Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 02:18 pm GMT

PDB ID	:	2C8M
Title	:	Structure of protein Ta0514, putative lipoate protein ligase from T. acidophilum with bound lipoic acid
Authors	:	McManus, E.; Perham, R.N.; Luisi, B.F.
Deposited on	:	2005-12-06
Resolution	:	1.89 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:

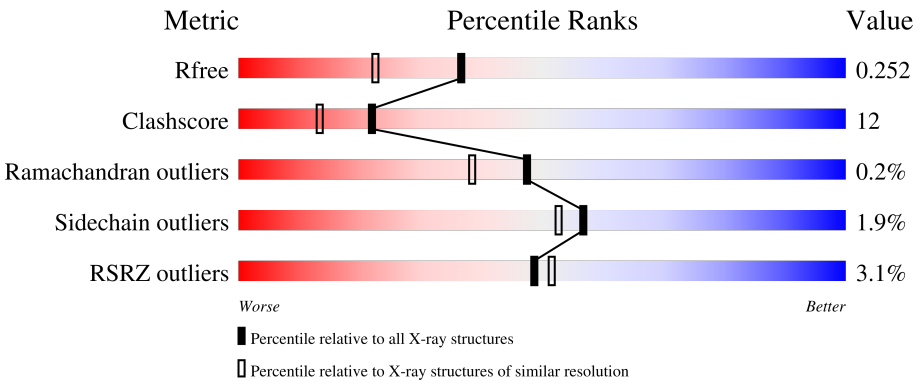
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	262	73% 18% • 8%
1	B	262	% 73% 18% • 6%
1	C	262	5% 67% 24% • 6%
1	D	262	5% 68% 22% • 8%

2 Entry composition (i)

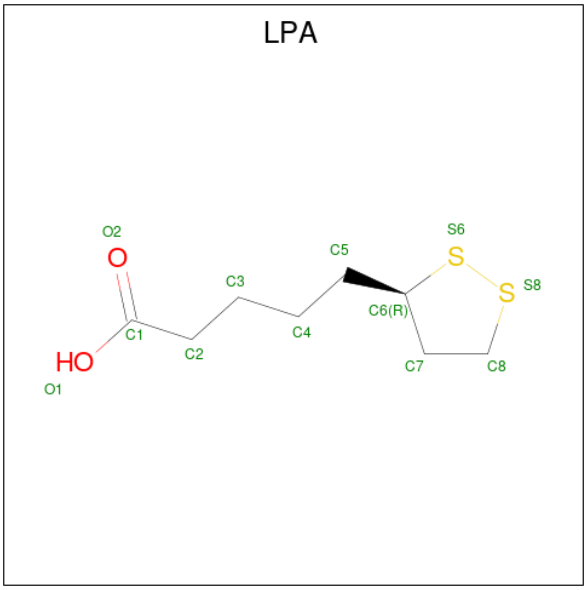
There are 3 unique types of molecules in this entry. The entry contains 8042 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	241	1886	1185	322	366	13	46	0	0
1	B	245	1920	1204	332	371	13	54	0	0
1	C	245	1882	1182	325	363	12	73	0	0
1	D	241	1822	1145	310	355	12	99	0	0

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



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

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

- Molecule 3 is water.

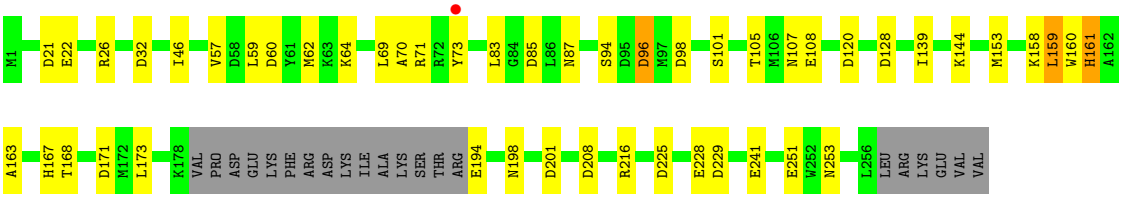
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	191	191	191	0	0
			Total	O		
3	B	162	162	162	0	0
			Total	O		
3	C	65	65	65	0	0
			Total	O		
3	D	66	66	66	0	0

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.

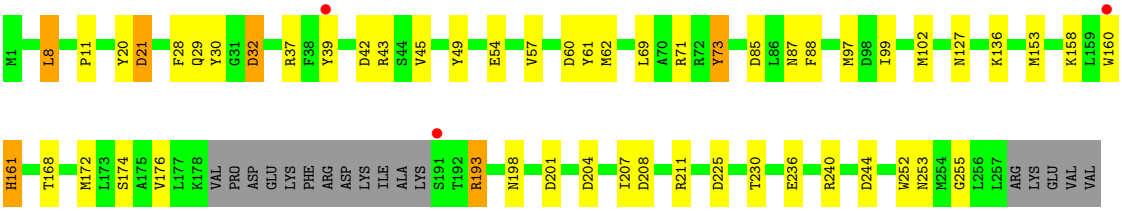
• Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain A:



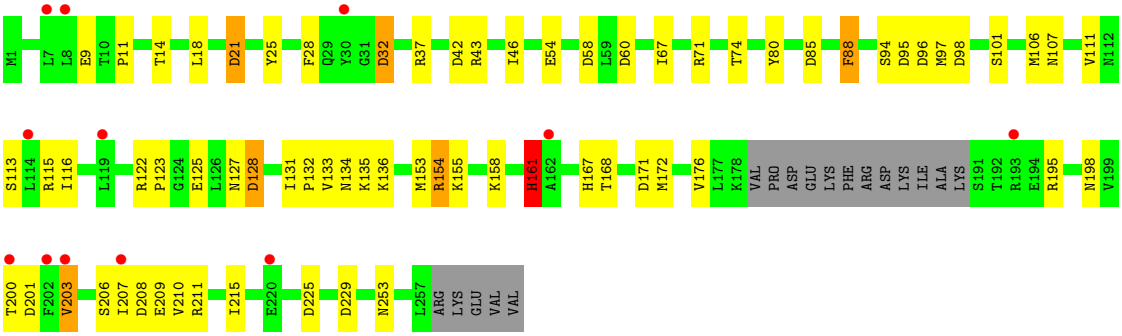
• Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain B:



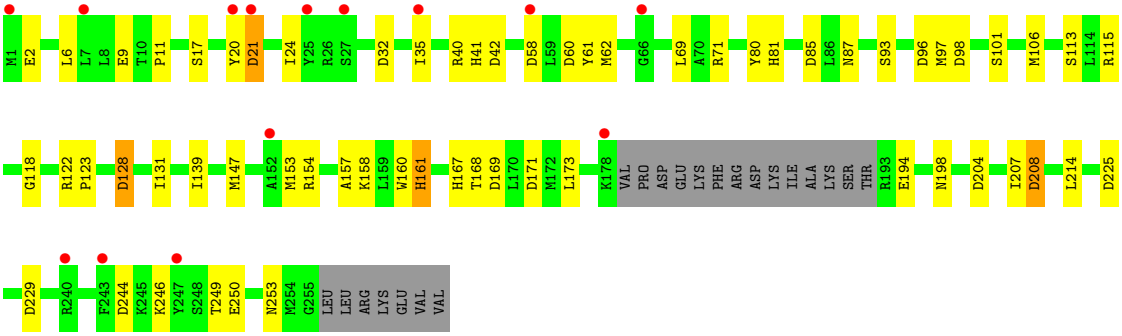
• Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain C:



• Molecule 1: LIPOATE-PROTEIN LIGASE A

Chain D:


M1
E2
L6
L7
L8
E9
T10
P11
S17
Y20
D21
I24
Y25
R26
S27
D32
I35
R40
H41
D42
D58
L59
D60
Y61
M62
G66
L69
A70
R71
Y80
H81
D85
L86
N87
S93
D96
M97
D98
S101
M106
S113
L114
R115
G118
R122
P123
D128
I131
I139
M147
A152
M153
R154
A157
K158
L159
W160
H161
H167
T168
D169
L170
D171
M172
L173
K178
VAL
PRO
ASP
GLU
LYS
PHE
ARG
ASP
LYS
ILE
ALA
LYS
SER
THR
R193
E194
N198
D204
I207
D208
L214
D225
D229
R240
F243
D244
K245
K246
Y247
S248
T249
E250
N253
M254
G255
LEU
LEU
ARG
LYS
GLU
VAL
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.38Å 117.88Å 105.66Å 90.00° 93.51° 90.00°	Depositor
Resolution (Å)	53.30 – 1.89 53.28 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (53.30-1.89) 99.2 (53.28-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.207 , 0.239 0.224 , 0.252	Depositor DCC
R_{free} test set	5132 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 73.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8042	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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)

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	0.63	3/1915 (0.2%)	0.87	16/2583 (0.6%)
1	B	0.53	3/1949 (0.2%)	0.86	11/2628 (0.4%)
1	C	0.41	2/1911 (0.1%)	0.73	14/2583 (0.5%)
1	D	0.47	4/1850 (0.2%)	0.94	22/2505 (0.9%)
All	All	0.52	12/7625 (0.2%)	0.85	63/10299 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	1	2
1	D	0	2
All	All	2	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	GLU	CD-OE2	-15.97	1.08	1.25
1	A	216	ARG	NE-CZ	11.85	1.48	1.33
1	D	40	ARG	CZ-NH2	-8.63	1.21	1.33
1	C	203	VAL	CB-CG1	-8.27	1.35	1.52
1	B	73	TYR	CG-CD1	8.01	1.49	1.39
1	B	20	TYR	C-N	-7.68	1.16	1.34
1	D	87	ASN	CG-OD1	-7.46	1.07	1.24
1	A	241	GLU	CD-OE2	-6.75	1.18	1.25
1	B	21	ASP	C-N	5.73	1.47	1.34
1	D	225	ASP	CA-CB	5.27	1.65	1.53
1	C	125	GLU	CB-CG	5.07	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	154	ARG	CZ-NH1	-5.05	1.26	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	154	ARG	NE-CZ-NH1	-23.09	108.76	120.30
1	B	211	ARG	NE-CZ-NH2	16.89	128.75	120.30
1	A	216	ARG	NE-CZ-NH1	-14.39	113.10	120.30
1	A	216	ARG	NE-CZ-NH2	13.98	127.29	120.30
1	D	40	ARG	NE-CZ-NH2	11.63	126.11	120.30
1	D	154	ARG	NH1-CZ-NH2	10.72	131.19	119.40
1	A	216	ARG	CD-NE-CZ	8.18	135.05	123.60
1	B	211	ARG	NH1-CZ-NH2	-7.98	110.63	119.40
1	A	241	GLU	OE1-CD-OE2	-6.38	115.65	123.30
1	D	225	ASP	CB-CA-C	-6.03	98.35	110.40
1	C	203	VAL	CG1-CB-CG2	-6.01	101.28	110.90
1	D	40	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
1	B	201	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	157	ALA	N-CA-CB	5.92	118.38	110.10
1	B	73	TYR	CD1-CE1-CZ	-5.87	114.51	119.80
1	C	229	ASP	CB-CG-OD2	5.74	123.46	118.30
1	D	250	GLU	OE1-CD-OE2	5.57	129.99	123.30
1	B	32	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	229	ASP	CB-CG-OD2	5.43	123.18	118.30
1	D	42	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	201	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	229	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	225	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	58	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	204	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	60	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	171	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	208	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	98	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	32	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	85	ASP	CB-CG-OD2	5.26	123.04	118.30
1	D	128	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	60	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	32	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	244	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	225	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	208	ASP	CB-CG-OD2	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	120	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	171	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	171	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	85	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	58	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	96	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	128	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	204	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	60	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	98	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	21	ASP	CB-CG-OD2	5.20	122.97	118.30
1	D	32	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	60	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	21	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	85	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	21	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	208	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	169	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	225	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	208	ASP	CB-CG-OD2	5.12	122.91	118.30
1	C	96	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	128	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	201	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	244	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	96	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	95	ASP	CB-CG-OD2	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	192	THR	CB
1	C	192	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	161	HIS	Peptide
1	C	207	ILE	Peptide
1	D	21	ASP	Peptide
1	D	61	TYR	Sidechain

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	1886	0	1836	41	0
1	B	1920	0	1871	52	1
1	C	1882	0	1806	43	0
1	D	1822	0	1718	32	1
2	A	12	0	13	0	0
2	B	12	0	13	0	0
2	C	12	0	13	0	0
2	D	12	0	13	0	0
3	A	191	0	0	3	1
3	B	162	0	0	6	1
3	C	65	0	0	3	0
3	D	66	0	0	3	0
All	All	8042	0	7283	166	2

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 12.

All (166) 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:C:94:SER:OG	1:C:158:LYS:HE3	1.63	0.98
1:C:80:TYR:OH	1:C:172:MET:SD	2.27	0.91
1:B:61:TYR:CE2	1:B:176:VAL:HG22	2.08	0.88
1:A:153:MET:HG2	1:A:158:LYS:HG2	1.54	0.87
1:B:127:ASN:OD1	1:B:136:LYS:HE2	1.78	0.83
1:D:208:ASP:CG	3:D:2062:HOH:O	2.15	0.83
1:B:57:VAL:HG21	1:B:62:MET:SD	2.18	0.83
1:D:62:MET:HE1	1:D:69:LEU:HB2	1.62	0.82
1:C:97:MET:HE1	3:C:2033:HOH:O	1.80	0.82
1:B:174:SER:OG	1:B:193:ARG:HB2	1.80	0.81
1:B:153:MET:HE2	1:B:158:LYS:CE	2.13	0.79
1:B:62:MET:HE1	1:B:69:LEU:HB2	1.66	0.76
1:B:45:VAL:HG21	1:B:62:MET:SD	2.26	0.76
1:B:49:TYR:O	3:B:2040:HOH:O	2.09	0.70
1:A:160:TRP:O	1:A:160:TRP:CE3	2.46	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:HIS:HD2	1:D:81:HIS:ND1	1.91	0.69
1:B:8:LEU:HB2	3:B:2007:HOH:O	1.92	0.68
1:B:39:TYR:CE1	1:B:87:ASN:CB	2.76	0.67
1:B:153:MET:HE2	1:B:158:LYS:HE3	1.76	0.67
1:B:252:TRP:O	3:B:2160:HOH:O	2.11	0.67
1:B:172:MET:O	1:B:176:VAL:HG23	1.96	0.66
1:C:133:VAL:HG11	1:C:195:ARG:HB3	1.77	0.66
1:B:39:TYR:CE1	1:B:87:ASN:HB2	2.31	0.65
1:C:206:SER:OG	1:C:209:GLU:HG3	1.97	0.65
1:D:6:LEU:CD1	1:D:35:ILE:HG21	2.26	0.65
1:C:97:MET:O	1:C:153:MET:HE1	1.97	0.64
1:A:94:SER:OG	1:A:158:LYS:NZ	2.19	0.64
1:A:62:MET:HE1	1:A:69:LEU:HB2	1.80	0.64
1:D:106:MET:CE	3:D:2009:HOH:O	2.44	0.64
1:D:106:MET:HE3	3:D:2009:HOH:O	1.98	0.64
1:C:106:MET:HE3	3:C:2032:HOH:O	1.96	0.64
1:C:167:HIS:ND1	1:C:167:HIS:O	2.33	0.62
1:B:57:VAL:CG2	1:B:62:MET:SD	2.86	0.62
1:D:168:THR:H	1:D:198:ASN:HD21	1.47	0.62
1:A:153:MET:SD	1:A:158:LYS:HE3	2.40	0.62
1:B:62:MET:HG3	1:B:176:VAL:CG1	2.30	0.62
1:B:160:TRP:O	1:B:160:TRP:CE3	2.53	0.62
1:B:39:TYR:CD1	1:B:87:ASN:HB2	2.34	0.62
1:B:61:TYR:CD2	1:B:176:VAL:HG22	2.35	0.61
1:D:9:GLU:HG3	1:D:11:PRO:HD3	1.82	0.60
1:B:61:TYR:HE2	1:B:176:VAL:HG22	1.62	0.60
1:D:6:LEU:CD1	1:D:35:ILE:CG2	2.82	0.58
1:A:101:SER:O	1:A:105:THR:HG23	2.02	0.58
1:D:6:LEU:HD11	1:D:35:ILE:HG21	1.85	0.57
1:C:67:ILE:HD13	1:C:176:VAL:HG11	1.84	0.57
1:B:153:MET:CE	1:B:158:LYS:CE	2.81	0.57
1:D:139:ILE:HB	1:D:147:MET:HB3	1.86	0.57
1:B:236:GLU:OE2	1:B:240:ARG:NE	2.31	0.56
1:A:46:ILE:HD12	1:A:46:ILE:N	2.19	0.56
1:A:71:ARG:H	1:A:253:ASN:HD22	1.52	0.56
1:D:173:LEU:HD23	1:D:173:LEU:C	2.25	0.56
1:A:167:HIS:O	1:A:167:HIS:CD2	2.59	0.56
1:B:39:TYR:CE1	1:B:87:ASN:HB3	2.39	0.56
1:A:73:TYR:CE1	1:A:159:LEU:HD22	2.41	0.56
1:D:17:SER:OG	1:D:41:HIS:HE1	1.89	0.56
1:A:22:GLU:HG2	1:A:26:ARG:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ARG:O	1:C:215:ILE:HG13	2.05	0.55
1:A:160:TRP:O	1:A:160:TRP:HE3	1.89	0.55
1:B:62:MET:HG3	1:B:176:VAL:HG13	1.88	0.55
1:D:113:SER:CB	1:D:214:LEU:HD23	2.36	0.55
1:C:172:MET:O	1:C:176:VAL:HG22	2.07	0.54
1:B:39:TYR:CZ	1:B:87:ASN:HB3	2.42	0.54
1:D:20:TYR:O	1:D:24:ILE:HG13	2.07	0.54
1:B:71:ARG:H	1:B:253:ASN:HD22	1.54	0.54
1:C:37:ARG:O	1:C:88:PHE:HA	2.08	0.53
1:A:73:TYR:OH	1:A:159:LEU:CD2	2.56	0.53
1:B:168:THR:H	1:B:198:ASN:HD21	1.56	0.52
1:B:161:HIS:O	1:B:161:HIS:HD2	1.91	0.52
1:D:160:TRP:CE3	1:D:160:TRP:O	2.63	0.52
1:A:73:TYR:CE1	1:A:159:LEU:CD2	2.93	0.52
1:D:6:LEU:HG	1:D:35:ILE:HG23	1.90	0.52
1:D:246:LYS:O	1:D:249:THR:OG1	2.24	0.52
1:A:144:LYS:HE3	3:A:2138:HOH:O	2.11	0.51
1:A:96:ASP:O	1:A:158:LYS:NZ	2.44	0.51
1:B:54:GLU:HG2	3:B:2041:HOH:O	2.10	0.50
1:C:107:ASN:O	1:C:111:VAL:HG23	2.10	0.50
1:C:206:SER:O	1:C:210:VAL:HG23	2.11	0.50
1:C:94:SER:HG	1:C:158:LYS:HE3	1.73	0.50
1:D:122:ARG:HB3	1:D:123:PRO:HD2	1.94	0.50
1:B:255:GLY:HA2	3:B:2160:HOH:O	2.11	0.50
1:D:168:THR:H	1:D:198:ASN:ND2	2.09	0.50
1:A:107:ASN:OD1	1:A:139:ILE:HD11	2.12	0.49
1:A:73:TYR:HE1	1:A:159:LEU:HD22	1.77	0.49
1:C:122:ARG:HG3	1:C:123:PRO:HD2	1.95	0.49
1:A:85:ASP:OD1	1:A:87:ASN:ND2	2.46	0.49
1:D:97:MET:O	1:D:153:MET:HE1	2.13	0.49
1:B:71:ARG:NH1	3:B:2040:HOH:O	2.44	0.48
1:C:161:HIS:O	1:C:161:HIS:HD2	1.96	0.48
1:A:168:THR:H	1:A:198:ASN:HD21	1.60	0.48
1:C:168:THR:H	1:C:198:ASN:HD21	1.59	0.48
1:C:71:ARG:H	1:C:253:ASN:HD22	1.62	0.48
1:D:6:LEU:HD12	1:D:35:ILE:HG21	1.96	0.48
1:A:173:LEU:C	1:A:173:LEU:HD23	2.34	0.48
1:B:102:MET:HE3	1:B:160:TRP:HB2	1.95	0.47
1:C:71:ARG:H	1:C:253:ASN:ND2	2.12	0.47
1:A:228:GLU:OE2	3:A:2164:HOH:O	2.20	0.47
1:C:74:THR:HG1	1:C:161:HIS:HE2	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:HB	1:C:132:PRO:HD2	1.97	0.47
1:B:21:ASP:HB2	1:B:37:ARG:NH1	2.30	0.47
1:B:168:THR:H	1:B:198:ASN:ND2	2.11	0.47
1:A:96:ASP:OD1	1:A:158:LYS:NZ	2.46	0.46
1:D:128:ASP:O	1:D:131:ILE:HG12	2.16	0.46
1:B:160:TRP:O	1:B:160:TRP:HE3	1.97	0.46
1:A:71:ARG:H	1:A:253:ASN:ND2	2.13	0.46
1:B:153:MET:CE	1:B:158:LYS:HE3	2.44	0.46
1:C:28:PHE:CZ	1:C:32:ASP:HB2	2.51	0.46
1:D:6:LEU:HD12	1:D:35:ILE:CG2	2.45	0.46
1:A:46:ILE:HA	1:A:70:ALA:O	2.15	0.46
1:C:128:ASP:O	1:C:135:LYS:HG2	2.15	0.46
1:A:94:SER:HB2	1:A:158:LYS:HG3	1.97	0.45
1:A:167:HIS:CD2	3:A:2147:HOH:O	2.69	0.45
1:C:127:ASN:OD1	1:C:136:LYS:CE	2.64	0.45
1:A:73:TYR:OH	1:A:159:LEU:HD21	2.15	0.45
1:B:161:HIS:O	1:B:161:HIS:CD2	2.69	0.45
1:D:17:SER:CB	1:D:41:HIS:HE1	2.30	0.45
1:C:133:VAL:O	1:C:134:ASN:CB	2.65	0.45
1:B:71:ARG:H	1:B:253:ASN:ND2	2.15	0.44
1:B:97:MET:CE	1:B:153:MET:HG3	2.47	0.44
1:A:22:GLU:HG2	1:A:26:ARG:HD3	1.98	0.44
1:A:87:ASN:HD22	1:A:163:ALA:HA	1.83	0.44
1:A:161:HIS:O	1:A:161:HIS:HD2	2.00	0.44
1:A:251:GLU:H	1:A:251:GLU:CD	2.21	0.44
1:D:93:SER:O	1:D:158:LYS:HE2	2.18	0.44
1:D:160:TRP:O	1:D:160:TRP:HE3	2.01	0.43
1:B:99:ILE:CG1	1:B:153:MET:HE3	2.48	0.43
1:C:167:HIS:O	1:C:167:HIS:CG	2.71	0.43
1:D:80:TYR:HB3	1:D:173:LEU:HG	2.00	0.43
1:D:115:ARG:O	1:D:118:GLY:N	2.46	0.43
1:A:144:LYS:HE2	1:A:194:GLU:O	2.16	0.43
1:B:28:PHE:CZ	1:B:32:ASP:HB2	2.53	0.43
1:C:168:THR:H	1:C:198:ASN:ND2	2.16	0.43
1:A:57:VAL:HG23	1:A:59:LEU:HD23	1.99	0.43
1:B:99:ILE:CA	1:B:153:MET:HE1	2.49	0.43
1:C:25:TYR:OH	1:C:154:ARG:HB2	2.19	0.43
1:D:167:HIS:O	1:D:167:HIS:CD2	2.72	0.43
1:B:45:VAL:CG2	1:B:62:MET:SD	3.04	0.42
1:A:73:TYR:OH	1:A:159:LEU:HD22	2.19	0.42
1:A:168:THR:H	1:A:198:ASN:ND2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:ARG:H	1:D:253:ASN:HD22	1.66	0.42
1:C:135:LYS:HB2	1:C:135:LYS:HE2	1.78	0.42
1:C:54:GLU:HG3	3:C:2019:HOH:O	2.18	0.42
1:C:42:ASP:O	1:C:43:ARG:C	2.57	0.42
1:D:161:HIS:HD2	1:D:161:HIS:O	2.03	0.42
1:C:14:THR:O	1:C:18:LEU:HG	2.20	0.42
1:A:107:ASN:CG	1:A:139:ILE:HD11	2.41	0.41
1:B:37:ARG:O	1:B:88:PHE:HA	2.20	0.41
1:B:42:ASP:O	1:B:43:ARG:C	2.58	0.41
1:B:97:MET:HE1	1:B:153:MET:HG3	2.02	0.41
1:B:102:MET:CE	1:B:160:TRP:HB2	2.51	0.41
1:A:83:LEU:HD12	1:B:11:PRO:HB2	2.02	0.41
1:C:80:TYR:CZ	1:C:172:MET:SD	3.13	0.41
1:B:99:ILE:HB	1:B:153:MET:CE	2.50	0.41
1:C:9:GLU:HG3	1:C:11:PRO:HD3	2.01	0.41
1:C:200:THR:HA	1:C:203:VAL:O	2.20	0.41
1:C:122:ARG:CG	1:C:123:PRO:HD2	2.50	0.41
1:A:62:MET:HE3	1:A:62:MET:HB3	1.93	0.41
1:C:113:SER:O	1:C:116:ILE:HB	2.21	0.41
1:B:29:GLN:O	1:B:30:TYR:C	2.58	0.41
1:C:88:PHE:CD2	1:C:88:PHE:N	2.89	0.41
1:C:161:HIS:O	1:C:161:HIS:CD2	2.74	0.41
1:A:22:GLU:OE2	1:A:26:ARG:HD2	2.20	0.41
1:B:39:TYR:CZ	1:B:87:ASN:CB	3.04	0.41
1:C:74:THR:OG1	1:C:161:HIS:NE2	2.43	0.41
1:C:98:ASP:OD2	1:C:101:SER:HB2	2.21	0.41
1:C:46:ILE:HD12	1:C:46:ILE:N	2.37	0.40
1:A:64:LYS:HG2	1:B:230:THR:HG21	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2008:HOH:O	3:B:2029:HOH:O[2_545]	1.86	0.34
1:B:73:TYR:O	1:D:122:ARG:NH1[2_555]	2.03	0.17

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	237/262 (90%)	231 (98%)	6 (2%)	0	100	100
1	B	241/262 (92%)	236 (98%)	5 (2%)	0	100	100
1	C	241/262 (92%)	227 (94%)	12 (5%)	2 (1%)	19	9
1	D	237/262 (90%)	228 (96%)	9 (4%)	0	100	100
All	All	956/1048 (91%)	922 (96%)	32 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	154	ARG
1	C	155	LYS

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	199/226 (88%)	197 (99%)	2 (1%)	76	76
1	B	202/226 (89%)	198 (98%)	4 (2%)	55	51
1	C	193/226 (85%)	189 (98%)	4 (2%)	53	48
1	D	183/226 (81%)	178 (97%)	5 (3%)	44	38
All	All	777/904 (86%)	762 (98%)	15 (2%)	57	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LEU
1	A	161	HIS
1	B	8	LEU
1	B	161	HIS
1	B	193	ARG
1	B	207	ILE
1	C	21	ASP
1	C	88	PHE
1	C	115	ARG
1	C	161	HIS
1	D	2	GLU
1	D	101	SER
1	D	161	HIS
1	D	194	GLU
1	D	207	ILE

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

Mol	Chain	Res	Type
1	A	87	ASN
1	A	167	HIS
1	A	198	ASN
1	A	253	ASN
1	B	161	HIS
1	B	198	ASN
1	B	253	ASN
1	C	161	HIS
1	C	198	ASN
1	C	253	ASN
1	D	41	HIS
1	D	167	HIS
1	D	198	ASN
1	D	253	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)

4 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	C	900	-	12,12,12	1.09	1 (8%)	14,14,14	1.56	2 (14%)
2	LPA	A	900	-	12,12,12	1.03	1 (8%)	14,14,14	2.01	4 (28%)
2	LPA	D	900	-	12,12,12	1.11	1 (8%)	14,14,14	1.60	3 (21%)
2	LPA	B	900	-	12,12,12	1.09	1 (8%)	14,14,14	1.53	2 (14%)

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	C	900	-	-	2/7/14/14	0/1/1/1
2	LPA	A	900	-	-	2/7/14/14	0/1/1/1
2	LPA	D	900	-	-	2/7/14/14	0/1/1/1
2	LPA	B	900	-	-	0/7/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	LPA	S6-S8	-2.90	1.82	2.04
2	D	900	LPA	S6-S8	-2.89	1.82	2.04
2	B	900	LPA	S6-S8	-2.77	1.83	2.04
2	A	900	LPA	S6-S8	-2.64	1.84	2.04

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	LPA	C8-S8-S6	4.94	112.24	95.01
2	C	900	LPA	C8-S8-S6	4.07	109.22	95.01
2	A	900	LPA	C7-C8-S8	-3.80	98.98	109.05
2	D	900	LPA	C8-S8-S6	3.69	107.88	95.01
2	B	900	LPA	C8-S8-S6	3.65	107.75	95.01
2	D	900	LPA	C7-C8-S8	-3.20	100.57	109.05
2	C	900	LPA	C7-C8-S8	-3.06	100.96	109.05
2	B	900	LPA	C7-C8-S8	-2.98	101.16	109.05
2	A	900	LPA	C6-S6-S8	-2.77	86.00	95.56
2	D	900	LPA	C6-S6-S8	-2.15	88.14	95.56
2	A	900	LPA	O1-C1-C2	2.14	120.92	114.03

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	900	LPA	O1-C1-C2-C3
2	D	900	LPA	O2-C1-C2-C3
2	A	900	LPA	O2-C1-C2-C3
2	A	900	LPA	O1-C1-C2-C3
2	C	900	LPA	O1-C1-C2-C3
2	C	900	LPA	O2-C1-C2-C3

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	20:TYR	C	21:ASP	N	1.16

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	241/262 (91%)	0.39	1 (0%)	92	93	19, 27, 38, 46	28 (11%)
1	B	245/262 (93%)	0.38	3 (1%)	79	81	19, 26, 39, 51	29 (11%)
1	C	245/262 (93%)	0.45	12 (4%)	29	33	24, 38, 46, 55	46 (18%)
1	D	241/262 (91%)	0.64	14 (5%)	23	25	24, 39, 47, 52	58 (24%)
All	All	972/1048 (92%)	0.46	30 (3%)	49	51	19, 33, 45, 55	161 (16%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.6
1	B	39	TYR	5.1
1	D	7	LEU	3.9
1	D	240	ARG	3.6
1	C	202	PHE	3.3
1	D	27	SER	3.3
1	A	73	TYR	2.9
1	C	200	THR	2.7
1	D	243	PHE	2.7
1	D	25	TYR	2.7
1	B	191	SER	2.7
1	D	20	TYR	2.7
1	D	247	TYR	2.7
1	C	207	ILE	2.6
1	D	178	LYS	2.6
1	B	160	TRP	2.6
1	D	35	ILE	2.6
1	D	66	GLY	2.6
1	D	21	ASP	2.5
1	C	193	ARG	2.5
1	C	114	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	58	ASP	2.4
1	D	152	ALA	2.4
1	C	220	GLU	2.4
1	C	203	VAL	2.3
1	C	7	LEU	2.3
1	C	8	LEU	2.2
1	C	162	ALA	2.1
1	C	30	TYR	2.1
1	C	119	LEU	2.1

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	LPA	C	900	12/12	0.89	0.20	14,20,24,25	12
2	LPA	A	900	12/12	0.92	0.24	7,12,19,22	12
2	LPA	B	900	12/12	0.93	0.24	6,8,16,18	12
2	LPA	D	900	12/12	0.93	0.20	15,23,29,35	12

6.5 Other polymers (i)

There are no such residues in this entry.