Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 10:31 PM EDT

PDB ID	:	1X2H
Title	:	Crystal Structure of Lipate-Protein Ligase A from Escherichia coli complexed with lipoic acid
Authors	:	Fujiwara, K.; Toma, S.; Okamura-Ikeda, K.; Motokawa, Y.; Nakagawa, A.; Taniguchi, H.
Deposited on	:	2005-04-23
Resolution	:	2.91 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:

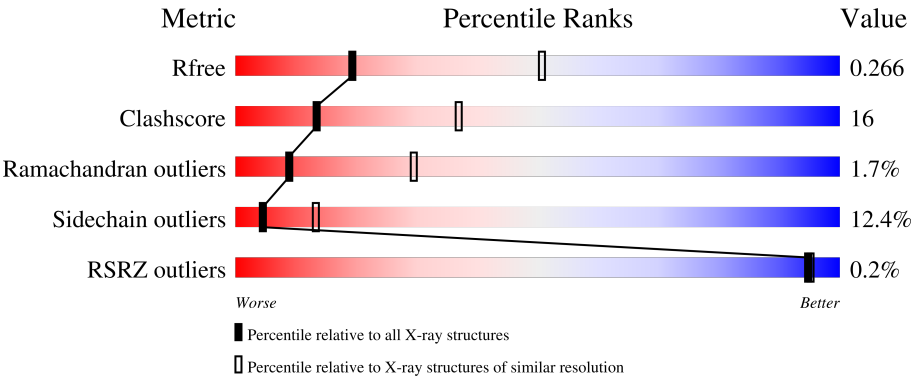
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	337	62% 31% 6% ·
1	B	337	68% 24% 5% ·
1	C	337	61% 32% 7% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7937 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.

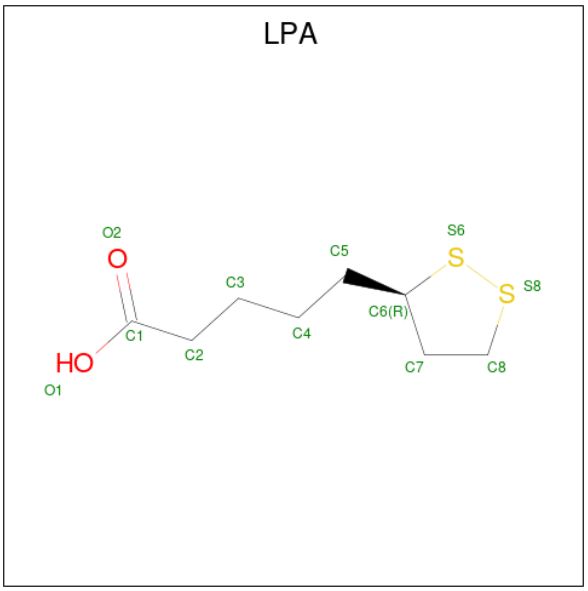
- Molecule 1 is a protein called Lipoate-protein ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	0	0
			2614	1644	466	493	6	5			
1	B	330	Total	C	N	O	S	Se	0	0	0
			2614	1644	466	493	6	5			
1	C	337	Total	C	N	O	S	Se	0	0	0
			2663	1673	476	503	6	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MSE	MET	modified residue	UNP P32099
A	60	MSE	MET	modified residue	UNP P32099
A	89	MSE	MET	modified residue	UNP P32099
A	306	MSE	MET	modified residue	UNP P32099
A	332	MSE	MET	modified residue	UNP P32099
B	27	MSE	MET	modified residue	UNP P32099
B	60	MSE	MET	modified residue	UNP P32099
B	89	MSE	MET	modified residue	UNP P32099
B	306	MSE	MET	modified residue	UNP P32099
B	332	MSE	MET	modified residue	UNP P32099
C	27	MSE	MET	modified residue	UNP P32099
C	60	MSE	MET	modified residue	UNP P32099
C	89	MSE	MET	modified residue	UNP P32099
C	306	MSE	MET	modified residue	UNP P32099
C	332	MSE	MET	modified residue	UNP P32099

- Molecule 2 is LIPOIC ACID (three-letter code: LPA) (formula: $C_8H_{14}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 12 8 2 2	0	0
2	B	1	Total C O S 12 8 2 2	0	0

- Molecule 3 is water.

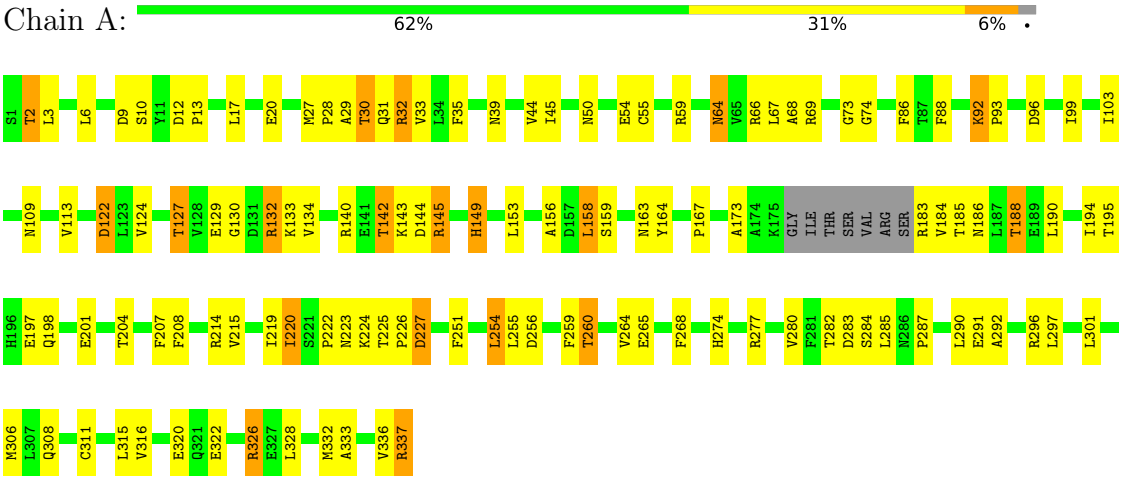
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	8	Total O 8 8	0	0
3	C	3	Total O 3 3	0	0

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.

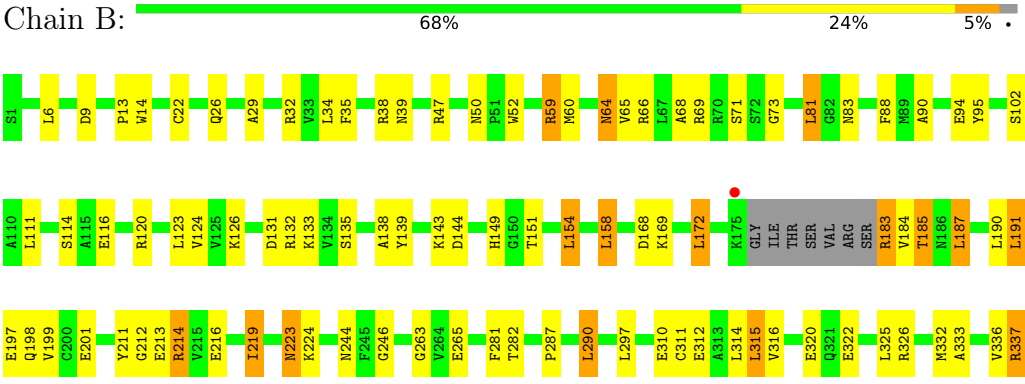
• Molecule 1: Lipoate-protein ligase A

Chain A:



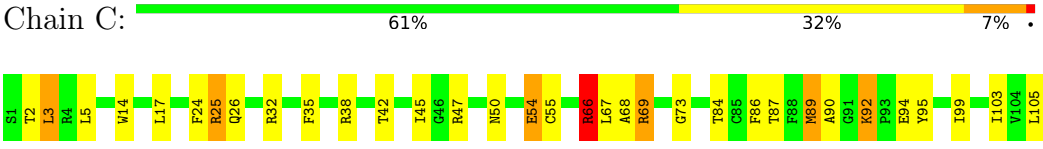
• Molecule 1: Lipoate-protein ligase A

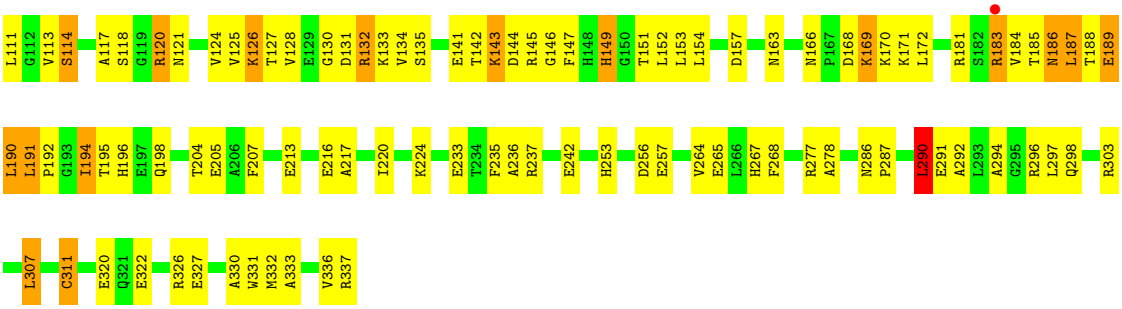
Chain B:



• Molecule 1: Lipoate-protein ligase A

Chain C:




L111 G112 V113 S114 A117 S118 G119 R120 N121 V124 V125 K126 T127 V128 E129 G130 D131 R132 K133 V134 S135 E141 T142 K143 D144 R145 G146 F147 H148 H149 G150 T151 L152 L153 L154 D157 N163 N166 P167 D168 K169 K170 K171 L172 R181 S182 R183 V184 T185 N186 L187 T188 E189
L190 L191 P192 G193 I194 T195 H196 E197 Q198 T204 E205 A206 F207 E213 E216 A217 I220 K224 E233 T234 F235 A236 R237 E242 H253 D256 E257 V264 E265 L266 H267 F268 R277 A278 N286 P287 L290 E291 A292 L293 A294 G295 R296 L297 Q298 R303
L307 C311 E320 Q321 E322 R326 E327 A330 W331 M332 A333 V336 R337

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	83.20Å 111.60Å 289.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.67 – 2.91 66.70 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.1 (66.67-2.91) 97.1 (66.70-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.271 0.184 , 0.266	Depositor DCC
R_{free} test set	1572 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7937	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

Bond lengths and bond angles in the following residue types are not validated in this section: LPA

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	0.97	2/2665 (0.1%)	0.97	4/3601 (0.1%)
1	B	0.95	3/2665 (0.1%)	0.96	4/3601 (0.1%)
1	C	0.93	3/2715 (0.1%)	0.96	5/3670 (0.1%)
All	All	0.95	8/8045 (0.1%)	0.96	13/10872 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	55	CYS	CB-SG	-6.64	1.71	1.82
1	B	197	GLU	CG-CD	6.40	1.61	1.51
1	A	197	GLU	CG-CD	6.29	1.61	1.51
1	C	311	CYS	CB-SG	-6.07	1.72	1.82
1	A	54	GLU	CG-CD	5.46	1.60	1.51
1	C	54	GLU	CD-OE2	5.33	1.31	1.25
1	B	139	TYR	CD1-CE1	5.06	1.47	1.39
1	B	311	CYS	CB-SG	-5.05	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	66	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	290	LEU	CA-CB-CG	-6.22	100.99	115.30
1	B	326	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	227	ASP	CB-CA-C	5.75	121.90	110.40
1	C	290	LEU	CA-CB-CG	-5.75	102.07	115.30
1	A	12	ASP	CB-CG-OD2	-5.52	113.34	118.30
1	A	3	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	172	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	111	LEU	CA-CB-CG	5.23	127.33	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	69	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	187	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	69	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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	2614	0	2551	94	0
1	B	2614	0	2551	73	0
1	C	2663	0	2605	97	0
2	A	12	0	13	0	0
2	B	12	0	13	1	0
3	A	11	0	0	1	0
3	B	8	0	0	2	0
3	C	3	0	0	1	0
All	All	7937	0	7733	252	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 16.

All (252) 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:332:MSE:SE	1:B:332:MSE:CE	2.15	1.42
1:B:158:LEU:HD12	1:B:158:LEU:H	1.17	1.04
1:A:282:THR:HG21	1:A:290:LEU:HD12	1.39	1.03
1:C:286:ASN:HB3	3:C:338:HOH:O	1.59	0.99
1:C:89:MSE:HE3	1:C:145:ARG:HB2	1.40	0.99
1:B:83:ASN:HD22	1:B:151:THR:HG21	1.30	0.94
1:A:142:THR:HG23	1:A:143:LYS:H	1.35	0.91
1:A:127:THR:HG22	1:A:129:GLU:H	1.35	0.89
1:A:92:LYS:HB2	1:A:92:LYS:NZ	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:CG2	1:A:143:LYS:N	2.36	0.88
1:C:2:THR:HG22	1:C:213:GLU:OE1	1.76	0.86
1:A:66:ARG:HH21	1:B:64:ASN:HD22	1.23	0.86
1:B:158:LEU:H	1:B:158:LEU:CD1	1.87	0.85
1:B:69:ARG:H	1:B:244:ASN:HD22	1.20	0.84
1:A:142:THR:HG23	1:A:143:LYS:N	1.95	0.82
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.43	0.81
1:B:183:ARG:HB3	1:B:183:ARG:HH11	1.43	0.80
1:A:132:ARG:HH11	1:A:132:ARG:HB3	1.45	0.79
1:B:158:LEU:HD12	1:B:158:LEU:N	1.97	0.79
1:C:89:MSE:CE	1:C:145:ARG:HB2	2.13	0.78
1:B:183:ARG:HB3	1:B:183:ARG:NH1	1.98	0.78
1:A:2:THR:OG1	1:A:32:ARG:NH1	2.19	0.76
1:B:59:ARG:HH11	1:B:59:ARG:HG2	1.52	0.75
1:B:69:ARG:H	1:B:244:ASN:ND2	1.85	0.74
1:C:127:THR:H	1:C:130:GLY:HA2	1.54	0.71
1:A:127:THR:CG2	1:A:129:GLU:H	2.03	0.71
1:A:158:LEU:HD12	1:A:159:SER:H	1.56	0.71
1:A:66:ARG:NH2	1:B:64:ASN:HD22	1.88	0.70
1:B:154:LEU:HD11	1:B:199:VAL:HG21	1.73	0.69
1:C:142:THR:HG22	1:C:143:LYS:N	2.07	0.69
1:C:303:ARG:O	1:C:307:LEU:HD12	1.92	0.69
1:C:26:GLN:HA	1:C:26:GLN:OE1	1.92	0.69
1:A:127:THR:HG22	1:A:129:GLU:N	2.07	0.69
1:B:123:LEU:HB2	1:B:135:SER:HB3	1.74	0.69
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.05	0.69
1:A:92:LYS:HB2	1:A:92:LYS:HZ3	1.55	0.68
1:B:126:LYS:HD3	1:B:131:ASP:OD1	1.92	0.68
1:B:183:ARG:NH1	3:B:346:HOH:O	2.25	0.68
1:C:89:MSE:HE3	1:C:145:ARG:CB	2.20	0.68
1:B:83:ASN:HB3	1:B:151:THR:CG2	2.25	0.66
1:A:2:THR:HG1	1:A:32:ARG:HH11	1.43	0.66
1:A:132:ARG:HB3	1:A:132:ARG:NH1	2.10	0.66
1:C:336:VAL:HG12	1:C:336:VAL:O	1.95	0.66
1:A:254:LEU:HD12	1:A:255:LEU:N	2.11	0.66
1:C:120:ARG:HB3	1:C:120:ARG:NH1	2.11	0.65
1:A:127:THR:HB	1:A:130:GLY:O	1.97	0.64
1:C:90:ALA:HB3	1:C:95:TYR:HB2	1.78	0.64
1:C:142:THR:HG22	1:C:144:ASP:H	1.61	0.64
1:A:20:GLU:OE2	1:A:149:HIS:ND1	2.31	0.64
1:C:109:ASN:HA	1:C:113:VAL:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:HB3	3:B:346:HOH:O	1.98	0.63
1:C:133:LYS:HD3	1:C:183:ARG:HH21	1.64	0.62
1:B:213:GLU:HG2	1:B:214:ARG:N	2.14	0.62
1:A:204:THR:O	1:A:207:PHE:HB3	2.01	0.61
1:B:47:ARG:HD3	1:B:71:SER:O	2.01	0.61
1:A:27:MSE:SE	1:A:33:VAL:HG21	2.51	0.61
1:C:2:THR:CG2	1:C:213:GLU:OE1	2.49	0.60
1:C:169:LYS:H	1:C:169:LYS:HD3	1.66	0.60
1:B:312:GLU:O	1:B:315:LEU:HB2	2.00	0.60
1:B:191:LEU:O	1:B:192:PRO:C	2.39	0.60
1:B:32:ARG:NH2	1:B:94:GLU:OE2	2.24	0.60
1:A:73:GLY:HA3	1:A:287:PRO:HD3	1.83	0.60
1:B:337:ARG:HG3	1:B:337:ARG:NH1	2.17	0.60
1:A:282:THR:CG2	1:A:290:LEU:HD12	2.25	0.59
1:B:68:ALA:HA	1:B:244:ASN:ND2	2.16	0.59
1:C:132:ARG:HH21	1:C:181:ARG:HH22	1.50	0.59
1:C:169:LYS:HD3	1:C:169:LYS:N	2.18	0.59
1:A:86:PHE:CD1	1:A:88:PHE:HE1	2.20	0.58
1:C:3:LEU:HD12	1:C:32:ARG:HB2	1.85	0.58
1:C:45:ILE:HG12	1:C:67:LEU:HD11	1.85	0.58
1:B:190:LEU:O	1:B:191:LEU:HG	2.04	0.57
1:A:156:ALA:H	1:A:186:ASN:HD21	1.51	0.57
1:C:89:MSE:HE2	1:C:90:ALA:C	2.24	0.57
1:A:92:LYS:HB2	1:A:92:LYS:HZ2	1.67	0.57
1:B:59:ARG:HG2	1:B:59:ARG:NH1	2.19	0.57
1:A:64:ASN:N	1:A:64:ASN:HD22	2.02	0.57
1:A:256:ASP:HA	1:A:264:VAL:O	2.06	0.56
1:C:253:HIS:HB2	1:C:268:PHE:O	2.05	0.56
1:B:216:GLU:OE1	1:B:216:GLU:HA	2.04	0.56
1:A:109:ASN:HA	1:A:113:VAL:O	2.05	0.56
1:A:301:LEU:HB3	1:A:306:MSE:HG3	1.87	0.55
1:C:142:THR:HG22	1:C:143:LYS:H	1.70	0.55
1:C:92:LYS:HE2	1:C:143:LYS:O	2.07	0.55
1:B:138:ALA:HB1	2:B:338:LPA:O2	2.06	0.55
1:B:223:ASN:C	1:B:223:ASN:HD22	2.10	0.55
1:B:83:ASN:ND2	1:B:151:THR:HG21	2.13	0.55
1:A:92:LYS:NZ	1:A:92:LYS:CB	2.64	0.54
1:B:290:LEU:N	1:B:290:LEU:HD12	2.23	0.54
1:A:225:THR:HG22	1:A:226:PRO:O	2.08	0.54
1:C:264:VAL:HG21	1:C:290:LEU:HD21	1.89	0.54
1:C:216:GLU:HA	1:C:216:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:SER:HB2	1:C:152:LEU:HD23	1.89	0.54
1:B:124:VAL:HG12	1:B:133:LYS:HA	1.88	0.53
1:C:294:ALA:O	1:C:298:GLN:NE2	2.39	0.53
1:C:113:VAL:HG23	1:C:191:LEU:HD23	1.91	0.53
1:C:142:THR:CG2	1:C:143:LYS:N	2.70	0.53
1:C:168:ASP:HB3	1:C:171:LYS:HG3	1.89	0.53
1:B:9:ASP:HB2	1:B:219:ILE:HG22	1.91	0.53
1:B:90:ALA:HB3	1:B:95:TYR:CG	2.44	0.53
1:C:90:ALA:HB3	1:C:95:TYR:CG	2.43	0.53
1:C:131:ASP:C	1:C:132:ARG:HD2	2.29	0.53
1:A:92:LYS:HZ3	1:A:92:LYS:CB	2.22	0.52
1:A:132:ARG:NH1	1:A:185:THR:OG1	2.41	0.52
1:B:69:ARG:N	1:B:244:ASN:HD22	1.97	0.52
1:C:109:ASN:O	1:C:111:LEU:N	2.43	0.52
1:C:135:SER:HB2	1:C:152:LEU:CD2	2.40	0.52
1:B:34:LEU:HD13	1:B:88:PHE:CE1	2.44	0.52
1:A:134:VAL:C	1:A:153:LEU:HD12	2.31	0.51
1:B:73:GLY:HA3	1:B:287:PRO:HD3	1.92	0.51
1:B:133:LYS:HB3	1:B:184:VAL:HG22	1.93	0.51
1:A:99:ILE:O	1:A:103:ILE:HD12	2.10	0.51
1:A:142:THR:HG22	1:A:143:LYS:N	2.20	0.51
1:C:169:LYS:H	1:C:169:LYS:CD	2.23	0.51
1:C:204:THR:O	1:C:207:PHE:HB3	2.11	0.51
1:B:290:LEU:HD12	1:B:290:LEU:H	1.74	0.50
1:A:122:ASP:OD1	1:A:122:ASP:N	2.39	0.50
1:A:220:ILE:HG21	1:A:226:PRO:HB3	1.93	0.50
1:C:5:LEU:HD23	1:C:217:ALA:HB2	1.93	0.50
1:C:143:LYS:H	1:C:143:LYS:HD3	1.76	0.50
1:A:290:LEU:CD2	1:A:328:LEU:HD11	2.42	0.50
1:B:60:MSE:HE3	1:B:65:VAL:HG12	1.92	0.50
1:A:28:PRO:C	1:A:30:THR:H	2.14	0.50
1:C:131:ASP:O	1:C:132:ARG:HD2	2.12	0.50
1:A:220:ILE:CG2	1:A:226:PRO:HB3	2.42	0.50
1:B:187:LEU:HB3	1:B:194:ILE:CD1	2.42	0.49
1:B:83:ASN:HB3	1:B:151:THR:HG23	1.94	0.49
1:C:126:LYS:HG3	1:C:130:GLY:O	2.11	0.49
1:A:156:ALA:H	1:A:186:ASN:ND2	2.10	0.49
1:C:120:ARG:HB3	1:C:120:ARG:HH11	1.74	0.49
1:A:195:THR:OG1	1:A:198:GLN:HB2	2.13	0.49
1:C:132:ARG:NH2	1:C:181:ARG:HH22	2.10	0.49
1:A:10:SER:HB2	1:A:222:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:CG2	1:A:144:ASP:OD1	2.61	0.49
1:B:211:TYR:O	1:B:213:GLU:N	2.46	0.49
1:A:64:ASN:HB3	1:B:64:ASN:HB2	1.95	0.49
1:C:166:ASN:N	1:C:166:ASN:ND2	2.61	0.49
1:C:195:THR:OG1	1:C:198:GLN:HG3	2.13	0.48
1:A:132:ARG:HH11	1:A:132:ARG:CB	2.20	0.48
1:C:90:ALA:HB3	1:C:95:TYR:CB	2.41	0.48
1:A:183:ARG:CZ	1:A:183:ARG:HB3	2.43	0.48
1:A:50:ASN:C	1:A:50:ASN:OD1	2.51	0.48
1:B:22:CYS:HA	1:B:26:GLN:HG2	1.95	0.48
1:C:24:PHE:HD1	1:C:147:PHE:CD1	2.31	0.48
1:A:142:THR:HG21	1:A:144:ASP:OD1	2.14	0.48
1:A:311:CYS:HB2	1:A:332:MSE:HE1	1.95	0.48
1:C:142:THR:CG2	1:C:143:LYS:H	2.26	0.48
1:C:132:ARG:HH21	1:C:181:ARG:NH2	2.12	0.47
1:A:44:VAL:HA	1:A:68:ALA:O	2.13	0.47
1:A:274:HIS:NE2	1:C:242:GLU:OE2	2.43	0.47
1:B:50:ASN:HB2	1:B:281:PHE:CD1	2.48	0.47
1:C:188:THR:O	1:C:192:PRO:HA	2.13	0.47
1:A:86:PHE:O	1:A:149:HIS:HA	2.14	0.47
1:A:282:THR:HG21	1:A:290:LEU:CD1	2.27	0.47
1:A:86:PHE:CD1	1:A:88:PHE:CE1	3.02	0.47
1:A:194:ILE:HA	1:A:198:GLN:OE1	2.15	0.47
1:A:277:ARG:HB3	1:C:277:ARG:HB3	1.97	0.47
1:C:67:LEU:HD12	1:C:68:ALA:N	2.29	0.47
1:C:114:SER:O	1:C:125:VAL:HG12	2.15	0.47
1:C:86:PHE:O	1:C:149:HIS:HA	2.14	0.46
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.63	0.46
1:A:92:LYS:HG2	1:A:93:PRO:HA	1.98	0.46
1:C:109:ASN:C	1:C:111:LEU:H	2.19	0.46
1:C:126:LYS:HA	1:C:130:GLY:HA2	1.98	0.46
1:A:92:LYS:NZ	1:A:143:LYS:O	2.47	0.46
1:C:117:ALA:O	1:C:118:SER:C	2.52	0.46
1:A:67:LEU:HG	1:A:68:ALA:N	2.31	0.46
1:B:194:ILE:H	1:B:194:ILE:HG12	1.57	0.46
1:B:132:ARG:HB3	1:B:185:THR:HB	1.98	0.46
1:C:166:ASN:N	1:C:166:ASN:HD22	2.14	0.45
1:C:330:ALA:O	1:C:333:ALA:HB3	2.16	0.45
1:A:183:ARG:HG2	1:A:183:ARG:O	2.17	0.45
1:B:6:LEU:O	1:B:35:PHE:HA	2.16	0.45
1:C:190:LEU:H	1:C:190:LEU:HG	1.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:CG	1:B:59:ARG:NH1	2.74	0.45
1:A:336:VAL:HG12	1:A:337:ARG:N	2.30	0.45
1:C:267:HIS:O	1:C:278:ALA:HA	2.17	0.45
1:C:84:THR:HG23	1:C:196:HIS:CE1	2.52	0.45
1:C:170:LYS:HE3	1:C:256:ASP:OD1	2.17	0.45
1:C:264:VAL:CG2	1:C:290:LEU:CD2	2.95	0.45
1:C:233:GLU:OE1	1:C:237:ARG:NE	2.43	0.44
1:C:95:TYR:HD2	1:C:146:GLY:HA3	1.82	0.44
1:C:311:CYS:CB	1:C:332:MSE:HE1	2.47	0.44
1:C:264:VAL:HG22	1:C:290:LEU:CD2	2.48	0.44
1:A:59:ARG:HG2	1:A:164:TYR:CE1	2.53	0.44
1:C:264:VAL:HG22	1:C:290:LEU:HD22	1.98	0.44
1:A:27:MSE:HE2	1:A:27:MSE:HB3	1.60	0.44
1:C:90:ALA:CB	1:C:95:TYR:HB2	2.46	0.44
1:B:38:ARG:NH1	1:B:81:LEU:O	2.47	0.44
1:A:96:ASP:C	1:A:96:ASP:OD1	2.56	0.43
1:A:292:ALA:HB2	1:C:292:ALA:HB2	2.00	0.43
1:B:47:ARG:NH2	1:B:287:PRO:HG2	2.33	0.43
1:C:154:LEU:HD13	1:C:194:ILE:HG22	1.99	0.43
1:C:186:ASN:HB3	1:C:187:LEU:H	1.52	0.43
1:A:260:THR:HG23	3:A:341:HOH:O	2.17	0.43
1:C:47:ARG:HA	1:C:69:ARG:HD3	2.00	0.43
1:B:108:LEU:O	1:B:109:ASN:C	2.57	0.43
1:C:134:VAL:O	1:C:153:LEU:HD12	2.18	0.43
1:A:208:PHE:CE2	1:A:214:ARG:HB3	2.54	0.43
1:A:251:PHE:CD1	1:A:251:PHE:N	2.87	0.43
1:A:259:PHE:O	1:A:260:THR:C	2.56	0.43
1:A:308:GLN:CD	1:A:333:ALA:HB2	2.38	0.43
1:B:213:GLU:CG	1:B:214:ARG:N	2.80	0.43
1:C:297:LEU:HD23	1:C:297:LEU:HA	1.86	0.43
1:A:223:ASN:HB3	1:B:52:TRP:CH2	2.53	0.42
1:C:35:PHE:HB3	1:C:87:THR:HB	2.00	0.42
1:A:74:GLY:HA2	1:A:283:ASP:O	2.19	0.42
1:B:102:SER:HA	1:B:105:LEU:HB2	2.01	0.42
1:A:223:ASN:HB3	1:B:52:TRP:CZ3	2.55	0.42
1:B:211:TYR:C	1:B:213:GLU:H	2.22	0.42
1:B:315:LEU:HD22	1:B:325:LEU:HD12	2.01	0.42
1:A:30:THR:HG22	1:A:31:GLN:HG2	2.02	0.42
1:C:105:LEU:O	1:C:108:LEU:HB2	2.19	0.42
1:A:6:LEU:O	1:A:35:PHE:HA	2.19	0.42
1:C:127:THR:N	1:C:130:GLY:HA2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:LYS:N	1:C:169:LYS:CD	2.81	0.42
1:A:9:ASP:HB2	1:A:219:ILE:CG2	2.50	0.42
1:C:143:LYS:HE3	1:C:143:LYS:HB2	1.86	0.42
1:C:132:ARG:HG3	1:C:185:THR:OG1	2.20	0.42
1:C:235:PHE:O	1:C:236:ALA:C	2.58	0.42
1:A:142:THR:HG22	1:A:145:ARG:H	1.84	0.42
1:A:308:GLN:NE2	1:A:333:ALA:HB2	2.35	0.42
1:B:168:ASP:O	1:B:172:LEU:HG	2.19	0.42
1:C:66:ARG:HA	1:C:66:ARG:HD3	1.44	0.42
1:A:291:GLU:OE2	1:C:296:ARG:HD2	2.20	0.41
1:A:296:ARG:HD2	1:C:291:GLU:OE2	2.20	0.41
1:A:268:PHE:N	1:A:268:PHE:CD1	2.88	0.41
1:A:326:ARG:HH12	1:C:25:ARG:HB2	1.85	0.41
1:B:90:ALA:HB3	1:B:95:TYR:CD2	2.54	0.41
1:A:92:LYS:CG	1:A:93:PRO:HA	2.50	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.91	0.41
1:B:314:LEU:O	1:B:315:LEU:C	2.58	0.41
1:C:73:GLY:HA3	1:C:287:PRO:HD3	2.03	0.41
1:B:13:PRO:HA	1:B:39:ASN:OD1	2.20	0.41
1:C:257:GLU:HB2	1:C:331:TRP:CE2	2.56	0.41
1:B:310:GLU:OE1	1:B:310:GLU:HA	2.21	0.41
1:C:42:THR:HA	1:C:66:ARG:O	2.20	0.41
1:A:45:ILE:HG13	1:A:69:ARG:HA	2.01	0.41
1:B:263:GLY:O	1:B:282:THR:HA	2.21	0.41
1:C:14:TRP:CH2	1:C:66:ARG:HD2	2.55	0.41
1:A:13:PRO:HB3	1:A:39:ASN:HB3	2.02	0.41
1:B:315:LEU:HD22	1:B:315:LEU:HA	1.87	0.41
1:B:332:MSE:O	1:B:333:ALA:C	2.59	0.41
1:C:2:THR:HG23	1:C:3:LEU:HD13	2.03	0.41
1:A:254:LEU:O	1:A:255:LEU:HD23	2.21	0.41
1:A:134:VAL:O	1:A:153:LEU:HD12	2.21	0.40
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.92	0.40
1:C:142:THR:HG21	1:C:144:ASP:OD1	2.21	0.40
1:A:280:VAL:HG11	1:A:290:LEU:HB3	2.02	0.40
1:A:296:ARG:NH1	1:C:291:GLU:OE2	2.51	0.40
1:B:14:TRP:CH2	1:B:66:ARG:HB3	2.56	0.40
1:A:64:ASN:N	1:A:64:ASN:ND2	2.69	0.40
1:C:99:ILE:O	1:C:103:ILE:HG13	2.22	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	326/337 (97%)	301 (92%)	20 (6%)	5 (2%)	10 32
1	B	326/337 (97%)	305 (94%)	16 (5%)	5 (2%)	10 32
1	C	335/337 (99%)	297 (89%)	31 (9%)	7 (2%)	7 24
All	All	987/1011 (98%)	903 (92%)	67 (7%)	17 (2%)	9 29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	THR
1	B	81	LEU
1	B	212	GLY
1	B	246	GLY
1	C	94	GLU
1	C	157	ASP
1	C	186	ASN
1	C	187	LEU
1	B	29	ALA
1	C	110	ALA
1	C	183	ARG
1	A	29	ALA
1	A	167	PRO
1	A	260	THR
1	C	189	GLU
1	A	173	ALA
1	B	192	PRO

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	276/277 (100%)	241 (87%)	35 (13%)	4	12
1	B	276/277 (100%)	246 (89%)	30 (11%)	6	18
1	C	282/277 (102%)	244 (86%)	38 (14%)	4	10
All	All	834/831 (100%)	731 (88%)	103 (12%)	4	13

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LEU
1	A	30	THR
1	A	32	ARG
1	A	55	CYS
1	A	64	ASN
1	A	92	LYS
1	A	122	ASP
1	A	124	VAL
1	A	127	THR
1	A	132	ARG
1	A	133	LYS
1	A	140	ARG
1	A	142	THR
1	A	149	HIS
1	A	158	LEU
1	A	163	ASN
1	A	184	VAL
1	A	188	THR
1	A	190	LEU
1	A	201	GLU
1	A	215	VAL
1	A	220	ILE
1	A	224	LYS
1	A	227	ASP
1	A	254	LEU
1	A	265	GLU
1	A	284	SER
1	A	297	LEU
1	A	315	LEU
1	A	316	VAL

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Mol	Chain	Res	Type
1	A	320	GLU
1	A	322	GLU
1	A	326	ARG
1	A	337	ARG
1	B	59	ARG
1	B	64	ASN
1	B	114	SER
1	B	116	GLU
1	B	120	ARG
1	B	143	LYS
1	B	144	ASP
1	B	149	HIS
1	B	154	LEU
1	B	158	LEU
1	B	169	LYS
1	B	172	LEU
1	B	183	ARG
1	B	185	THR
1	B	191	LEU
1	B	194	ILE
1	B	195	THR
1	B	198	GLN
1	B	201	GLU
1	B	214	ARG
1	B	219	ILE
1	B	223	ASN
1	B	224	LYS
1	B	265	GLU
1	B	315	LEU
1	B	316	VAL
1	B	320	GLU
1	B	322	GLU
1	B	336	VAL
1	B	337	ARG
1	C	3	LEU
1	C	17	LEU
1	C	25	ARG
1	C	38	ARG
1	C	50	ASN
1	C	54	GLU
1	C	66	ARG
1	C	89	MSE

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Mol	Chain	Res	Type
1	C	92	LYS
1	C	114	SER
1	C	120	ARG
1	C	121	ASN
1	C	124	VAL
1	C	126	LYS
1	C	128	VAL
1	C	132	ARG
1	C	141	GLU
1	C	143	LYS
1	C	149	HIS
1	C	151	THR
1	C	163	ASN
1	C	169	LYS
1	C	184	VAL
1	C	189	GLU
1	C	190	LEU
1	C	191	LEU
1	C	194	ILE
1	C	205	GLU
1	C	220	ILE
1	C	224	LYS
1	C	265	GLU
1	C	290	LEU
1	C	307	LEU
1	C	320	GLU
1	C	322	GLU
1	C	326	ARG
1	C	327	GLU
1	C	337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	155	ASN
1	A	186	ASN
1	A	247	GLN
1	A	267	HIS
1	A	279	GLN
1	B	64	ASN
1	B	83	ASN

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Mol	Chain	Res	Type
1	B	166	ASN
1	B	210	HIS
1	B	223	ASN
1	B	244	ASN
1	B	247	GLN
1	B	298	GLN
1	C	50	ASN
1	C	64	ASN
1	C	121	ASN
1	C	166	ASN
1	C	198	GLN
1	C	247	GLN
1	C	253	HIS
1	C	308	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	LPA	B	338	-	12,12,12	0.92	0	14,14,14	1.79	4 (28%)
2	LPA	A	338	-	12,12,12	0.78	0	14,14,14	1.40	1 (7%)

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	LPA	B	338	-	-	5/7/14/14	0/1/1/1
2	LPA	A	338	-	-	2/7/14/14	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	338	LPA	C3-C2-C1	-4.52	103.07	114.47
2	A	338	LPA	C6-S6-S8	3.10	106.28	95.56
2	B	338	LPA	C4-C3-C2	-2.31	104.90	113.19
2	B	338	LPA	O2-C1-C2	-2.27	115.77	123.08
2	B	338	LPA	O1-C1-C2	2.16	120.98	114.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	338	LPA	C3-C4-C5-C6
2	B	338	LPA	C1-C2-C3-C4
2	B	338	LPA	C3-C4-C5-C6
2	B	338	LPA	C2-C3-C4-C5
2	A	338	LPA	C4-C5-C6-S6
2	B	338	LPA	O2-C1-C2-C3
2	B	338	LPA	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	338	LPA	1	0

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, 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	325/337 (96%)	-0.15	0	100	100	16, 34, 53, 80	0
1	B	325/337 (96%)	-0.03	1 (0%)	94	94	19, 33, 63, 83	0
1	C	332/337 (98%)	0.14	1 (0%)	94	94	23, 41, 73, 79	0
All	All	982/1011 (97%)	-0.02	2 (0%)	95	95	16, 35, 67, 83	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	LYS	2.9
1	C	183	ARG	2.2

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	LPA	A	338	12/12	0.86	0.33	74,78,82,84	0
2	LPA	B	338	12/12	0.91	0.34	74,76,79,80	0

6.5 Other polymers (i)

There are no such residues in this entry.