



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2026 – 04:30 PM EDT

PDB ID : 13LD / pdb_000013ld
Title : Deuterated alanine racemase from *Geobacillus stearothermophilus*
Authors : Leber, L.B.; Kovalevsky, A.Y.; Mueser, T.C.
Deposited on : 2026-05-12
Resolution : 1.90 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

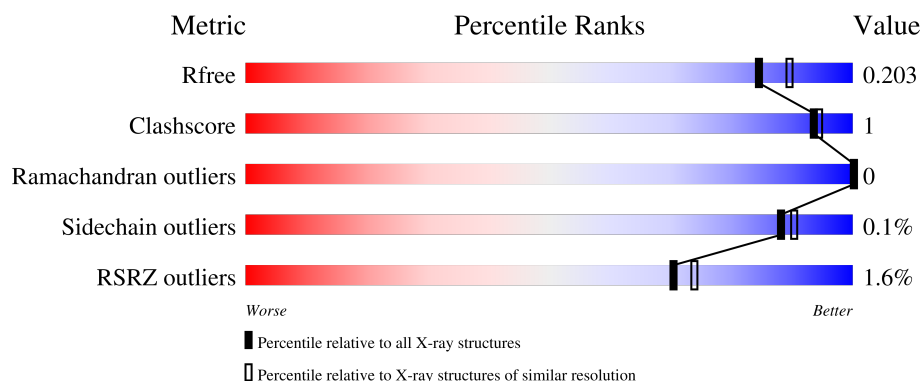
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	388	<div> <div>0%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
1	B	388	<div> <div>2%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	C	388	<div> <div>2%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
1	D	388	<div> <div>2%</div> <div>95%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12757 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 Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	P	S	0	2	0
			3055	1953	540	548	1	13			
1	B	381	Total	C	N	O	P	S	0	3	0
			3072	1962	547	549	1	13			
1	C	382	Total	C	N	O	P	S	0	3	0
			3073	1964	545	550	1	13			
1	D	381	Total	C	N	O	P	S	0	2	0
			3058	1954	541	548	1	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	VAL	LEU	conflict	UNP P10724
A	383	ALA	ARG	conflict	UNP P10724
B	163	VAL	LEU	conflict	UNP P10724
B	383	ALA	ARG	conflict	UNP P10724
C	163	VAL	LEU	conflict	UNP P10724
C	383	ALA	ARG	conflict	UNP P10724
D	163	VAL	LEU	conflict	UNP P10724
D	383	ALA	ARG	conflict	UNP P10724

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

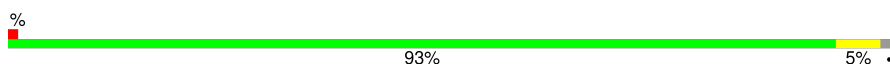
- Molecule 3 is water.

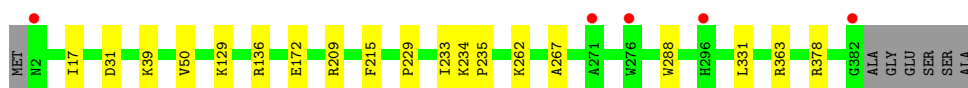
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	130	Total O 130 130	0	0
3	B	119	Total O 119 119	0	0
3	C	126	Total O 126 126	0	0
3	D	108	Total O 108 108	0	0

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.

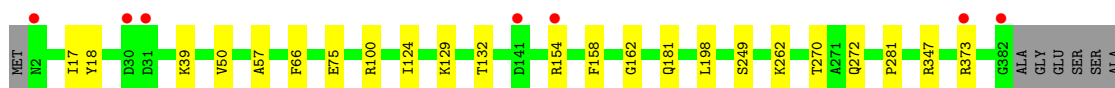
- Molecule 1: Alanine racemase

Chain A: 



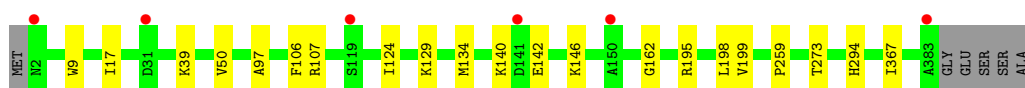
- Molecule 1: Alanine racemase

Chain B: 



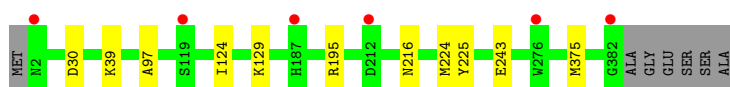
- Molecule 1: Alanine racemase

Chain C: 



- Molecule 1: Alanine racemase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.44Å 109.92Å 90.18Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	27.81 – 1.90 27.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.81-1.90) 99.3 (27.81-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.164 , 0.204 0.166 , 0.203	Depositor DCC
R_{free} test set	6737 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12757	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: KCX, ACT, 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	0.60	0/3095	0.75	2/4207 (0.0%)
1	B	0.59	0/3113	0.72	0/4230
1	C	0.61	1/3114 (0.0%)	0.75	2/4233 (0.0%)
1	D	0.56	0/3098	0.69	0/4210
All	All	0.59	1/12420 (0.0%)	0.73	4/16880 (0.0%)

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	A	0	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	LYS	C-N	-8.12	1.21	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	LYS	CA-C-N	6.75	133.67	122.73
1	C	140	LYS	C-N-CA	6.75	133.67	122.73
1	A	215	PHE	CA-C-N	-6.00	113.06	122.49
1	A	215	PHE	C-N-CA	-6.00	113.06	122.49

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ARG	Sidechain
1	A	378	ARG	Sidechain
1	B	154	ARG	Sidechain
1	B	373	ARG	Sidechain

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	3055	0	3030	9	0
1	B	3072	0	3044	11	0
1	C	3073	0	3045	11	0
1	D	3058	0	3030	6	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	130	0	0	1	0
3	B	119	0	0	0	0
3	C	126	0	0	3	0
3	D	108	0	0	1	0
All	All	12757	0	12161	34	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 1.

All (34) 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:262:LYS:HD3	1:A:267:ALA:HB1	1.72	0.71
1:D:97:ALA:HB2	1:D:124:ILE:HG12	1.75	0.68
1:D:243:GLU:HG2	3:D:559:HOH:O	1.99	0.61
1:B:17:ILE:HD13	1:B:50:VAL:HG22	1.87	0.56
1:A:288:TRP:CE2	1:A:331:LEU:HD23	2.42	0.54
1:A:229:PRO:HB2	1:A:233:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:HD2	1:C:199:VAL:HG21	1.92	0.50
1:C:134:MET:HB3	3:C:583:HOH:O	2.12	0.50
1:A:31:ASP:HB3	3:A:605:HOH:O	2.13	0.49
1:C:294[B]:HIS:CE1	3:C:505:HOH:O	2.66	0.48
1:A:234:LYS:N	1:A:235:PRO:HD2	2.28	0.48
1:C:294[B]:HIS:HE1	3:C:505:HOH:O	1.95	0.48
1:B:262:LYS:HE3	1:B:270:THR:OG1	2.15	0.47
1:C:106:PHE:CD1	1:C:107:ARG:HG3	2.51	0.45
1:C:97:ALA:HB2	1:C:124:ILE:HG12	1.98	0.45
1:A:17:ILE:HD13	1:A:50:VAL:HG22	1.99	0.44
1:A:363:ARG:HG2	1:B:66:PHE:HZ	1.82	0.44
1:C:259:PRO:HG3	1:C:273:THR:HA	2.00	0.44
1:C:17:ILE:HD13	1:C:50:VAL:HG22	1.98	0.44
1:A:172:GLU:O	1:A:209:ARG:NH2	2.51	0.43
1:B:347:ARG:HD3	1:D:30:ASP:O	2.18	0.43
1:B:100:ARG:HG3	1:B:100:ARG:HH11	1.84	0.42
1:C:162:GLY:HA2	1:C:198:LEU:O	2.19	0.42
1:B:124:ILE:HD12	1:B:158:PHE:CE1	2.55	0.42
1:C:142:GLU:O	1:C:146:LYS:HG3	2.19	0.42
1:D:195:ARG:HH12	1:D:216:ASN:HD21	1.67	0.41
1:B:132:THR:O	1:B:181:GLN:HG2	2.20	0.41
1:B:18:TYR:CD1	1:B:57:ALA:HB2	2.56	0.41
1:B:162:GLY:HA2	1:B:198:LEU:O	2.20	0.41
1:C:9:TRP:CD1	1:C:367:ILE:HD12	2.56	0.41
1:B:272:GLN:HB2	1:D:375[A]:MET:HE3	2.03	0.41
1:B:249:SER:OG	1:B:281:PRO:HD2	2.21	0.40
1:D:224:MET:HE3	1:D:225:TYR:CZ	2.56	0.40
1:A:288:TRP:CZ2	1:A:331:LEU:HD23	2.57	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	379/388 (98%)	368 (97%)	11 (3%)	0	100	100
1	B	380/388 (98%)	367 (97%)	13 (3%)	0	100	100
1	C	381/388 (98%)	372 (98%)	9 (2%)	0	100	100
1	D	378/388 (97%)	366 (97%)	12 (3%)	0	100	100
All	All	1518/1552 (98%)	1473 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	318/320 (99%)	318 (100%)	0	100	100
1	B	319/320 (100%)	318 (100%)	1 (0%)	86	88
1	C	319/320 (100%)	319 (100%)	0	100	100
1	D	318/320 (99%)	318 (100%)	0	100	100
All	All	1274/1280 (100%)	1273 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	302	GLN
1	B	125	HIS
1	B	157	HIS
1	B	258	GLN
1	C	5	HIS
1	C	98	GLN

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Mol	Chain	Res	Type
1	C	253	HIS
1	C	272	GLN
1	D	258	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	KCX	C	129	1	10,11,12	2.24	2 (20%)	6,12,14	2.70	4 (66%)
1	LLP	C	39	1	23,24,25	1.47	6 (26%)	25,32,34	1.98	10 (40%)
1	KCX	D	129	1	10,11,12	2.08	2 (20%)	6,12,14	2.71	3 (50%)
1	LLP	B	39	1	23,24,25	1.43	4 (17%)	25,32,34	1.93	10 (40%)
1	KCX	B	129	1	10,11,12	2.05	2 (20%)	6,12,14	1.90	1 (16%)
1	LLP	A	39	1	23,24,25	1.52	4 (17%)	25,32,34	2.00	9 (36%)
1	LLP	D	39	1	23,24,25	1.47	5 (21%)	25,32,34	2.03	9 (36%)
1	KCX	A	129	1	10,11,12	2.01	2 (20%)	6,12,14	2.46	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
1	KCX	C	129	1	-	1/9/10/12	-
1	LLP	C	39	1	-	1/16/17/19	0/1/1/1
1	KCX	D	129	1	-	1/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	39	1	-	2/16/17/19	0/1/1/1
1	KCX	B	129	1	-	1/9/10/12	-
1	LLP	A	39	1	-	1/16/17/19	0/1/1/1
1	LLP	D	39	1	-	1/16/17/19	0/1/1/1
1	KCX	A	129	1	-	1/9/10/12	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	KCX	CX-NZ	5.69	1.45	1.35
1	D	129	KCX	CX-NZ	5.55	1.45	1.35
1	B	129	KCX	CX-NZ	5.31	1.44	1.35
1	A	129	KCX	CX-NZ	4.68	1.43	1.35
1	A	39	LLP	C3-C2	4.08	1.45	1.41
1	D	39	LLP	C3-C2	3.58	1.44	1.41
1	C	129	KCX	OQ1-CX	3.33	1.27	1.21
1	C	39	LLP	C3-C2	3.20	1.44	1.41
1	B	39	LLP	C3-C2	3.14	1.44	1.41
1	A	39	LLP	C6-N1	-3.12	1.28	1.34
1	D	39	LLP	C6-N1	-3.00	1.28	1.34
1	B	129	KCX	OQ1-CX	2.97	1.27	1.21
1	C	39	LLP	C6-N1	-2.94	1.28	1.34
1	B	39	LLP	C6-N1	-2.86	1.28	1.34
1	A	129	KCX	OQ1-CX	2.67	1.26	1.21
1	D	129	KCX	OQ1-CX	2.61	1.26	1.21
1	C	39	LLP	CD-CE	2.46	1.59	1.51
1	D	39	LLP	CD-CE	2.42	1.59	1.51
1	B	39	LLP	CD-CE	2.37	1.59	1.51
1	A	39	LLP	CD-CE	2.36	1.59	1.51
1	B	39	LLP	CB-CA	2.33	1.57	1.53
1	C	39	LLP	CB-CA	2.28	1.57	1.53
1	C	39	LLP	P-OP4	2.12	1.67	1.60
1	D	39	LLP	P-OP4	2.10	1.67	1.60
1	A	39	LLP	C4-C3	2.06	1.44	1.41
1	C	39	LLP	C4-C3	2.05	1.44	1.41
1	D	39	LLP	CB-CA	2.02	1.56	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	KCX	OQ1-CX-NZ	-5.40	116.72	124.92
1	D	129	KCX	OQ1-CX-NZ	-4.67	117.83	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	LLP	OP4-C5'-C5	-4.48	100.95	109.36
1	C	129	KCX	CE-NZ-CX	-4.35	114.60	121.98
1	C	39	LLP	C6-N1-C2	4.26	126.92	119.20
1	A	39	LLP	C6-N1-C2	4.16	126.74	119.20
1	B	39	LLP	C6-N1-C2	4.15	126.72	119.20
1	D	39	LLP	C6-N1-C2	4.15	126.72	119.20
1	C	39	LLP	OP4-C5'-C5	-4.06	101.75	109.36
1	B	129	KCX	OQ1-CX-NZ	-4.04	118.78	124.92
1	D	129	KCX	CE-NZ-CX	-4.01	115.18	121.98
1	C	129	KCX	OQ1-CX-NZ	-3.99	118.86	124.92
1	B	39	LLP	OP4-C5'-C5	-3.69	102.44	109.36
1	A	39	LLP	OP4-C5'-C5	-3.40	102.98	109.36
1	A	39	LLP	C2'-C2-C3	3.32	124.68	120.80
1	A	39	LLP	C3-C4-C5	-3.21	115.70	118.28
1	D	39	LLP	C3-C4-C5	-3.01	115.86	118.28
1	B	39	LLP	C3-C4-C5	-2.99	115.88	118.28
1	A	39	LLP	C3-C2-N1	-2.95	117.25	120.96
1	C	39	LLP	C3-C4-C5	-2.87	115.97	118.28
1	D	39	LLP	C3-C2-N1	-2.82	117.40	120.96
1	A	39	LLP	CE-NZ-C4'	2.73	127.47	118.72
1	A	39	LLP	CD-CE-NZ	-2.71	103.65	110.83
1	C	39	LLP	C3-C2-N1	-2.65	117.62	120.96
1	D	39	LLP	C2'-C2-C3	2.64	123.89	120.80
1	B	39	LLP	C3-C2-N1	-2.64	117.63	120.96
1	C	39	LLP	C5-C6-N1	-2.63	119.55	123.83
1	B	39	LLP	C5-C6-N1	-2.63	119.56	123.83
1	D	39	LLP	CD-CE-NZ	-2.62	103.89	110.83
1	D	39	LLP	CE-NZ-C4'	2.61	127.07	118.72
1	B	39	LLP	CE-NZ-C4'	2.61	127.06	118.72
1	C	39	LLP	C4-C3-C2	-2.60	118.68	120.14
1	C	39	LLP	CE-NZ-C4'	2.60	127.06	118.72
1	B	39	LLP	CD-CE-NZ	-2.47	104.30	110.83
1	A	39	LLP	C4-C3-C2	-2.47	118.75	120.14
1	D	39	LLP	C5-C6-N1	-2.45	119.84	123.83
1	A	129	KCX	CD-CG-CB	-2.43	104.45	113.62
1	C	39	LLP	CD-CE-NZ	-2.41	104.46	110.83
1	D	39	LLP	C4-C3-C2	-2.34	118.82	120.14
1	C	39	LLP	C2'-C2-C3	2.31	123.50	120.80
1	A	39	LLP	C5-C6-N1	-2.27	120.14	123.83
1	C	39	LLP	O3-C3-C4	2.14	125.22	119.44
1	B	39	LLP	C2'-C2-C3	2.13	123.29	120.80
1	B	39	LLP	O3-C3-C4	2.13	125.18	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	LLP	C4-C3-C2	-2.08	118.97	120.14
1	D	129	KCX	CD-CG-CB	-2.05	105.91	113.62
1	C	129	KCX	CD-CG-CB	-2.01	106.04	113.62
1	C	129	KCX	CD-CE-NZ	2.01	117.83	112.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	129	KCX	CG-CD-CE-NZ
1	B	39	LLP	CG-CD-CE-NZ
1	A	39	LLP	CG-CD-CE-NZ
1	C	39	LLP	CG-CD-CE-NZ
1	D	129	KCX	CG-CD-CE-NZ
1	A	129	KCX	CG-CD-CE-NZ
1	D	39	LLP	CG-CD-CE-NZ
1	B	129	KCX	CG-CD-CE-NZ
1	B	39	LLP	C3-C4-C4'-NZ

There are no ring outliers.

No monomer is involved in short contacts.

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	ACT	B	401	-	3,3,3	1.46	1 (33%)	3,3,3	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	D	401	-	3,3,3	1.30	1 (33%)	3,3,3	0.74	0
2	ACT	C	401	-	3,3,3	1.30	0	3,3,3	0.72	0
2	ACT	A	401	-	3,3,3	1.30	1 (33%)	3,3,3	0.71	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ACT	OXT-C	-2.24	1.20	1.30
2	A	401	ACT	OXT-C	-2.01	1.21	1.30
2	D	401	ACT	OXT-C	-2.00	1.21	1.30

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 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	379/388 (97%)	-0.17	5 (1%) 75 78	10, 24, 47, 67	2 (0%)
1	B	379/388 (97%)	-0.01	7 (1%) 67 71	13, 27, 49, 69	3 (0%)
1	C	380/388 (97%)	-0.11	6 (1%) 70 74	12, 25, 47, 62	3 (0%)
1	D	379/388 (97%)	-0.08	6 (1%) 70 74	13, 26, 49, 67	2 (0%)
All	All	1517/1552 (97%)	-0.09	24 (1%) 70 74	10, 26, 48, 69	10 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	383	ALA	4.2
1	B	373	ARG	3.4
1	C	141	ASP	3.3
1	B	141	ASP	3.1
1	D	2[A]	ASN	3.0
1	B	154	ARG	3.0
1	A	271	ALA	2.8
1	B	30	ASP	2.8
1	B	2	ASN	2.7
1	D	276	TRP	2.6
1	B	382	GLY	2.6
1	A	2	ASN	2.5
1	A	276	TRP	2.4
1	D	119	SER	2.4
1	D	187	HIS	2.3
1	A	296	HIS	2.3
1	C	2	ASN	2.3
1	A	382	GLY	2.3
1	D	382	GLY	2.2
1	B	31	ASP	2.2
1	C	119	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	31	ASP	2.1
1	C	150	ALA	2.0
1	D	212	ASP	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, 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
1	KCX	C	129	12/13	0.95	0.06	21,26,32,32	0
1	KCX	B	129	12/13	0.96	0.06	21,25,31,31	0
1	LLP	A	39	24/25	0.97	0.06	9,16,21,23	0
1	KCX	A	129	12/13	0.97	0.06	15,19,24,24	0
1	KCX	D	129	12/13	0.97	0.05	18,22,26,27	0
1	LLP	B	39	24/25	0.98	0.04	13,20,22,25	0
1	LLP	D	39	24/25	0.98	0.05	11,16,22,25	0
1	LLP	C	39	24/25	0.98	0.05	12,18,22,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	ACT	C	401	4/4	0.89	0.13	23,24,24,26	0
2	ACT	A	401	4/4	0.91	0.12	26,27,27,28	0
2	ACT	D	401	4/4	0.92	0.12	25,25,26,27	0
2	ACT	B	401	4/4	0.93	0.14	24,25,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.