Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2024 – 12:09 PM JST

PDB ID	:	9IVE
Title	:	Structure of wild-type aminotransferase from Mycolicibacterium neoaurum in complex with LLP and ALA
Authors	:	Wei, H.; Cong, L.; You, S.; Liu, W.
Deposited on	:	2024-07-23
Resolution	:	1.93 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:

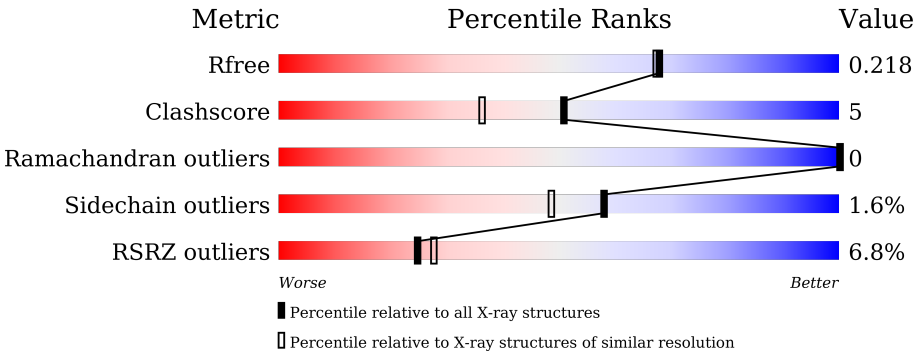
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 1.93 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}	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	335	5% 86% 10%
1	B	335	7% 88% 8%
1	C	335	3% 88% 7%
1	D	335	10% 85% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11152 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 Branched-chain amino acid transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	P	S	0	0	0
			2493	1574	425	485	1	8			
1	B	323	Total	C	N	O	P	S	0	0	0
			2493	1574	425	485	1	8			
1	C	320	Total	C	N	O	P	S	0	0	0
			2475	1564	422	480	1	8			
1	D	323	Total	C	N	O	P	S	0	0	0
			2493	1574	425	485	1	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP V5X927
A	2	SER	-	expression tag	UNP V5X927
A	3	THR	-	expression tag	UNP V5X927
A	4	GLY	-	expression tag	UNP V5X927
A	5	THR	-	expression tag	UNP V5X927
A	6	SER	-	expression tag	UNP V5X927
A	7	ASN	-	expression tag	UNP V5X927
A	8	LEU	-	expression tag	UNP V5X927
A	9	VAL	-	expression tag	UNP V5X927
A	119	SER	ALA	conflict	UNP V5X927
A	259	ILE	LEU	conflict	UNP V5X927
A	261	ASP	GLU	conflict	UNP V5X927
A	279	ASP	GLU	conflict	UNP V5X927
A	302	ALA	PRO	conflict	UNP V5X927
A	307	ALA	GLU	conflict	UNP V5X927
A	310	PRO	GLU	conflict	UNP V5X927
B	1	MET	-	initiating methionine	UNP V5X927
B	2	SER	-	expression tag	UNP V5X927
B	3	THR	-	expression tag	UNP V5X927
B	4	GLY	-	expression tag	UNP V5X927
B	5	THR	-	expression tag	UNP V5X927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP V5X927
B	7	ASN	-	expression tag	UNP V5X927
B	8	LEU	-	expression tag	UNP V5X927
B	9	VAL	-	expression tag	UNP V5X927
B	119	SER	ALA	conflict	UNP V5X927
B	259	ILE	LEU	conflict	UNP V5X927
B	261	ASP	GLU	conflict	UNP V5X927
B	279	ASP	GLU	conflict	UNP V5X927
B	302	ALA	PRO	conflict	UNP V5X927
B	307	ALA	GLU	conflict	UNP V5X927
B	310	PRO	GLU	conflict	UNP V5X927
C	1	MET	-	initiating methionine	UNP V5X927
C	2	SER	-	expression tag	UNP V5X927
C	3	THR	-	expression tag	UNP V5X927
C	4	GLY	-	expression tag	UNP V5X927
C	5	THR	-	expression tag	UNP V5X927
C	6	SER	-	expression tag	UNP V5X927
C	7	ASN	-	expression tag	UNP V5X927
C	8	LEU	-	expression tag	UNP V5X927
C	9	VAL	-	expression tag	UNP V5X927
C	119	SER	ALA	conflict	UNP V5X927
C	259	ILE	LEU	conflict	UNP V5X927
C	261	ASP	GLU	conflict	UNP V5X927
C	279	ASP	GLU	conflict	UNP V5X927
C	302	ALA	PRO	conflict	UNP V5X927
C	307	ALA	GLU	conflict	UNP V5X927
C	310	PRO	GLU	conflict	UNP V5X927
D	1	MET	-	initiating methionine	UNP V5X927
D	2	SER	-	expression tag	UNP V5X927
D	3	THR	-	expression tag	UNP V5X927
D	4	GLY	-	expression tag	UNP V5X927
D	5	THR	-	expression tag	UNP V5X927
D	6	SER	-	expression tag	UNP V5X927
D	7	ASN	-	expression tag	UNP V5X927
D	8	LEU	-	expression tag	UNP V5X927
D	9	VAL	-	expression tag	UNP V5X927
D	119	SER	ALA	conflict	UNP V5X927
D	259	ILE	LEU	conflict	UNP V5X927
D	261	ASP	GLU	conflict	UNP V5X927
D	279	ASP	GLU	conflict	UNP V5X927
D	302	ALA	PRO	conflict	UNP V5X927
D	307	ALA	GLU	conflict	UNP V5X927

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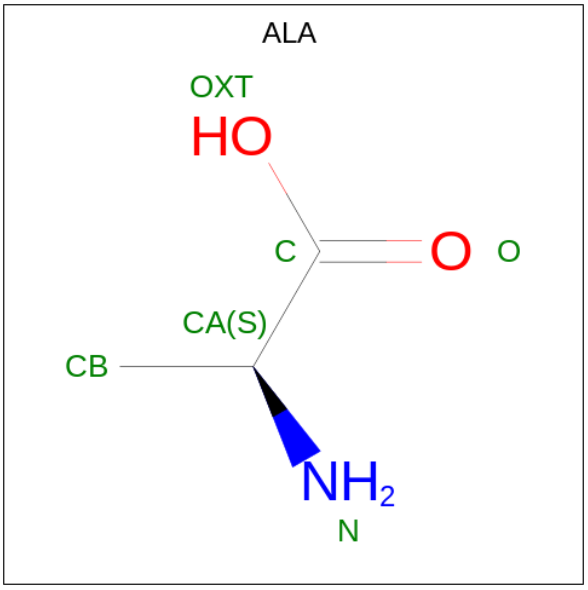
Chain	Residue	Modelled	Actual	Comment	Reference
D	310	PRO	GLU	conflict	UNP V5X927

- Molecule 2 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 6 3 1 2	0	0
2	B	1	Total C N O 6 3 1 2	0	0
2	C	1	Total C N O 6 3 1 2	0	0
2	D	1	Total C N O 6 3 1 2	0	0

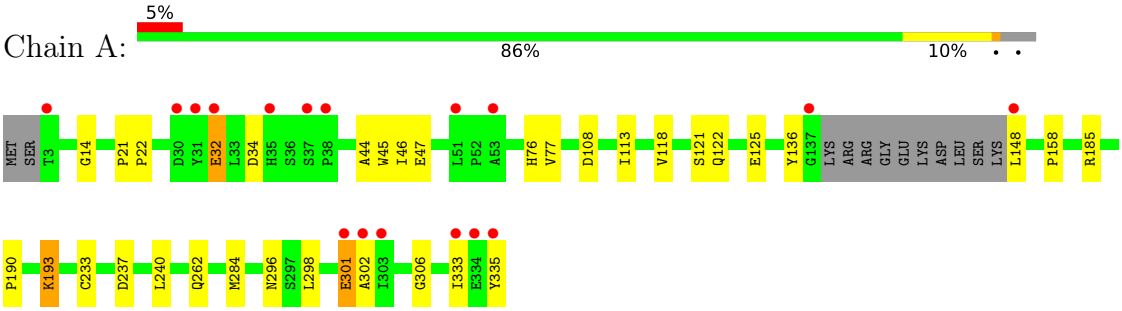
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	284	Total O 284 284	0	0
3	B	327	Total O 327 327	0	0
3	C	302	Total O 302 302	0	0
3	D	261	Total O 261 261	0	0

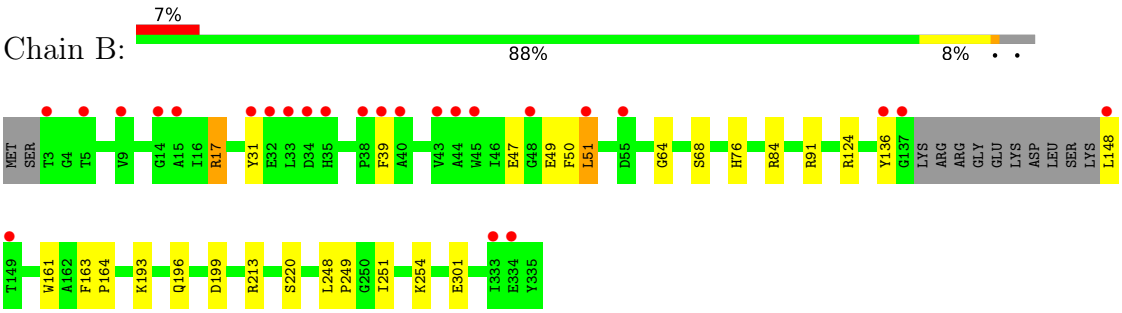
3 Residue-property plots (i)

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.

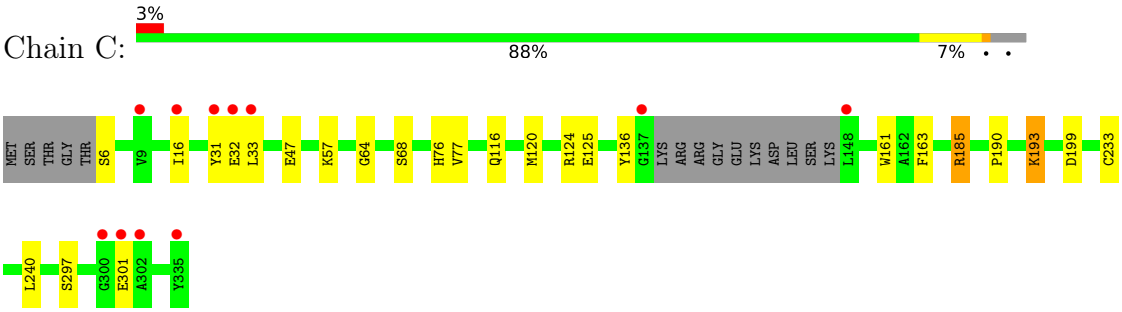
• Molecule 1: Branched-chain amino acid transferase



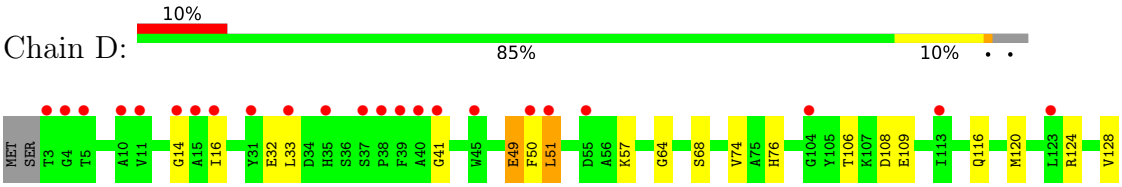
• Molecule 1: Branched-chain amino acid transferase

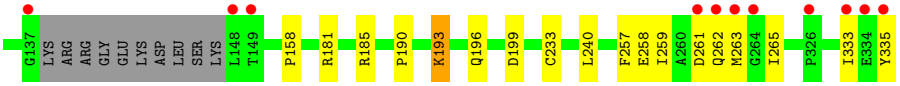


• Molecule 1: Branched-chain amino acid transferase



• Molecule 1: Branched-chain amino acid transferase




G137
LYS
ARG
ARG
GLY
GLU
LYS
ASP
LEU
SER
LYS
L148
T149
P158
R181
R185
P190
K193
Q196
D199
C233
L240
F257
E258
I259
A260
D261
Q262
M263
G264
I265
P326
I333
E334
Y335

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.93Å 78.81Å 92.09Å 96.84° 108.76° 112.90°	Depositor
Resolution (Å)	35.94 – 1.93 35.94 – 1.93	Depositor EDS
% Data completeness (in resolution range)	94.9 (35.94-1.93) 94.8 (35.94-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.182 , 0.215 0.186 , 0.218	Depositor DCC
R_{free} test set	112416 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11152	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: LLP

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	0.40	0/2525	0.62	0/3440
1	B	0.46	0/2525	0.64	0/3440
1	C	0.38	0/2507	0.61	0/3415
1	D	0.43	0/2525	0.63	0/3440
All	All	0.42	0/10082	0.63	0/13735

There are no bond length outliers.

There are no bond angle outliers.

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	2493	0	2409	28	0
1	B	2493	0	2409	20	0
1	C	2475	0	2392	20	0
1	D	2493	0	2409	32	0
2	A	6	0	4	0	0
2	B	6	0	4	0	0
2	C	6	0	4	0	0
2	D	6	0	4	0	0
3	A	284	0	0	4	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	327	0	0	1	2
3	C	302	0	0	4	1
3	D	261	0	0	7	0
All	All	11152	0	9635	99	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 5.

All (99) 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:A:302:ALA:HB1	1:A:306:GLY:CA	1.66	1.25
1:D:116:GLN:HG2	3:D:504:HOH:O	1.39	1.19
1:A:302:ALA:HB1	1:A:306:GLY:HA3	1.30	1.07
1:D:57:LYS:NZ	3:D:501:HOH:O	1.95	0.98
1:D:16:ILE:HD12	1:D:16:ILE:H	1.38	0.87
1:A:302:ALA:HB1	1:A:306:GLY:HA2	1.57	0.84
1:D:120:MET:SD	3:D:504:HOH:O	2.33	0.84
1:D:41:GLY:O	3:D:502:HOH:O	2.01	0.78
1:D:263:MET:O	1:D:265:ILE:HG13	1.87	0.75
1:C:301:GLU:OE1	3:C:2401:HOH:O	2.06	0.74
1:D:49:GLU:CG	1:D:51:LEU:HD21	2.19	0.72
1:B:50:PHE:C	1:B:51:LEU:HD23	2.09	0.72
1:C:47:GLU:OE2	1:C:136:TYR:OH	2.07	0.72
1:C:6:SER:N	3:C:2402:HOH:O	2.23	0.71
1:A:237:ASP:OD2	3:A:501:HOH:O	2.09	0.69
1:A:302:ALA:CB	1:A:306:GLY:HA3	2.17	0.69
1:B:47:GLU:OE2	1:B:136:TYR:OH	2.10	0.68
1:D:49:GLU:CD	1:D:51:LEU:HD21	2.14	0.68
1:C:32:GLU:HA	1:C:32:GLU:OE1	1.95	0.67
1:B:51:LEU:HD23	1:B:51:LEU:N	2.10	0.66
1:A:296:ASN:O	1:A:302:ALA:HA	1.95	0.66
1:A:148:LEU:N	3:A:506:HOH:O	2.28	0.66
1:B:164:PRO:HD3	1:B:213:ARG:HH21	1.63	0.64
1:B:301:GLU:HG3	3:C:2427:HOH:O	1.98	0.63
1:C:16:ILE:HG12	1:C:33:LEU:HD11	1.80	0.63
1:D:106:THR:OG1	1:D:109:GLU:HG3	1.99	0.61
1:D:50:PHE:C	1:D:51:LEU:HG	2.19	0.61
1:B:213:ARG:NE	3:B:503:HOH:O	2.29	0.59
1:C:297:SER:HB2	1:C:301:GLU:O	2.02	0.59
1:A:302:ALA:CB	1:A:306:GLY:CA	2.61	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HG12	1:C:33:LEU:CD1	2.34	0.57
1:D:257:PHE:O	1:D:261:ASP:HB2	2.04	0.57
1:D:233:CYS:HB3	1:D:240:LEU:HD11	1.87	0.57
1:D:16:ILE:HD12	1:D:16:ILE:N	2.17	0.56
1:A:47:GLU:OE2	1:A:136:TYR:OH	2.23	0.55
1:B:31:TYR:CE1	1:B:124:ARG:HB2	2.42	0.54
1:D:116:GLN:NE2	3:D:504:HOH:O	2.32	0.54
1:D:258:GLU:O	1:D:261:ASP:HB3	2.07	0.54
1:C:57:LYS:NZ	3:C:2408:HOH:O	2.39	0.54
1:D:14:GLY:O	1:D:158:PRO:HG2	2.10	0.51
1:D:16:ILE:HG22	3:D:538:HOH:O	2.11	0.51
1:D:16:ILE:H	1:D:16:ILE:CD1	2.16	0.50
1:A:302:ALA:HB1	1:A:306:GLY:N	2.22	0.50
1:D:16:ILE:HG12	1:D:33:LEU:HD11	1.93	0.50
1:A:44:ALA:HB1	1:A:46:ILE:HD11	1.94	0.49
1:D:185:ARG:HA	1:D:190:PRO:HD2	1.94	0.49
1:D:64:GLY:O	1:D:68:SER:HA	2.12	0.49
1:C:31:TYR:CE1	1:C:124:ARG:HB2	2.47	0.48
1:B:39:PHE:HE1	1:B:51:LEU:HA	1.79	0.48
1:C:16:ILE:CG1	1:C:33:LEU:HD11	2.42	0.48
1:A:34:ASP:H	1:A:122:GLN:HE22	1.61	0.48
1:A:302:ALA:CB	1:A:306:GLY:HA2	2.34	0.48
1:A:233:CYS:HB3	1:A:240:LEU:HD11	1.96	0.48
1:C:185:ARG:HA	1:C:190:PRO:HD2	1.96	0.48
1:B:49:GLU:O	1:B:51:LEU:CD2	2.62	0.47
1:C:233:CYS:HB3	1:C:240:LEU:HD11	1.97	0.47
1:D:49:GLU:HG3	1:D:51:LEU:HD21	1.94	0.47
1:A:118:VAL:HG11	1:A:333:ILE:HG13	1.98	0.46
1:A:233:CYS:HB2	1:A:284:MET:HG2	1.97	0.46
1:C:116:GLN:O	1:C:120:MET:HG3	2.16	0.46
1:B:84:ARG:NH2	1:B:254:LYS:HD3	2.31	0.46
1:C:297:SER:CB	1:C:301:GLU:O	2.64	0.46
1:B:164:PRO:HD3	1:B:213:ARG:NH2	2.28	0.45
1:D:193:LLP:HE2	1:D:193:LLP:O3	2.17	0.45
1:B:64:GLY:O	1:B:68:SER:HA	2.17	0.45
1:B:17:ARG:NH2	1:B:31:TYR:H	2.15	0.45
1:B:164:PRO:CD	1:B:213:ARG:HH21	2.29	0.45
1:B:199:ASP:OD1	1:B:199:ASP:N	2.50	0.44
1:B:49:GLU:O	1:B:51:LEU:HD23	2.17	0.44
1:A:77:VAL:O	1:A:125:GLU:HA	2.17	0.44
3:A:528:HOH:O	1:C:57:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLU:CD	1:A:32:GLU:N	2.71	0.44
1:A:121:SER:O	1:A:122:GLN:HB2	2.17	0.43
1:C:64:GLY:O	1:C:68:SER:HA	2.18	0.43
1:D:49:GLU:HG3	1:D:51:LEU:CD2	2.48	0.43
1:A:193:LLP:HE2	1:A:193:LLP:O3	2.18	0.43
1:D:259:ILE:O	1:D:263:MET:N	2.48	0.43
1:A:14:GLY:O	1:A:158:PRO:HG2	2.18	0.43
1:D:333:ILE:O	1:D:335:TYR:CD1	2.72	0.43
1:A:45:TRP:CZ2	1:A:113:ILE:HD13	2.54	0.42
1:D:199:ASP:OD1	1:D:199:ASP:N	2.52	0.42
1:D:108:ASP:OD1	3:D:503:HOH:O	2.21	0.42
1:D:263:MET:HB3	1:D:265:ILE:HD12	2.02	0.42
1:A:21:PRO:HA	1:A:22:PRO:HD3	1.90	0.41
1:A:233:CYS:HB2	1:A:284:MET:CG	2.49	0.41
1:A:333:ILE:HB	1:A:335:TYR:CE2	2.55	0.41
1:D:259:ILE:O	1:D:262:GLN:N	2.50	0.41
1:C:161:TRP:HB3	1:C:163:PHE:O	2.20	0.41
1:A:298:LEU:O	1:A:301:GLU:HB2	2.20	0.41
1:A:185:ARG:HA	1:A:190:PRO:HD2	2.01	0.41
1:B:248:LEU:HD12	1:B:249:PRO:HD2	2.02	0.41
1:D:74:VAL:HA	1:D:128:VAL:O	2.20	0.41
1:B:196:GLN:HB3	1:D:196:GLN:HB3	2.02	0.41
1:C:193:LLP:O3	1:C:193:LLP:HE2	2.20	0.41
1:C:77:VAL:O	1:C:125:GLU:HA	2.21	0.41
1:B:161:TRP:HB3	1:B:163:PHE:O	2.21	0.41
1:C:199:ASP:OD1	1:C:199:ASP:N	2.47	0.40
1:B:91:ARG:NH1	1:B:251:ILE:HG12	2.35	0.40
1:A:108:ASP:OD1	3:A:502:HOH:O	2.22	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:727:HOH:O	3:B:788:HOH:O[1_444]	1.97	0.23
3:B:768:HOH:O	3:C:2687:HOH:O[1_665]	2.02	0.18

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	318/335 (95%)	310 (98%)	8 (2%)	0	100	100
1	B	318/335 (95%)	310 (98%)	8 (2%)	0	100	100
1	C	315/335 (94%)	308 (98%)	7 (2%)	0	100	100
1	D	318/335 (95%)	306 (96%)	12 (4%)	0	100	100
All	All	1269/1340 (95%)	1234 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	259/270 (96%)	255 (98%)	4 (2%)	60	52
1	B	259/270 (96%)	254 (98%)	5 (2%)	52	41
1	C	257/270 (95%)	255 (99%)	2 (1%)	79	76
1	D	259/270 (96%)	253 (98%)	6 (2%)	45	33
All	All	1034/1080 (96%)	1017 (98%)	17 (2%)	58	49

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	76	HIS

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Mol	Chain	Res	Type
1	A	262	GLN
1	A	301	GLU
1	B	17	ARG
1	B	51	LEU
1	B	76	HIS
1	B	148	LEU
1	B	220	SER
1	C	76	HIS
1	C	185	ARG
1	D	32	GLU
1	D	49	GLU
1	D	51	LEU
1	D	76	HIS
1	D	124	ARG
1	D	181	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	262	GLN
1	B	116	GLN
1	D	35	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	LLP	C	193	1	23,24,25	1.21	1 (4%)	25,32,34	1.92	9 (36%)
1	LLP	A	193	1	23,24,25	1.13	1 (4%)	25,32,34	2.02	11 (44%)
1	LLP	D	193	1	23,24,25	1.20	1 (4%)	25,32,34	1.79	7 (28%)
1	LLP	B	193	1	23,24,25	1.27	2 (8%)	25,32,34	2.07	12 (48%)

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
1	LLP	C	193	1	-	4/16/17/19	0/1/1/1
1	LLP	A	193	1	-	5/16/17/19	0/1/1/1
1	LLP	D	193	1	-	4/16/17/19	0/1/1/1
1	LLP	B	193	1	-	5/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	LLP	P-OP4	3.88	1.72	1.60
1	D	193	LLP	P-OP4	3.84	1.72	1.60
1	A	193	LLP	P-OP4	3.73	1.72	1.60
1	C	193	LLP	P-OP4	3.72	1.72	1.60
1	B	193	LLP	O3-C3	-2.28	1.31	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	193	LLP	CE-NZ-C4'	4.61	133.05	118.90
1	A	193	LLP	CE-NZ-C4'	4.57	132.93	118.90
1	B	193	LLP	CE-NZ-C4'	4.54	132.85	118.90
1	D	193	LLP	CE-NZ-C4'	4.26	131.97	118.90
1	A	193	LLP	CD-CE-NZ	3.71	120.01	110.93
1	C	193	LLP	CD-CE-NZ	3.70	120.01	110.93
1	D	193	LLP	CD-CE-NZ	3.65	119.87	110.93
1	B	193	LLP	CD-CE-NZ	3.54	119.60	110.93
1	B	193	LLP	C5-C4-C4'	-3.35	116.05	121.56
1	A	193	LLP	OP3-P-OP4	-3.29	97.98	106.73
1	A	193	LLP	C5-C4-C4'	-3.14	116.40	121.56
1	B	193	LLP	C3-C4-C4'	3.13	126.25	120.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	193	LLP	OP3-P-OP4	-2.94	98.92	106.73
1	D	193	LLP	C5-C4-C4'	-2.88	116.82	121.56
1	C	193	LLP	C5-C4-C4'	-2.76	117.01	121.56
1	C	193	LLP	OP3-P-OP4	-2.71	99.53	106.73
1	B	193	LLP	OP3-P-OP2	2.55	117.40	107.64
1	A	193	LLP	CD-CG-CB	2.54	122.61	113.62
1	D	193	LLP	CD-CG-CB	2.43	122.22	113.62
1	C	193	LLP	C3-C4-C4'	2.43	124.94	120.41
1	D	193	LLP	C3-C4-C4'	2.35	124.79	120.41
1	C	193	LLP	CD-CG-CB	2.34	121.89	113.62
1	C	193	LLP	CG-CD-CE	-2.32	105.49	113.57
1	B	193	LLP	C4-C3-C2	-2.31	118.76	120.19
1	A	193	LLP	C3-C4-C4'	2.27	124.65	120.41
1	A	193	LLP	C4-C3-C2	-2.26	118.79	120.19
1	A	193	LLP	OP4-C5'-C5	2.26	113.66	109.35
1	B	193	LLP	CG-CD-CE	-2.26	105.70	113.57
1	B	193	LLP	OP4-C5'-C5	2.24	113.62	109.35
1	D	193	LLP	OP3-P-OP2	2.22	116.13	107.64
1	D	193	LLP	OP3-P-OP4	-2.20	100.87	106.73
1	C	193	LLP	OP3-P-OP2	2.17	115.93	107.64
1	A	193	LLP	CG-CD-CE	-2.16	106.03	113.57
1	B	193	LLP	OP4-P-OP1	-2.12	100.54	106.47
1	A	193	LLP	OP3-P-OP2	2.11	115.70	107.64
1	B	193	LLP	OP3-P-OP1	2.10	118.92	110.68
1	A	193	LLP	OP3-P-OP1	2.08	118.83	110.68
1	B	193	LLP	CD-CG-CB	2.06	120.92	113.62
1	C	193	LLP	OP4-C5'-C5	2.01	113.18	109.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	193	LLP	C4-C4'-NZ-CE
1	A	193	LLP	CG-CD-CE-NZ
1	B	193	LLP	C4-C4'-NZ-CE
1	B	193	LLP	O-C-CA-CB
1	B	193	LLP	CG-CD-CE-NZ
1	C	193	LLP	C4-C4'-NZ-CE
1	C	193	LLP	CG-CD-CE-NZ
1	D	193	LLP	C4-C4'-NZ-CE
1	D	193	LLP	CG-CD-CE-NZ
1	A	193	LLP	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	B	193	LLP	N-CA-CB-CG
1	C	193	LLP	N-CA-CB-CG
1	D	193	LLP	N-CA-CB-CG
1	B	193	LLP	C3-C4-C4'-NZ
1	A	193	LLP	C3-C4-C4'-NZ
1	C	193	LLP	C3-C4-C4'-NZ
1	D	193	LLP	C3-C4-C4'-NZ
1	A	193	LLP	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	193	LLP	1	0
1	A	193	LLP	1	0
1	D	193	LLP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	ALA	D	401	-	5,5,5	0.86	0	6,6,6	1.54	2 (33%)
2	ALA	C	401	-	5,5,5	1.08	1 (20%)	6,6,6	1.53	1 (16%)
2	ALA	A	401	-	5,5,5	1.11	1 (20%)	6,6,6	1.25	1 (16%)
2	ALA	B	401	-	5,5,5	0.96	0	6,6,6	1.52	2 (33%)

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	ALA	D	401	-	-	0/4/4/4	-
2	ALA	C	401	-	-	2/4/4/4	-
2	ALA	A	401	-	-	2/4/4/4	-
2	ALA	B	401	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ALA	OXT-C	-2.20	1.23	1.30
2	A	401	ALA	OXT-C	-2.18	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	ALA	OXT-C-O	-3.23	116.77	124.09
2	D	401	ALA	OXT-C-O	-2.64	118.10	124.09
2	A	401	ALA	OXT-C-O	-2.58	118.24	124.09
2	B	401	ALA	OXT-C-CA	2.56	123.30	114.06
2	D	401	ALA	OXT-C-CA	2.44	122.87	114.06
2	B	401	ALA	OXT-C-O	-2.36	118.73	124.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ALA	O-C-CA-CB
2	C	401	ALA	O-C-CA-CB
2	C	401	ALA	OXT-C-CA-CB
2	A	401	ALA	OXT-C-CA-CB

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 (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	322/335 (96%)	0.42	17 (5%)	33	37	14, 24, 46, 64	0
1	B	322/335 (96%)	0.41	25 (7%)	20	23	14, 23, 45, 72	0
1	C	319/335 (95%)	0.32	11 (3%)	48	53	14, 25, 41, 63	0
1	D	322/335 (96%)	0.65	34 (10%)	13	15	15, 26, 47, 64	0
All	All	1285/1340 (95%)	0.45	87 (6%)	25	28	14, 24, 46, 72	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	ALA	12.9
1	A	301	GLU	7.9
1	D	261	ASP	6.6
1	D	16	ILE	6.5
1	D	3	THR	6.4
1	A	335	TYR	6.0
1	D	262	GLN	5.3
1	C	33	LEU	5.1
1	B	148	LEU	4.8
1	A	3	THR	4.7
1	D	263	MET	4.6
1	C	32	GLU	4.3
1	C	302	ALA	4.2
1	D	51	LEU	4.1
1	B	33	LEU	4.0
1	B	32	GLU	3.9
1	C	300	GLY	3.9
1	A	334	GLU	3.8
1	B	3	THR	3.7
1	A	37	SER	3.5
1	C	31	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	15	ALA	3.2
1	A	53	ALA	3.2
1	C	301	GLU	3.1
1	B	31	TYR	3.1
1	D	335	TYR	3.1
1	A	333	ILE	3.0
1	B	43	VAL	3.0
1	B	14	GLY	2.9
1	B	15	ALA	2.9
1	D	333	ILE	2.9
1	B	55	ASP	2.9
1	B	334	GLU	2.9
1	D	33	LEU	2.8
1	B	51	LEU	2.8
1	B	39	PHE	2.8
1	D	334	GLU	2.8
1	A	30	ASP	2.8
1	D	14	GLY	2.7
1	A	137	GLY	2.7
1	D	45	TRP	2.7
1	C	148	LEU	2.6
1	D	326	PRO	2.6
1	D	4	GLY	2.6
1	D	35	HIS	2.6
1	D	38	PRO	2.6
1	D	37	SER	2.6
1	D	50	PHE	2.5
1	A	303	ILE	2.5
1	A	32	GLU	2.5
1	D	31	TYR	2.5
1	A	38	PRO	2.5
1	C	16	ILE	2.5
1	D	10	ALA	2.5
1	A	31	TYR	2.4
1	B	137	GLY	2.4
1	D	5	THR	2.4
1	D	137	GLY	2.4
1	B	149	THR	2.4
1	B	45	TRP	2.4
1	D	113	ILE	2.4
1	D	39	PHE	2.4
1	B	5	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	104	GLY	2.4
1	D	40	ALA	2.3
1	D	11	VAL	2.3
1	C	137	GLY	2.3
1	D	41	GLY	2.3
1	A	148	LEU	2.3
1	B	35	HIS	2.2
1	D	148	LEU	2.2
1	B	44	ALA	2.2
1	D	55	ASP	2.2
1	A	35	HIS	2.2
1	D	149	THR	2.1
1	D	264	GLY	2.1
1	D	123	LEU	2.1
1	B	34	ASP	2.1
1	B	136	TYR	2.1
1	B	48	GLY	2.1
1	C	9	VAL	2.1
1	A	51	LEU	2.1
1	B	40	ALA	2.1
1	B	333	ILE	2.1
1	C	335	TYR	2.1
1	B	9	VAL	2.0
1	B	38	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
1	LLP	C	193	24/25	0.94	0.10	15,19,31,34	0
1	LLP	B	193	24/25	0.95	0.08	15,19,25,34	0
1	LLP	A	193	24/25	0.95	0.08	14,17,25,31	0
1	LLP	D	193	24/25	0.95	0.09	16,20,30,37	0

6.3 Carbohydrates (i)

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	ALA	C	401	6/6	0.62	0.23	40,46,47,48	0
2	ALA	D	401	6/6	0.68	0.20	34,43,48,49	0
2	ALA	B	401	6/6	0.73	0.20	35,41,43,47	0
2	ALA	A	401	6/6	0.74	0.20	37,39,40,50	0

6.5 Other polymers

There are no such residues in this entry.