1	C	188	THR
1	C	207	LEU
1	C	239	SER
1	C	259	GLU
1	C	311	ASP
1	C	366	LYS
1	C	378	ILE
1	C	380	MET
1	C	387	SER
1	C	417	LEU
1	C	433	GLU
1	C	434	LYS
1	C	450	SER
1	C	452	LYS
1	C	458	LEU
1	C	459	LEU
1	C	460	LEU
1	D	72	SER
1	D	126	SER
1	D	144	GLU
1	D	149	LEU
1	D	156	LEU
1	D	160	SER
1	D	174	THR
1	D	207	LEU
1	D	237	GLN
1	D	239	SER
1	D	282	GLU
1	D	283	MET

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Mol	Chain	Res	Type
1	D	311	ASP
1	D	320	THR
1	D	324	GLU
1	D	340	GLN
1	D	366	LYS
1	D	380	MET
1	D	387	SER
1	D	417	LEU
1	D	433	GLU
1	D	457	LEU
1	D	458	LEU
1	D	459	LEU
1	D	460	LEU
1	E	72	SER
1	E	109	SER
1	E	126	SER
1	E	156	LEU
1	E	182	LEU
1	E	191	LEU
1	E	239	SER
1	E	259	GLU
1	E	270	GLU
1	E	289	LEU
1	E	295	LEU
1	E	311	ASP
1	E	317	GLU
1	E	327	THR
1	E	340	GLN
1	E	350	SER
1	E	358	GLU
1	E	361	GLN
1	E	366	LYS
1	E	378	ILE
1	E	380	MET
1	E	389	LEU
1	E	404	ARG
1	E	433	GLU
1	E	434	LYS
1	E	452	LYS
1	E	458	LEU
1	E	459	LEU
1	E	460	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	HIS
1	B	97	HIS
1	B	187	HIS
1	B	376	ASN
1	C	124	GLN
1	C	332	GLN
1	C	353	GLN
1	C	381	HIS
1	D	179	GLN
1	D	340	GLN
1	D	456	ASN
1	E	97	HIS
1	E	124	GLN
1	E	441	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 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%)
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.

All (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
2	E	501	LEU	C-CA-CB-CG
2	A	501	LEU	C-CA-CB-CG
2	C	501	LEU	CA-CB-CG-CD1
2	A	501	LEU	CA-CB-CG-CD1
2	E	501	LEU	N-CA-CB-CG
2	C	501	LEU	O-C-CA-N
2	D	501	LEU	O-C-CA-N
2	C	501	LEU	N-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 ⓘ

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	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

All (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
1	C	310	PRO	5.7
1	B	233	PRO	5.3
1	A	310	PRO	5.1
1	D	233	PRO	4.9
1	B	281	GLU	4.8
1	B	310	PRO	4.8
1	D	269	GLN	4.8
1	A	240	PRO	4.7
1	C	270	GLU	4.6
1	B	295	LEU	4.6
1	A	233	PRO	4.5
1	C	220	GLY	4.4
1	D	295	LEU	4.3
1	E	281	GLU	4.2
1	E	233	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	240	PRO	4.0
1	C	233	PRO	4.0
1	A	236	GLU	4.0
1	C	295	LEU	3.8
1	B	236	GLU	3.8
1	E	295	LEU	3.8
1	B	271	SER	3.6
1	C	327	THR	3.5
1	B	220	GLY	3.5
1	D	324	GLU	3.5
1	D	327	THR	3.5
1	D	329	ARG	3.4
1	D	256	ARG	3.3
1	A	281	GLU	3.3
1	D	281	GLU	3.2
1	C	236	GLU	3.2
1	C	326	PHE	3.1
1	D	184	THR	3.0
1	E	185	GLY	3.0
1	A	239	SER	3.0
1	E	239	SER	3.0
1	E	269	GLN	3.0
1	B	256	ARG	2.9
1	A	271	SER	2.9
1	D	239	SER	2.9
1	C	239	SER	2.8
1	B	269	GLN	2.8
1	E	221	ASP	2.8
1	C	259	GLU	2.8
1	E	184	THR	2.8
1	A	266	GLN	2.7
1	A	295	LEU	2.7
1	C	186	GLU	2.7
1	E	186	GLU	2.6
1	E	270	GLU	2.6
1	D	236	GLU	2.6
1	E	329	ARG	2.6
1	B	186	GLU	2.6
1	E	327	THR	2.6
1	C	256	ARG	2.5
1	E	236	GLU	2.5
1	E	331	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	283	MET	2.4
1	C	329	ARG	2.4
1	D	480	THR	2.4
1	A	238	SER	2.4
1	E	240	PRO	2.4
1	C	283	MET	2.4
1	B	329	ARG	2.4
1	E	183	LYS	2.3
1	B	270	GLU	2.3
1	A	327	THR	2.3
1	D	186	GLU	2.3
1	B	311	ASP	2.2
1	D	66	GLY	2.2
1	A	311	ASP	2.1
1	A	269	GLN	2.1
1	D	311	ASP	2.1
1	D	284	GLU	2.1
1	B	66	GLY	2.1
1	D	221	ASP	2.0
1	B	239	SER	2.0
1	A	407	ASP	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 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($\text{\AA}^2$)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.