Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2016 – 03:05 PM EDT

PDB ID	:	5T0N
Title	:	Pseudo-apo structure of Sestrin2 at 3.0 angstrom resolution
Authors	:	Saxton, R.A.; Knockenhauer, K.E.; Schwartz, T.U.
Deposited on	:	2016-08-16
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

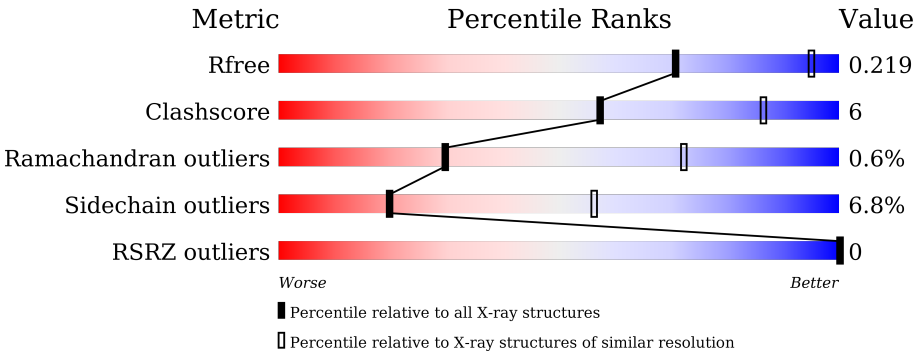
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	63% 12% • 24%
1	B	480	63% 11% • 24%
1	C	480	60% 14% • 25%
1	D	480	60% 13% • 25%
1	E	480	57% 16% • 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LEU	A	501	-	-	-	X
2	LEU	B	501	-	-	-	X
2	LEU	C	501	-	-	-	X
2	LEU	D	501	-	-	-	X

2 Entry composition

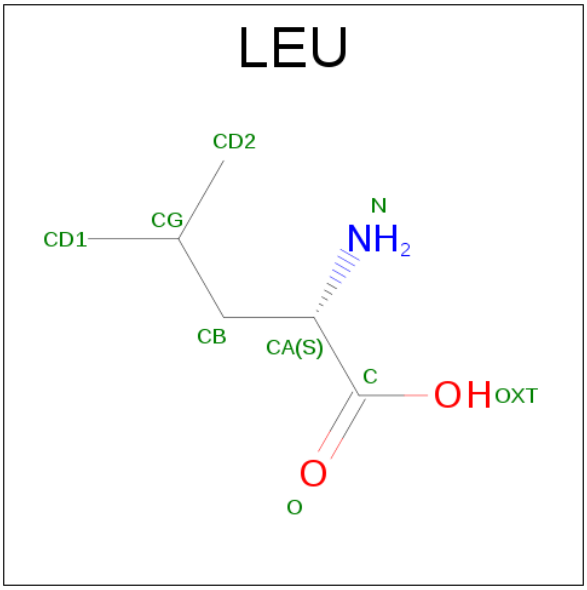
There are 2 unique types of molecules in this entry. The entry contains 14648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	363	Total	C	N	O	S	0	0	0
			2925	1878	505	524	18			
1	B	363	Total	C	N	O	S	0	0	0
			2925	1878	505	524	18			
1	C	360	Total	C	N	O	S	0	0	0
			2915	1873	506	518	18			
1	D	361	Total	C	N	O	S	0	0	0
			2909	1870	504	517	18			
1	E	362	Total	C	N	O	S	0	0	0
			2929	1880	506	525	18			

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



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

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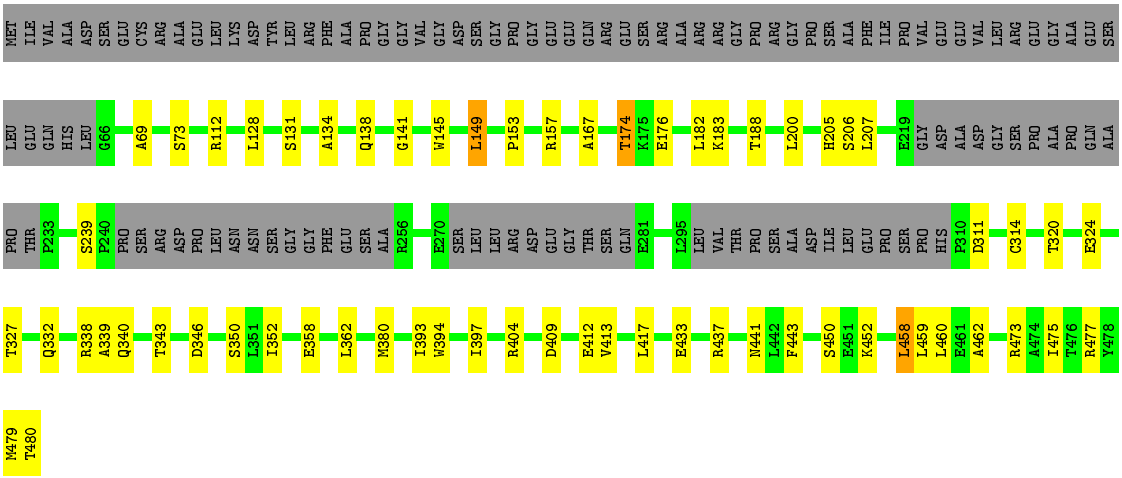
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			9	6	1	2		
2	C	1	Total	C	N	O	0	0
			9	6	1	2		
2	D	1	Total	C	N	O	0	0
			9	6	1	2		
2	E	1	Total	C	N	O	0	0
			9	6	1	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

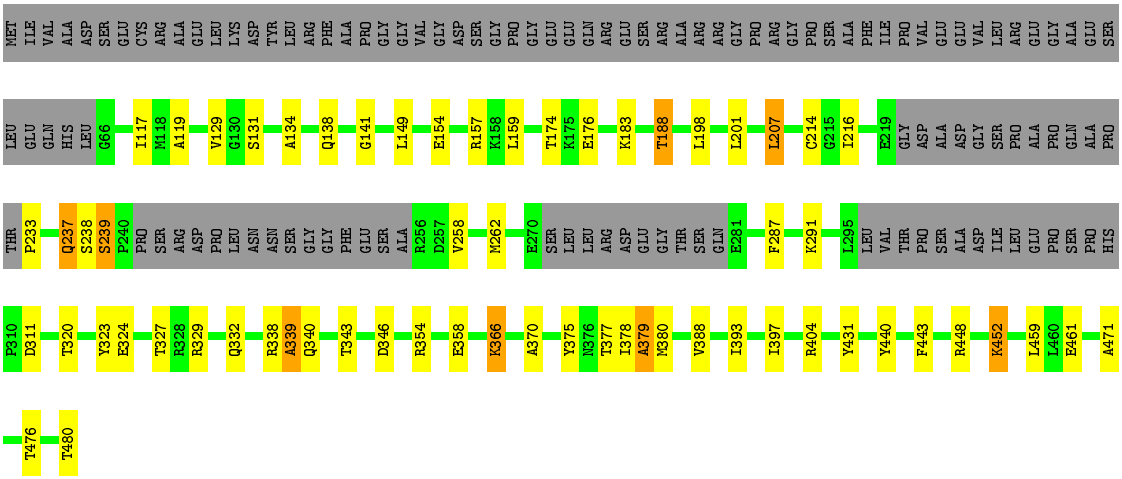
- Molecule 1: Sestrin-2

Chain A:



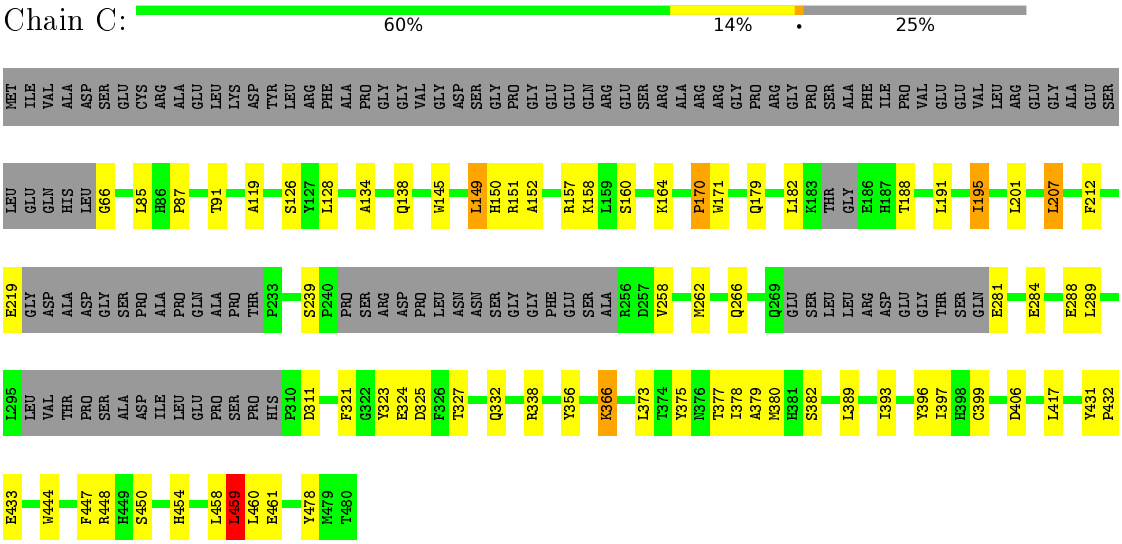
- Molecule 1: Sestrin-2

Chain B:



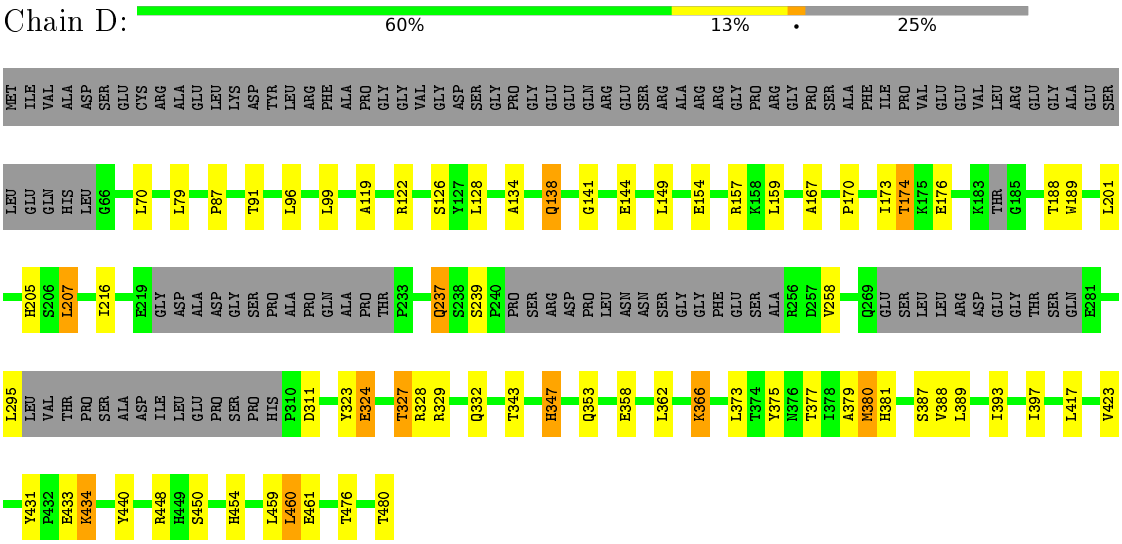
- Molecule 1: Sestrin-2

Chain C:



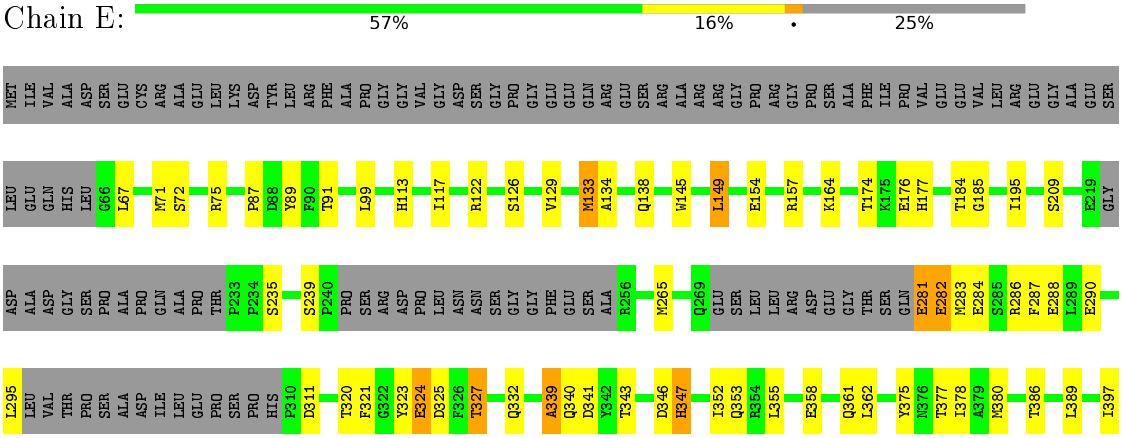
- Molecule 1: Sestrin-2

Chain D:



- Molecule 1: Sestrin-2

Chain E:




B404
G411
E412
V413
N414
Q415
L416
L417
V423
Y431
P432
E433
K434
R437
L457
L458
L459
L460
R463
L469
R473
T476
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	292.26Å 292.26Å 292.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.33 – 3.00 119.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (103.33-3.00) 93.1 (119.32-3.00)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.189 , 0.225 0.181 , 0.219	Depositor DCC
R_{free} test set	1523 reflections (1.99%)	DCC
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.002 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14648	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% 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

5.1 Standard geometry

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	0.50	0/3002	0.63	1/4069 (0.0%)
1	B	0.50	0/3002	0.64	0/4069
1	C	0.46	0/2991	0.59	1/4050 (0.0%)
1	D	0.45	0/2985	0.59	1/4043 (0.0%)
1	E	0.45	0/3006	0.60	0/4072
All	All	0.48	0/14986	0.61	3/20303 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	458	LEU	CB-CG-CD2	-5.64	101.40	111.00
1	C	459	LEU	CA-CB-CG	5.32	127.54	115.30
1	D	460	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2925	0	2828	27	0
1	B	2925	0	2828	36	0
1	C	2915	0	2833	36	0
1	D	2909	0	2821	38	0
1	E	2929	0	2846	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	14648	0	14206	172	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 6.

All (172) 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:B:174:THR:HG22	1:B:176:GLU:H	1.41	0.85
1:B:338:ARG:HG3	1:B:404:ARG:HH21	1.44	0.82
1:C:338:ARG:NH2	1:C:406:ASP:OD2	2.21	0.74
1:E:339:ALA:O	1:E:341:ASP:N	2.23	0.71
1:B:343:THR:OG1	1:B:346:ASP:OD1	2.06	0.71
1:A:338:ARG:HG3	1:A:404:ARG:HH21	1.56	0.70
1:A:324:GLU:HA	1:A:332:GLN:HB2	1.75	0.68
1:C:149:LEU:HD22	1:C:157:ARG:HG3	1.75	0.68
1:D:79:LEU:HA	1:D:216:ILE:HD13	1.77	0.67
1:C:134:ALA:O	1:C:138:GLN:HG2	1.95	0.67
1:E:174:THR:HG23	1:E:176:GLU:H	1.58	0.67
1:B:323:TYR:O	1:B:431:TYR:OH	2.11	0.67
1:E:413:VAL:HG13	1:E:417:LEU:HD12	1.79	0.64
1:A:134:ALA:O	1:A:138:GLN:HG2	1.97	0.64
1:E:323:TYR:O	1:E:431:TYR:OH	2.14	0.63
1:B:329:ARG:NH1	1:E:311:ASP:OD1	2.34	0.60
1:D:149:LEU:HD22	1:D:157:ARG:HG2	1.83	0.60
1:A:480:THR:HG22	1:B:480:THR:HA	1.84	0.60
1:C:324:GLU:OE1	1:C:332:GLN:N	2.34	0.59
1:E:87:PRO:O	1:E:91:THR:HG23	2.02	0.59
1:C:152:ALA:O	1:C:157:ARG:NH1	2.36	0.59
1:C:87:PRO:O	1:C:91:THR:HG23	2.02	0.58
1:D:379:ALA:O	1:D:448:ARG:NH1	2.33	0.58
1:A:149:LEU:HD22	1:A:157:ARG:HG2	1.86	0.58
1:B:174:THR:HG22	1:B:176:GLU:N	2.16	0.58
1:C:325:ASP:OD1	1:C:327:THR:HG22	2.04	0.57
1:D:87:PRO:O	1:D:91:THR:HG23	2.05	0.57
1:A:443:PHE:CZ	1:A:452:LYS:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:GLU:HA	1:E:157:ARG:HE	1.69	0.56
1:C:324:GLU:HA	1:C:332:GLN:HB2	1.86	0.56
1:A:343:THR:OG1	1:A:346:ASP:OD1	2.23	0.56
1:D:324:GLU:HB2	1:D:431:TYR:OH	2.06	0.56
1:E:343:THR:OG1	1:E:346:ASP:OD1	2.24	0.56
1:E:67:LEU:O	1:E:71:MET:HG3	2.06	0.55
1:D:324:GLU:HA	1:D:332:GLN:HB2	1.88	0.55
1:B:258:VAL:O	1:B:262:MET:HG3	2.06	0.54
1:E:134:ALA:O	1:E:138:GLN:HG2	2.07	0.54
1:A:413:VAL:HG13	1:A:417:LEU:HD22	1.90	0.54
1:B:346:ASP:OD1	1:B:346:ASP:N	2.37	0.54
1:E:99:LEU:HD22	1:E:358:GLU:HG3	1.90	0.54
1:C:195:ILE:HG21	1:C:356:TYR:HB2	1.88	0.54
1:B:393:ILE:O	1:B:397:ILE:HD12	2.08	0.53
1:C:444:TRP:HB3	1:C:447:PHE:HB2	1.89	0.53
1:A:338:ARG:HH11	1:A:340:GLN:HB2	1.73	0.53
1:E:117:ILE:HG23	1:E:129:VAL:HG13	1.91	0.53
1:D:393:ILE:O	1:D:397:ILE:HD12	2.09	0.52
1:D:431:TYR:HB3	1:D:434:LYS:HG3	1.92	0.52
1:B:134:ALA:O	1:B:138:GLN:HG2	2.08	0.52
1:E:281:GLU:OE1	1:E:281:GLU:N	2.42	0.52
1:A:182:LEU:HD13	1:B:354:ARG:HD2	1.91	0.52
1:B:379:ALA:O	1:B:448:ARG:NH1	2.43	0.52
1:D:373:LEU:HD23	1:D:454:HIS:CE1	2.45	0.52
1:B:154:GLU:HG3	1:B:157:ARG:NH1	2.25	0.51
1:B:339:ALA:O	1:B:340:GLN:HB2	2.10	0.51
1:A:473:ARG:HD2	1:A:477:ARG:NH2	2.25	0.51
1:C:128:LEU:HD11	1:C:207:LEU:HB3	1.92	0.51
1:D:323:TYR:O	1:D:431:TYR:OH	2.21	0.51
1:B:183:LYS:O	1:B:188:THR:HG23	2.10	0.51
1:A:324:GLU:H	1:A:332:GLN:HE21	1.57	0.51
1:A:339:ALA:O	1:A:340:GLN:HB2	2.11	0.51
1:B:443:PHE:O	1:B:452:LYS:NZ	2.44	0.51
1:B:198:LEU:HD13	1:B:471:ALA:HB1	1.93	0.50
1:C:164:LYS:HD2	1:C:321:PHE:CG	2.45	0.50
1:E:149:LEU:HD22	1:E:157:ARG:HG2	1.93	0.50
1:C:397:ILE:HD13	1:C:459:LEU:HA	1.94	0.50
1:D:128:LEU:HD11	1:D:207:LEU:HB3	1.93	0.50
1:B:214:CYS:HB2	1:B:216:ILE:HD12	1.94	0.50
1:D:154:GLU:HA	1:D:157:ARG:HE	1.77	0.50
1:A:393:ILE:O	1:A:397:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:LYS:HD2	1:D:461:GLU:OE2	2.12	0.49
1:D:327:THR:HG22	1:D:328:ARG:HG2	1.93	0.49
1:A:128:LEU:HD11	1:A:207:LEU:HB3	1.94	0.49
1:A:338:ARG:HG3	1:A:404:ARG:NH2	2.26	0.49
1:C:284:GLU:O	1:C:288:GLU:HG2	2.12	0.49
1:C:119:ALA:HB2	1:C:201:LEU:HD23	1.95	0.48
1:D:380:MET:HG2	1:D:381:HIS:CD2	2.48	0.48
1:C:366:LYS:HD2	1:C:461:GLU:OE2	2.13	0.48
1:D:237:GLN:HG2	1:D:440:TYR:CG	2.48	0.48
1:E:324:GLU:HA	1:E:332:GLN:HB2	1.96	0.48
1:E:265:MET:HE1	1:E:386:THR:HA	1.94	0.48
1:D:174:THR:HG22	1:D:176:GLU:H	1.79	0.48
1:A:112:ARG:HG2	1:A:200:LEU:HD11	1.96	0.48
1:A:183:LYS:O	1:A:188:THR:HG23	2.14	0.48
1:E:99:LEU:HD22	1:E:362:LEU:HD12	1.96	0.47
1:C:66:GLY:C	1:D:329:ARG:HH22	2.18	0.47
1:B:149:LEU:HD22	1:B:157:ARG:HG2	1.97	0.47
1:D:324:GLU:OE1	1:D:332:GLN:N	2.32	0.47
1:D:343:THR:O	1:D:347:HIS:HB2	2.14	0.47
1:E:473:ARG:HD2	1:E:477:ARG:NH2	2.30	0.47
1:D:159:LEU:HD22	1:D:189:TRP:CZ2	2.50	0.46
1:E:209:SER:OG	1:E:463:ARG:NH1	2.48	0.46
1:E:343:THR:O	1:E:347:HIS:HB2	2.15	0.46
1:D:119:ALA:HB2	1:D:201:LEU:HD23	1.98	0.46
1:C:262:MET:O	1:C:266:GLN:HG2	2.16	0.46
1:E:174:THR:HG22	1:E:177:HIS:ND1	2.31	0.46
1:A:394:TRP:CE3	1:A:462:ALA:HB2	2.51	0.46
1:D:79:LEU:HD11	1:D:207:LEU:HG	1.97	0.46
1:D:134:ALA:O	1:D:138:GLN:HG2	2.15	0.46
1:D:99:LEU:HD22	1:D:358:GLU:HG3	1.98	0.46
1:B:320:THR:HG21	1:E:320:THR:HG21	1.98	0.46
1:B:370:ALA:CB	1:B:461:GLU:HG3	2.46	0.46
1:A:145:TRP:CZ2	1:A:153:PRO:HD3	2.51	0.45
1:C:195:ILE:CG2	1:C:356:TYR:HB2	2.45	0.45
1:E:113:HIS:O	1:E:117:ILE:HG13	2.16	0.45
1:E:282:GLU:O	1:E:286:ARG:HG3	2.16	0.45
1:A:475:ILE:O	1:A:479:MET:HG2	2.16	0.45
1:C:170:PRO:HD2	1:C:171:TRP:CE3	2.52	0.45
1:B:119:ALA:HB2	1:B:201:LEU:HD23	1.98	0.45
1:B:207:LEU:HA	1:B:207:LEU:HD12	1.73	0.45
1:B:338:ARG:HH11	1:B:340:GLN:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HA	1:D:159:LEU:HD12	1.76	0.44
1:D:375:TYR:O	1:D:377:THR:HG23	2.18	0.44
1:E:295:LEU:HB3	1:E:423:VAL:HG22	1.98	0.44
1:D:70:LEU:H	1:E:133:MET:HE1	1.83	0.44
1:E:290:GLU:OE1	1:E:414:ASN:ND2	2.43	0.44
1:D:174:THR:CG2	1:D:176:GLU:H	2.31	0.44
1:B:340:GLN:H	1:B:343:THR:HG23	1.82	0.44
1:E:195:ILE:HA	1:E:195:ILE:HD13	1.90	0.44
1:A:206:SER:HB2	1:A:460:LEU:HB2	1.99	0.43
1:B:237:GLN:HG2	1:B:440:TYR:CG	2.53	0.43
1:B:291:LYS:HB3	1:B:291:LYS:HE3	1.77	0.43
1:E:287:PHE:CG	1:E:404:ARG:HG3	2.53	0.43
1:E:284:GLU:O	1:E:288:GLU:HG2	2.18	0.43
1:B:323:TYR:O	1:B:324:GLU:HB2	2.18	0.43
1:C:373:LEU:HD23	1:C:454:HIS:CE1	2.53	0.43
1:C:158:LYS:HE3	1:C:158:LYS:HB2	1.87	0.43
1:C:393:ILE:O	1:C:397:ILE:HD12	2.19	0.43
1:A:167:ALA:HB2	1:A:205:HIS:CE1	2.54	0.43
1:B:476:THR:O	1:B:480:THR:HG23	2.19	0.43
1:D:170:PRO:O	1:D:173:ILE:HG13	2.19	0.43
1:E:411:GLY:O	1:E:415:GLN:HG3	2.19	0.43
1:C:258:VAL:O	1:C:262:MET:HG3	2.18	0.42
1:D:295:LEU:HB3	1:D:423:VAL:HG22	2.00	0.42
1:C:323:TYR:O	1:C:431:TYR:OH	2.17	0.42
1:D:96:LEU:HD22	1:D:366:LYS:HE2	2.00	0.42
1:E:397:ILE:HD13	1:E:459:LEU:HA	2.01	0.42
1:B:443:PHE:CZ	1:B:452:LYS:HG2	2.54	0.42
1:B:324:GLU:HA	1:B:332:GLN:HB2	2.02	0.42
1:D:167:ALA:HB2	1:D:205:HIS:CE1	2.55	0.42
1:C:182:LEU:O	1:C:188:THR:OG1	2.36	0.42
1:D:476:THR:O	1:D:480:THR:HG22	2.20	0.42
1:B:375:TYR:O	1:B:377:THR:HG23	2.19	0.42
1:C:375:TYR:O	1:C:377:THR:HG23	2.19	0.42
1:C:145:TRP:CD1	1:C:145:TRP:N	2.88	0.42
1:E:375:TYR:O	1:E:377:THR:HG23	2.19	0.42
1:E:89:TYR:CE2	1:E:457:LEU:HD22	2.55	0.42
1:E:325:ASP:OD1	1:E:327:THR:HB	2.20	0.42
1:E:352:ILE:HG23	1:E:352:ILE:HD12	1.77	0.42
1:E:469:LEU:HA	1:E:469:LEU:HD23	1.83	0.42
1:A:69:ALA:O	1:A:73:SER:HB3	2.20	0.41
1:D:258:VAL:HB	1:D:380:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ARG:NH1	1:A:441:ASN:HD21	2.18	0.41
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.81	0.41
1:C:379:ALA:O	1:C:448:ARG:NH1	2.47	0.41
1:D:138:GLN:HG2	1:D:138:GLN:H	1.66	0.41
1:C:396:TYR:O	1:C:399:CYS:HB3	2.20	0.41
1:C:212:PHE:CD2	1:C:432:PRO:HB2	2.56	0.41
1:E:164:LYS:HD2	1:E:321:PHE:CG	2.56	0.41
1:A:409:ASP:O	1:A:412:GLU:HG3	2.21	0.41
1:B:366:LYS:HD2	1:B:461:GLU:OE2	2.21	0.41
1:C:195:ILE:HD13	1:C:195:ILE:HA	1.83	0.41
1:D:362:LEU:HD23	1:D:362:LEU:HA	1.83	0.41
1:A:174:THR:CG2	1:A:176:GLU:H	2.34	0.40
1:C:150:HIS:CD2	1:C:151:ARG:HD3	2.56	0.40
1:C:219:GLU:H	1:C:219:GLU:HG2	1.63	0.40
1:C:179:GLN:HG3	1:C:478:TYR:HE2	1.85	0.40
1:B:287:PHE:CE2	1:B:404:ARG:HB2	2.56	0.40
1:E:145:TRP:N	1:E:145:TRP:CD1	2.88	0.40
1:E:184:THR:HG22	1:E:185:GLY:N	2.36	0.40
1:D:173:ILE:HD13	1:D:173:ILE:HG21	1.85	0.40
1:B:117:ILE:HG23	1:B:129:VAL:HG13	2.03	0.40
1:E:476:THR:O	1:E:480:THR:HG23	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	353/480 (74%)	339 (96%)	13 (4%)	1 (0%)	46 84
1	B	353/480 (74%)	339 (96%)	10 (3%)	4 (1%)	17 58
1	C	348/480 (72%)	338 (97%)	10 (3%)	0	100 100
1	D	349/480 (73%)	337 (97%)	10 (3%)	2 (1%)	30 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	352/480 (73%)	338 (96%)	10 (3%)	4 (1%)	17 58
All	All	1755/2400 (73%)	1691 (96%)	53 (3%)	11 (1%)	30 72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	339	ALA
1	E	340	GLN
1	D	141	GLY
1	B	239	SER
1	B	339	ALA
1	D	347	HIS
1	B	141	GLY
1	B	379	ALA
1	E	324	GLU
1	E	347	HIS
1	A	141	GLY

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	306/410 (75%)	289 (94%)	17 (6%)	26 65
1	B	306/410 (75%)	289 (94%)	17 (6%)	26 65
1	C	306/410 (75%)	284 (93%)	22 (7%)	18 53
1	D	304/410 (74%)	280 (92%)	24 (8%)	15 48
1	E	309/410 (75%)	286 (93%)	23 (7%)	17 52
All	All	1531/2050 (75%)	1428 (93%)	103 (7%)	20 57

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	SER

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Mol	Chain	Res	Type
1	A	149	LEU
1	A	174	THR
1	A	239	SER
1	A	311	ASP
1	A	314	CYS
1	A	320	THR
1	A	327	THR
1	A	350	SER
1	A	352	ILE
1	A	358	GLU
1	A	362	LEU
1	A	380	MET
1	A	433	GLU
1	A	450	SER
1	A	458	LEU
1	A	459	LEU
1	B	131	SER
1	B	159	LEU
1	B	188	THR
1	B	207	LEU
1	B	233	PRO
1	B	237	GLN
1	B	238	SER
1	B	239	SER
1	B	311	ASP
1	B	327	THR
1	B	358	GLU
1	B	366	LYS
1	B	378	ILE
1	B	380	MET
1	B	388	VAL
1	B	452	LYS
1	B	459	LEU
1	C	85	LEU
1	C	126	SER
1	C	149	LEU
1	C	160	SER
1	C	170	PRO
1	C	195	ILE
1	C	207	LEU
1	C	239	SER
1	C	281	GLU

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Mol	Chain	Res	Type
1	C	289	LEU
1	C	311	ASP
1	C	366	LYS
1	C	378	ILE
1	C	380	MET
1	C	382	SER
1	C	389	LEU
1	C	417	LEU
1	C	433	GLU
1	C	450	SER
1	C	458	LEU
1	C	459	LEU
1	C	460	LEU
1	D	122	ARG
1	D	126	SER
1	D	138	GLN
1	D	144	GLU
1	D	174	THR
1	D	188	THR
1	D	207	LEU
1	D	237	GLN
1	D	239	SER
1	D	311	ASP
1	D	324	GLU
1	D	327	THR
1	D	353	GLN
1	D	366	LYS
1	D	380	MET
1	D	387	SER
1	D	388	VAL
1	D	389	LEU
1	D	417	LEU
1	D	433	GLU
1	D	434	LYS
1	D	450	SER
1	D	459	LEU
1	D	460	LEU
1	E	72	SER
1	E	75	ARG
1	E	122	ARG
1	E	126	SER
1	E	133	MET

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Mol	Chain	Res	Type
1	E	149	LEU
1	E	235	SER
1	E	239	SER
1	E	281	GLU
1	E	282	GLU
1	E	283	MET
1	E	327	THR
1	E	353	GLN
1	E	355	LEU
1	E	361	GLN
1	E	378	ILE
1	E	380	MET
1	E	389	LEU
1	E	433	GLU
1	E	434	LYS
1	E	437	ARG
1	E	459	LEU
1	E	460	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	332	GLN
1	A	441	ASN
1	B	332	GLN
1	B	368	GLN
1	B	441	ASN
1	C	102	HIS
1	D	454	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	A	501	-	5,8,8	0.40	0	5,10,10	1.44	1 (20%)
2	LEU	B	501	-	5,8,8	0.30	0	5,10,10	0.85	0
2	LEU	C	501	-	5,8,8	0.48	0	5,10,10	0.72	0
2	LEU	D	501	-	5,8,8	0.23	0	5,10,10	0.35	0
2	LEU	E	501	-	5,8,8	0.29	0	5,10,10	0.59	0

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	A	501	-	-	0/4/8/8	0/0/0/0
2	LEU	B	501	-	-	0/4/8/8	0/0/0/0
2	LEU	C	501	-	-	0/4/8/8	0/0/0/0
2	LEU	D	501	-	-	0/4/8/8	0/0/0/0
2	LEU	E	501	-	-	0/4/8/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	LEU	CG-CB-CA	3.22	121.66	114.80

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	363/480 (75%)	0.08	0	100	100	20, 32, 69, 96	0
1	B	363/480 (75%)	0.08	0	100	100	19, 31, 67, 94	0
1	C	360/480 (75%)	0.11	0	100	100	26, 41, 73, 97	0
1	D	361/480 (75%)	0.19	0	100	100	26, 40, 74, 95	0
1	E	362/480 (75%)	0.03	0	100	100	26, 39, 72, 87	0
All	All	1809/2400 (75%)	0.10	0	100	100	19, 37, 72, 97	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	LEU	C	501	9/9	0.97	0.44	3.72	32,35,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LEU	B	501	9/9	0.97	0.36	2.59	26,28,33,34	0
2	LEU	D	501	9/9	0.97	0.34	2.38	29,31,35,36	0
2	LEU	A	501	9/9	0.97	0.39	2.37	27,31,34,35	0
2	LEU	E	501	9/9	0.95	0.29	1.15	29,35,37,38	0

6.5 Other polymers (i)

There are no such residues in this entry.