Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:18 PM GMT

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
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:

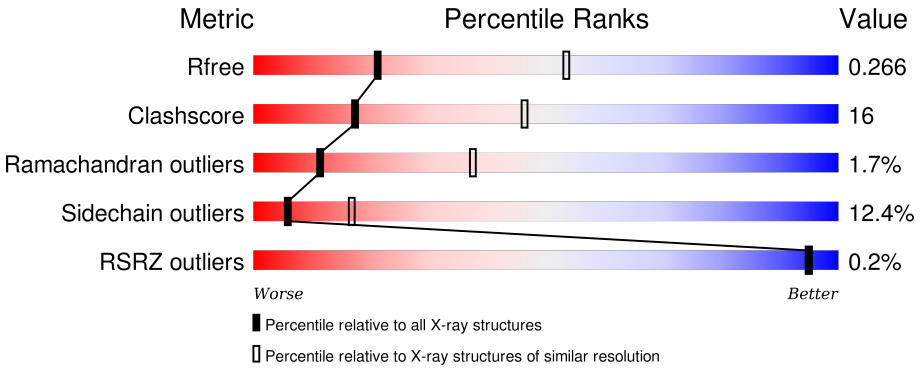
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (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 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	337	62% 31% 6% •
1	B	337	68% 24% 5% •
1	C	337	61% 32% 7% •

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	LPA	A	338	-	-	-	X
2	LPA	B	338	-	-	-	X

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.

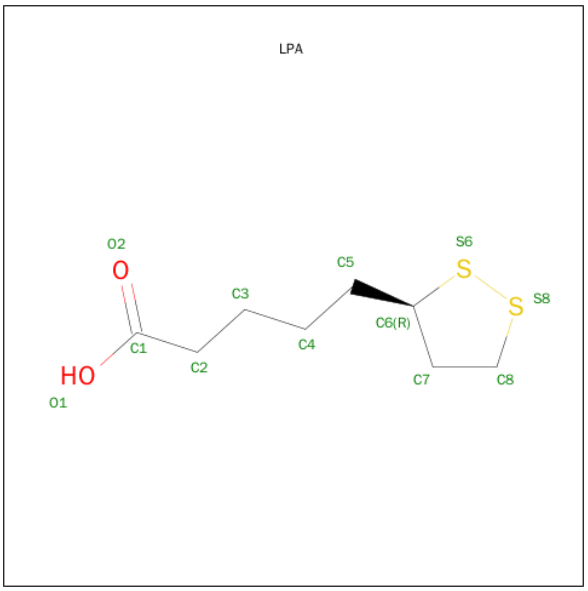
- Molecule 1 is a protein called Lipoate-protein ligase A.

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.

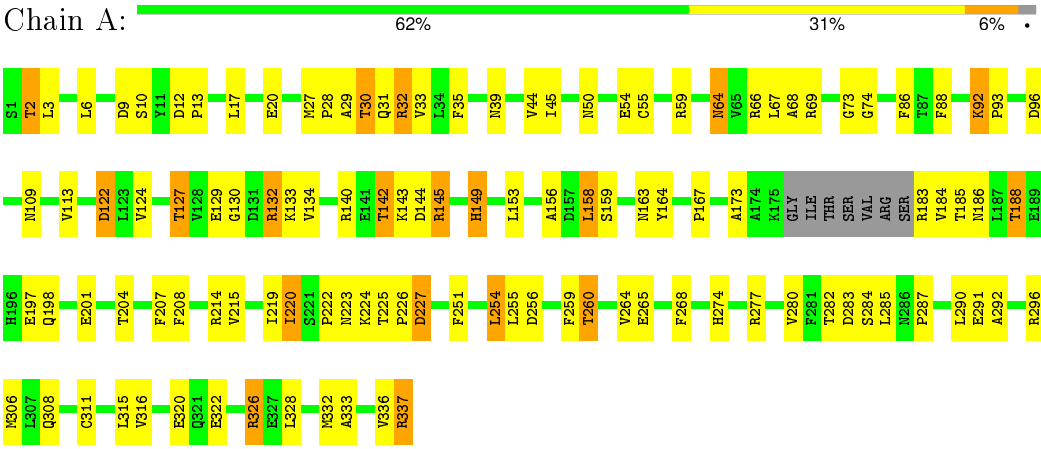
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	8	Total O 8 8	0	0
3	C	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

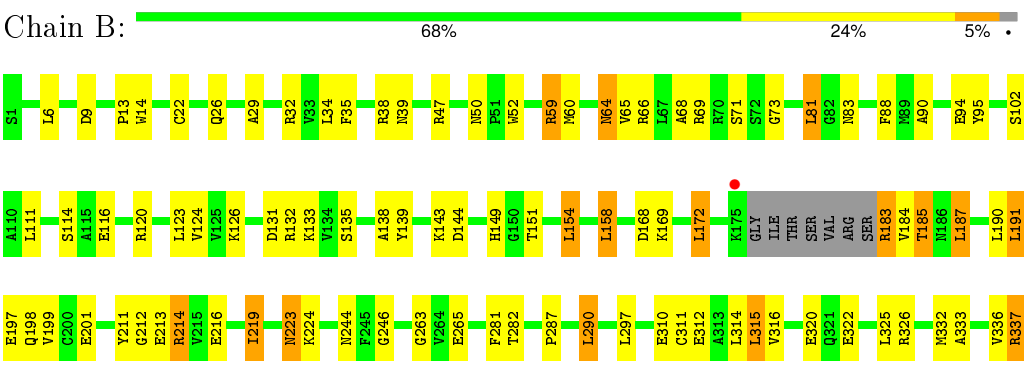
- Molecule 1: Lipoate-protein ligase A

Chain A:



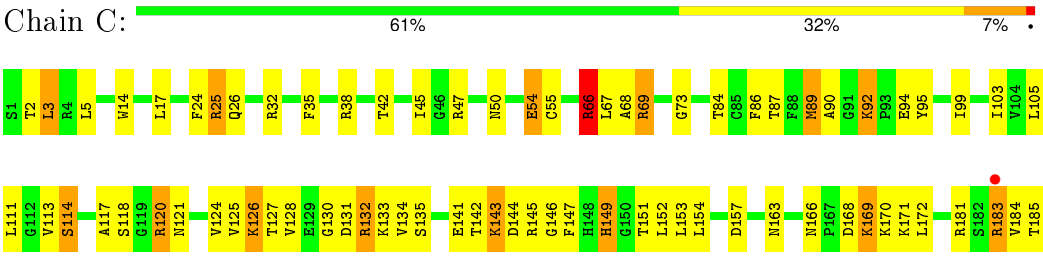
- Molecule 1: Lipoate-protein ligase A

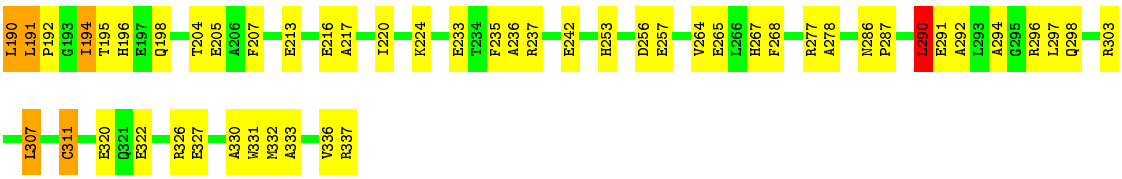
Chain B:



- Molecule 1: Lipoate-protein ligase A

Chain C:




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 (5.68%)	DCC
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 , 44.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 30079 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

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:NZ	1:A:92:LYS:HB2	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:CD1	1:B:158:LEU:H	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:HH11	1:B:337:ARG:HG3	1.43	0.81
1:B:183:ARG:HH11	1:B:183:ARG:HB3	1.43	0.80
1:A:132:ARG:HB3	1:A:132:ARG:HH11	1.45	0.79
1:B:158:LEU:N	1:B:158:LEU:HD12	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:OE1	1:C:26:GLN:HA	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:HZ3	1:A:92:LYS:HB2	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:132:ARG:HB3	1:A:132:ARG:NH1	2.10	0.66
1:A:2:THR:HG1	1:A:32:ARG:HH11	1.43	0.66
1:C:336:VAL:O	1:C:336:VAL:HG12	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:HD3	1:C:169:LYS:H	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:B:337:ARG:HG3	1:B:337:ARG:NH1	2.17	0.60
1:A:73:GLY:HA3	1:A:287:PRO:HD3	1.83	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:HZ2	1:A:92:LYS:HB2	1.67	0.57
1:B:59:ARG:NH1	1:B:59:ARG:HG2	2.19	0.57
1:A:64:ASN:HD22	1:A:64:ASN:N	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:223:ASN:C	1:B:223:ASN:HD22	2.10	0.55
1:B:138:ALA:HB1	2:B:338:LPA:O2	2.06	0.55
1:B:83:ASN:ND2	1:B:151:THR:HG21	2.13	0.55
1:A:92:LYS:CB	1:A:92:LYS:NZ	2.64	0.54
1:B:290:LEU:HD12	1:B:290:LEU:N	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:C:294:ALA:O	1:C:298:GLN:NE2	2.39	0.53
1:B:124:VAL:HG12	1:B:133:LYS:HA	1.88	0.53
1:C:142:THR:CG2	1:C:143:LYS:N	2.70	0.53
1:C:113:VAL:HG23	1:C:191:LEU:HD23	1.91	0.53
1:C:168:ASP:HB3	1:C:171:LYS:HG3	1.89	0.53
1:C:90:ALA:HB3	1:C:95:TYR:CG	2.43	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:131:ASP:C	1:C:132:ARG:HD2	2.29	0.53
1:A:92:LYS:CB	1:A:92:LYS:HZ3	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:142:THR:HG22	1:A:143:LYS:N	2.20	0.51
1:A:99:ILE:O	1:A:103:ILE:HD12	2.10	0.51
1:C:169:LYS:CD	1:C:169:LYS:H	2.23	0.51
1:C:204:THR:O	1:C:207:PHE:HB3	2.11	0.51
1:B:290:LEU:H	1:B:290:LEU:HD12	1.74	0.50
1:A:122:ASP:OD1	1:A:122:ASP:N	2.39	0.50
1:C:143:LYS:H	1:C:143:LYS:HD3	1.76	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: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:C:131:ASP:O	1:C:132:ARG:HD2	2.12	0.50
1:A:28:PRO:C	1:A:30:THR:H	2.14	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:HH11	1:C:120:ARG:HB3	1.74	0.49
1:C:132:ARG:NH2	1:C:181:ARG:HH22	2.10	0.49
1:A:195:THR:OG1	1:A:198:GLN:HB2	2.13	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:ND2	1:C:166:ASN:N	2.61	0.49
1:C:195:THR:OG1	1:C:198:GLN:HG3	2.13	0.48
1:A:132:ARG:CB	1:A:132:ARG:HH11	2.20	0.48
1:C:90:ALA:HB3	1:C:95:TYR:CB	2.41	0.48
1:A:183:ARG:HB3	1:A:183:ARG:CZ	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:C:142:THR:CG2	1:C:143:LYS:H	2.26	0.48
1:A:311:CYS:HB2	1:A:332:MSE:HE1	1.95	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:C:188:THR:O	1:C:192:PRO:HA	2.13	0.47
1:B:50:ASN:HB2	1:B:281:PHE:CD1	2.48	0.47
1:A:274:HIS:NE2	1:C:242:GLU:OE2	2.43	0.47
1:A:282:THR:HG21	1:A:290:LEU:CD1	2.27	0.47
1:A:86:PHE:O	1:A:149:HIS:HA	2.14	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:C:67:LEU:HD12	1:C:68:ALA:N	2.29	0.47
1:A:277:ARG:HB3	1:C:277:ARG:HB3	1.97	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:HA	1:B:81:LEU:HD23	1.63	0.46
1:A:92:LYS:HG2	1:A:93:PRO:HA	1.98	0.46
1:C:126:LYS:HA	1:C:130:GLY:HA2	1.98	0.46
1:C:109:ASN:C	1:C:111:LEU:H	2.19	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:B:194:ILE:H	1:B:194:ILE:HG12	1.57	0.46
1:A:67:LEU:HG	1:A:68:ALA:N	2.31	0.46
1:B:132:ARG:HB3	1:B:185:THR:HB	1.98	0.46
1:C:166:ASN:HD22	1:C:166:ASN:N	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:C:267:HIS:O	1:C:278:ALA:HA	2.17	0.45
1:A:336:VAL:HG12	1:A:337:ARG:N	2.30	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:C:264:VAL:HG22	1:C:290:LEU:HD22	1.98	0.44
1:A:59:ARG:HG2	1:A:164:TYR:CE1	2.53	0.44
1:C:90:ALA:CB	1:C:95:TYR:HB2	2.46	0.44
1:A:27:MSE:HB3	1:A:27:MSE:HE2	1.60	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:B:47:ARG:NH2	1:B:287:PRO:HG2	2.33	0.43
1:C:186:ASN:HB3	1:C:187:LEU:H	1.52	0.43
1:C:154:LEU:HD13	1:C:194:ILE:HG22	1.99	0.43
1:A:292:ALA:HB2	1:C:292:ALA:HB2	2.00	0.43
1:C:47:ARG:HA	1:C:69:ARG:HD3	2.00	0.43
1:A:260:THR:HG23	3:A:341:HOH:O	2.17	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:259:PHE:O	1:A:260:THR:C	2.56	0.43
1:A:251:PHE:CD1	1:A:251:PHE:N	2.87	0.43
1:A:308:GLN:CD	1:A:333:ALA:HB2	2.38	0.43
1:A:208:PHE:CE2	1:A:214:ARG:HB3	2.54	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:B:102:SER:HA	1:B:105:LEU:HB2	2.01	0.42
1:A:74:GLY:HA2	1:A:283:ASP:O	2.19	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:223:ASN:HB3	1:B:52:TRP:CZ3	2.55	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:C:127:THR:N	1:C:130:GLY:HA2	2.30	0.42
1:C:169:LYS:CD	1:C:169:LYS:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:O	1:A:35:PHE:HA	2.19	0.42
1:C:143:LYS:HB2	1:C:143:LYS:HE3	1.86	0.42
1:A:9:ASP:HB2	1:A:219:ILE:CG2	2.50	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:C:66:ARG:HA	1:C:66:ARG:HD3	1.44	0.42
1:B:168:ASP:O	1:B:172:LEU:HG	2.19	0.42
1:A:296:ARG:HD2	1:C:291:GLU:OE2	2.20	0.41
1:A:291:GLU:OE2	1:C:296:ARG:HD2	2.20	0.41
1:B:90:ALA:HB3	1:B:95:TYR:CD2	2.54	0.41
1:A:268:PHE:CD1	1:A:268:PHE:N	2.88	0.41
1:A:326:ARG:HH12	1:C:25:ARG:HB2	1.85	0.41
1:A:92:LYS:CG	1:A:93:PRO:HA	2.50	0.41
1:B:314:LEU:O	1:B:315:LEU:C	2.58	0.41
1:A:285:LEU:HA	1:A:285:LEU:HD23	1.91	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:C:42:THR:HA	1:C:66:ARG:O	2.20	0.41
1:B:310:GLU:HA	1:B:310:GLU:OE1	2.21	0.41
1:C:14:TRP:CH2	1:C:66:ARG:HD2	2.55	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: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:B:315:LEU:HA	1:B:315:LEU:HD22	1.87	0.41
1:A:13:PRO:HB3	1:A:39:ASN:HB3	2.02	0.41
1:A:254:LEU:O	1:A:255:LEU:HD23	2.21	0.41
1:C:142:THR:HG21	1:C:144:ASP:OD1	2.21	0.40
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: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

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	326/337 (97%)	301 (92%)	20 (6%)	5 (2%)	13	41
1	B	326/337 (97%)	305 (94%)	16 (5%)	5 (2%)	13	41
1	C	335/337 (99%)	297 (89%)	31 (9%)	7 (2%)	9	32
All	All	987/1011 (98%)	903 (92%)	67 (7%)	17 (2%)	11	37

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

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%)	5 16
1	B	276/277 (100%)	246 (89%)	30 (11%)	8 23
1	C	282/277 (102%)	244 (86%)	38 (14%)	5 13
All	All	834/831 (100%)	731 (88%)	103 (12%)	6 17

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

Some 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 carbohydrates 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	A	338	-	8,12,12	0.52	0	6,14,14	0.96	0
2	LPA	B	338	-	8,12,12	0.59	0	6,14,14	1.35	1 (16%)

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

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	B	338	LPA	C4-C3-C2	-2.13	104.90	113.90

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.14	0 100 100	16, 34, 53, 80	0
1	B	325/337 (96%)	-0.02	1 (0%) 94 93	19, 33, 63, 83	0
1	C	332/337 (98%)	0.15	1 (0%) 94 93	23, 41, 73, 79	0
All	All	982/1011 (97%)	-0.00	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	3.0
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 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	LPA	B	338	12/12	0.91	0.34	4.86	74,76,79,80	0
2	LPA	A	338	12/12	0.86	0.33	4.82	74,78,82,84	0

6.5 Other polymers (i)

There are no such residues in this entry.