Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 09:09 AM EDT

PDB ID	:	5DJ4
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 (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:

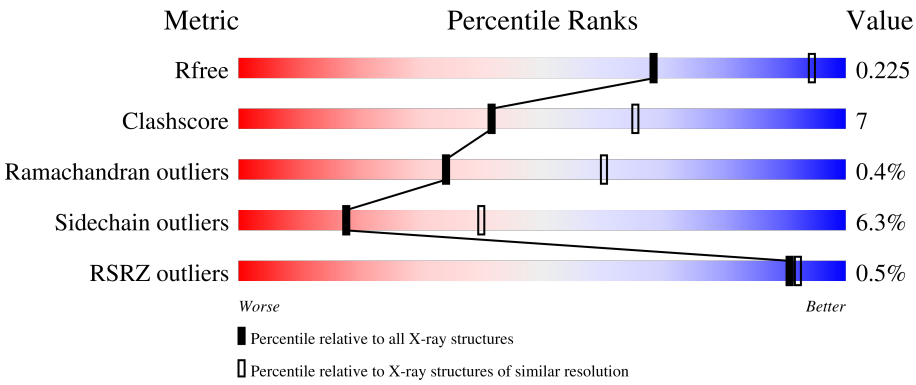
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	64% 11% • 24%
1	B	480	62% 13% 24%
1	C	480	% 59% 15% • 24%
1	D	480	60% 15% • 24%
1	E	480	61% 13% • 24%

2 Entry composition (i)

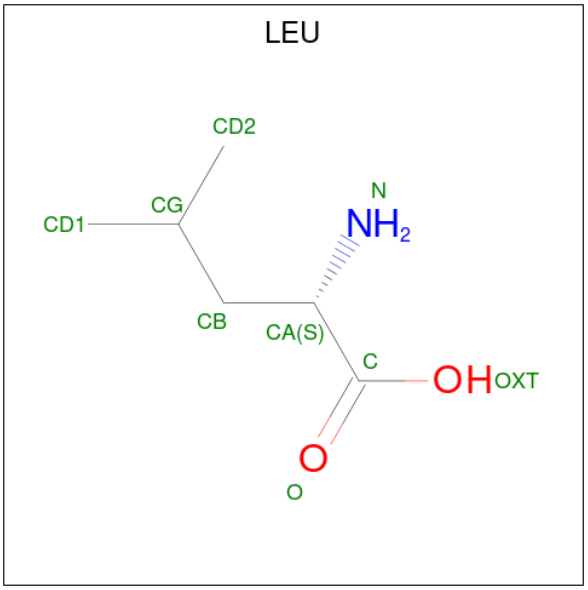
There are 3 unique types of molecules in this entry. The entry contains 14911 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$).



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

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

- Molecule 3 is water.

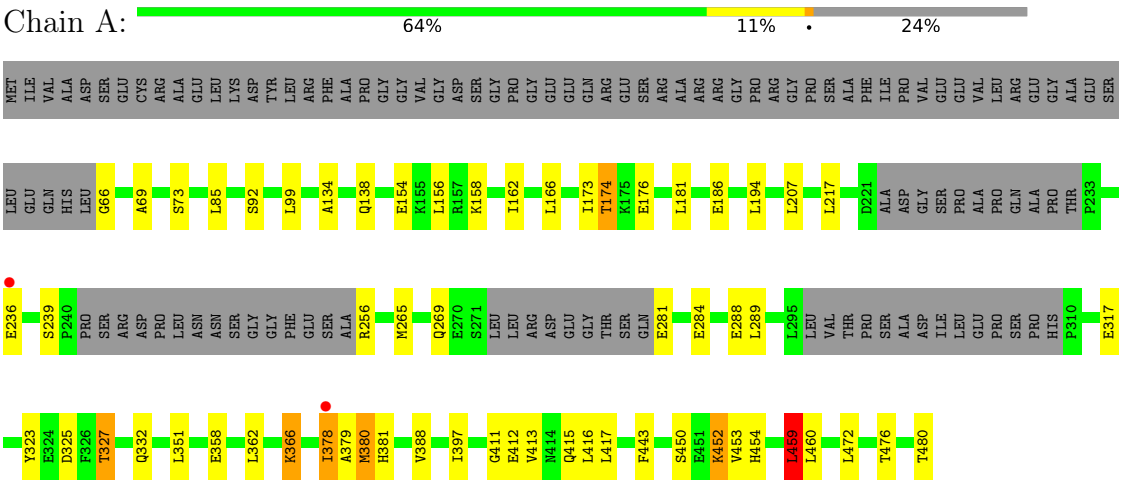
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	37	37	37	0	0
3	B	24	24	24	0	0
3	C	16	16	16	0	0
3	D	17	17	17	0	0
3	E	21	21	21	0	0

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.

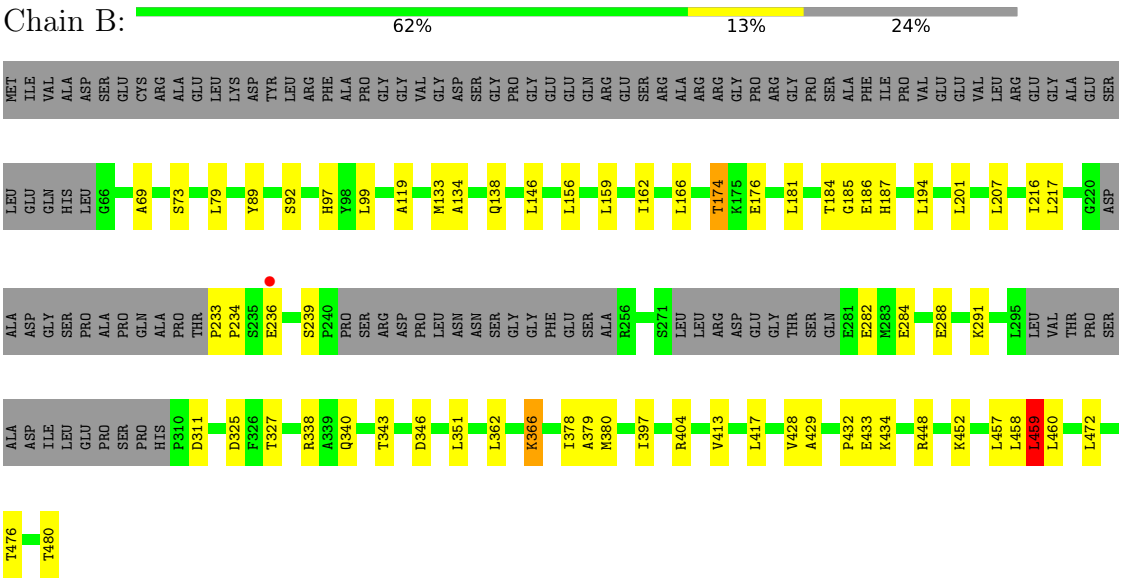
• Molecule 1: Sestrin-2

Chain A:



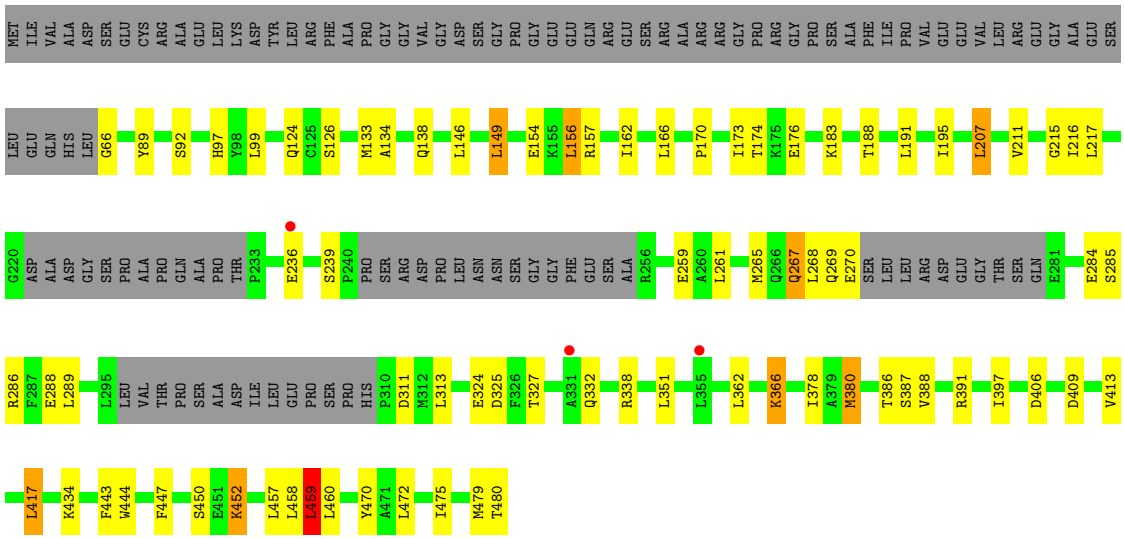
• Molecule 1: Sestrin-2

Chain B:



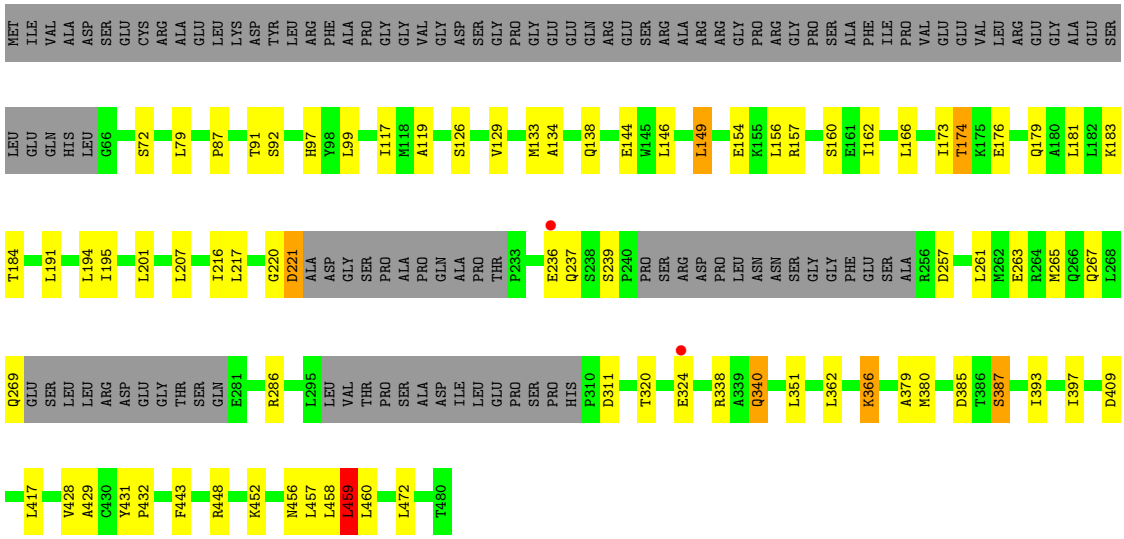
• Molecule 1: Sestrin-2

Chain C:



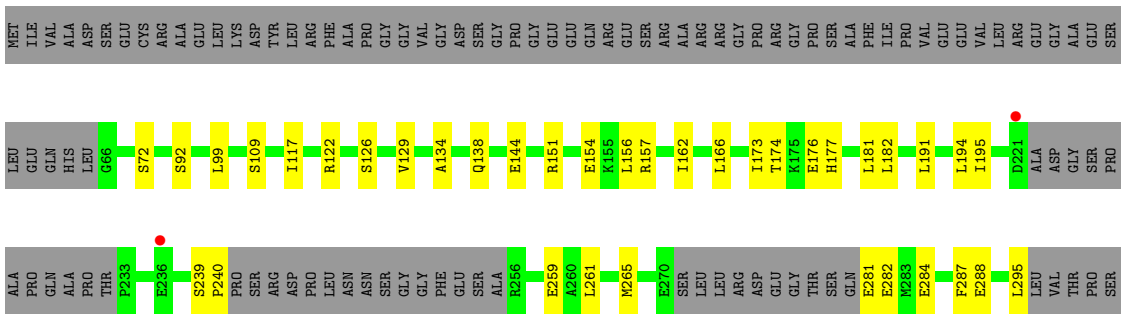
- Molecule 1: Sestrin-2

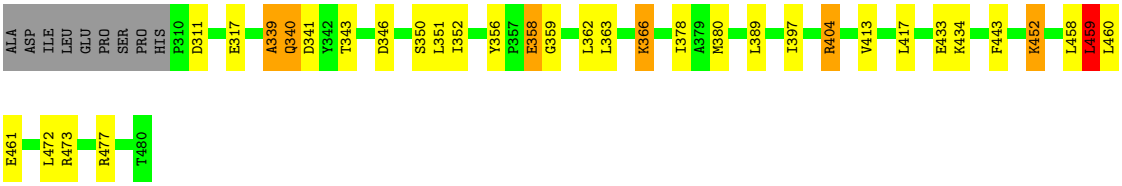
Chain D: 60% 15% • 24%



- Molecule 1: Sestrin-2

Chain E: 61% 13% • 24%




ALA
ASP
ILE
LEU
GLU
PRO
SER
PRO
HIS
P310
D311
E317
A339
Q340
D341
Y342
T343
D346
S350
L351
I352
Y356
P357
E358
G359
L362
L363
K366
I378
A379
M380
L389
I397
R404
V413
L417
E433
K434
F443
K452
L458
L459
L460
E461
L472
R473
R477
T480

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.196 , 0.223 0.200 , 0.225	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 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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)

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	0.57	0/3039	0.58	1/4115 (0.0%)
1	B	0.58	0/3013	0.59	1/4083 (0.0%)
1	C	0.47	0/3029	0.53	1/4101 (0.0%)
1	D	0.46	0/3022	0.53	1/4093 (0.0%)
1	E	0.50	0/3033	0.55	1/4107 (0.0%)
All	All	0.52	0/15136	0.56	5/20499 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	459	LEU	CA-CB-CG	6.58	130.44	115.30
1	A	459	LEU	CA-CB-CG	6.44	130.10	115.30
1	E	459	LEU	CA-CB-CG	6.27	129.72	115.30
1	D	459	LEU	CA-CB-CG	6.08	129.29	115.30
1	B	459	LEU	CA-CB-CG	5.61	128.21	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	2962	0	2875	37	0
1	B	2936	0	2839	33	0
1	C	2952	0	2870	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2945	0	2857	58	0
1	E	2956	0	2870	36	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	205	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 (205) 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:C:97:HIS:ND1	3:C:601:HOH:O	1.99	0.95
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:480:THR:OXT	1:C:480:THR:OG1	2.31	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:B:433:GLU:H	1:B:433:GLU:CD	2.22	0.42
1:C:413:VAL:O	1:C:417:LEU:HB2	2.20	0.42
1:C:149:LEU:HD22	1:C:157:ARG:HG3	2.01	0.42
1:C:265:MET:HE1	1:C:386:THR:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:380:MET:HE3	1:A:380:MET:HB2	1.90	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: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 (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%)	41 66
1	B	355/480 (74%)	346 (98%)	9 (2%)	0	100 100
1	C	354/480 (74%)	342 (97%)	10 (3%)	2 (1%)	25 50
1	D	354/480 (74%)	344 (97%)	8 (2%)	2 (1%)	25 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	355/480 (74%)	343 (97%)	10 (3%)	2 (1%)	25	50
All	All	1774/2400 (74%)	1721 (97%)	46 (3%)	7 (0%)	34	60

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 (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	313/410 (76%)	298 (95%)	15 (5%)	25	53
1	B	308/410 (75%)	293 (95%)	15 (5%)	25	52
1	C	312/410 (76%)	292 (94%)	20 (6%)	17	39
1	D	311/410 (76%)	289 (93%)	22 (7%)	14	34
1	E	312/410 (76%)	287 (92%)	25 (8%)	12	27
All	All	1556/2050 (76%)	1459 (94%)	97 (6%)	18	40

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LEU
1	A	174	THR
1	A	239	SER
1	A	256	ARG
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	317	GLU
1	A	327	THR
1	A	358	GLU
1	A	366	LYS
1	A	378	ILE
1	A	380	MET
1	A	450	SER
1	A	452	LYS
1	A	459	LEU
1	A	460	LEU
1	B	156	LEU
1	B	159	LEU
1	B	174	THR
1	B	207	LEU
1	B	239	SER
1	B	282	GLU
1	B	311	ASP
1	B	366	LYS
1	B	378	ILE
1	B	380	MET
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	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	434	LYS
1	C	450	SER
1	C	452	LYS

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Mol	Chain	Res	Type
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	221	ASP
1	D	237	GLN
1	D	239	SER
1	D	311	ASP
1	D	320	THR
1	D	340	GLN
1	D	366	LYS
1	D	380	MET
1	D	387	SER
1	D	417	LEU
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	295	LEU
1	E	311	ASP
1	E	317	GLU
1	E	340	GLN
1	E	350	SER
1	E	358	GLU
1	E	366	LYS
1	E	378	ILE
1	E	380	MET

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Mol	Chain	Res	Type
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	HIS
1	C	124	GLN
1	D	179	GLN
1	D	340	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 monosaccharides 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	C	501	-	7,8,8	0.95	1 (14%)	9,10,10	1.24	1 (11%)
2	LEU	D	501	-	7,8,8	1.04	1 (14%)	9,10,10	1.13	1 (11%)
2	LEU	B	501	-	7,8,8	0.94	1 (14%)	9,10,10	1.39	2 (22%)
2	LEU	A	501	-	7,8,8	1.06	1 (14%)	9,10,10	1.32	2 (22%)
2	LEU	E	501	-	7,8,8	0.98	1 (14%)	9,10,10	1.60	2 (22%)

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	C	501	-	-	3/8/8/8	-
2	LEU	D	501	-	-	3/8/8/8	-
2	LEU	B	501	-	-	2/8/8/8	-
2	LEU	A	501	-	-	3/8/8/8	-
2	LEU	E	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	-2.72	1.21	1.30
2	D	501	LEU	OXT-C	-2.65	1.21	1.30
2	E	501	LEU	OXT-C	-2.47	1.22	1.30
2	C	501	LEU	OXT-C	-2.34	1.22	1.30
2	B	501	LEU	OXT-C	-2.33	1.22	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	LEU	OXT-C-O	-3.73	115.63	124.09
2	A	501	LEU	OXT-C-O	-3.26	116.68	124.09
2	B	501	LEU	OXT-C-O	-3.17	116.89	124.09
2	C	501	LEU	OXT-C-O	-3.17	116.89	124.09
2	E	501	LEU	OXT-C-CA	2.93	123.37	113.38
2	D	501	LEU	OXT-C-O	-2.68	118.00	124.09
2	B	501	LEU	OXT-C-CA	2.65	122.41	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	LEU	OXT-C-CA	2.18	120.80	113.38

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 (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%)	0.24	2 (0%)	91	92	36, 48, 84, 105	0
1	B	365/480 (76%)	0.20	1 (0%)	94	95	34, 46, 82, 101	0
1	C	364/480 (75%)	0.21	3 (0%)	86	87	42, 59, 91, 110	0
1	D	364/480 (75%)	0.09	2 (0%)	91	92	38, 57, 94, 109	0
1	E	365/480 (76%)	0.14	2 (0%)	91	92	41, 57, 89, 102	0
All	All	1824/2400 (76%)	0.18	10 (0%)	91	92	34, 54, 90, 110	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	GLU	3.3
1	C	331	ALA	3.1
1	E	221	ASP	2.9
1	A	378	ILE	2.7
1	C	236	GLU	2.4
1	D	324	GLU	2.4
1	B	236	GLU	2.4
1	E	236	GLU	2.2
1	D	236	GLU	2.1
1	C	355	LEU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LEU	E	501	9/9	0.96	0.19	46,50,51,51	0
2	LEU	B	501	9/9	0.97	0.22	43,46,48,52	0
2	LEU	D	501	9/9	0.98	0.27	47,51,52,54	0
2	LEU	C	501	9/9	0.98	0.24	50,53,56,56	0
2	LEU	A	501	9/9	0.99	0.23	46,50,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.