



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 07:10 PM EDT

PDB ID : 2IAE
Title : Crystal structure of a protein phosphatase 2A (PP2A) holoenzyme.
Authors : Cho, U.S.; Xu, W.
Deposited on : unknown
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

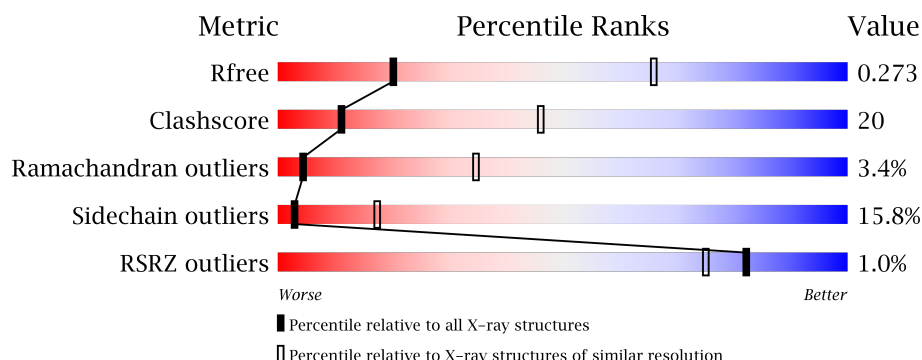
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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 $\leq 5\%$. 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	589	<div> <div>3%</div> <div>61%</div> <div>32%</div> <div>6%</div> <div>.</div> </div>
1	D	589	<div> <div>65%</div> <div>29%</div> <div>5%</div> <div>..</div> </div>
2	B	407	<div> <div>52%</div> <div>32%</div> <div>7%</div> <div>8%</div> </div>
2	E	407	<div> <div>47%</div> <div>36%</div> <div>9%</div> <div>7%</div> </div>
3	C	309	<div> <div>%</div> <div>52%</div> <div>37%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	309	
4	M	7	
4	N	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
4	DAM	M	7	-	-	X	-
4	ACB	N	3	-	-	X	-
4	DAM	N	7	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19955 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4541	2885	765	864	27			
1	D	583	Total	C	N	O	S	0	0	0
			4541	2885	765	864	27			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	376	Total	C	N	O	S	0	0	0
			2974	1945	486	533	10			
2	E	377	Total	C	N	O	S	0	0	0
			2987	1958	487	531	11			

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	306	Total	C	N	O	S	0	0	0
			2430	1538	415	462	15			
3	F	291	Total	C	N	O	S	0	0	0
			2336	1479	402	440	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	ASN	ASP	ENGINEERED	UNP P67775
F	88	ASN	ASP	ENGINEERED	UNP P67775

- Molecule 4 is a protein called microcystin-LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	7	Total	C	N	O	0	0	0
			71	49	10	12			
4	N	7	Total	C	N	O	0	0	0
			71	49	10	12			

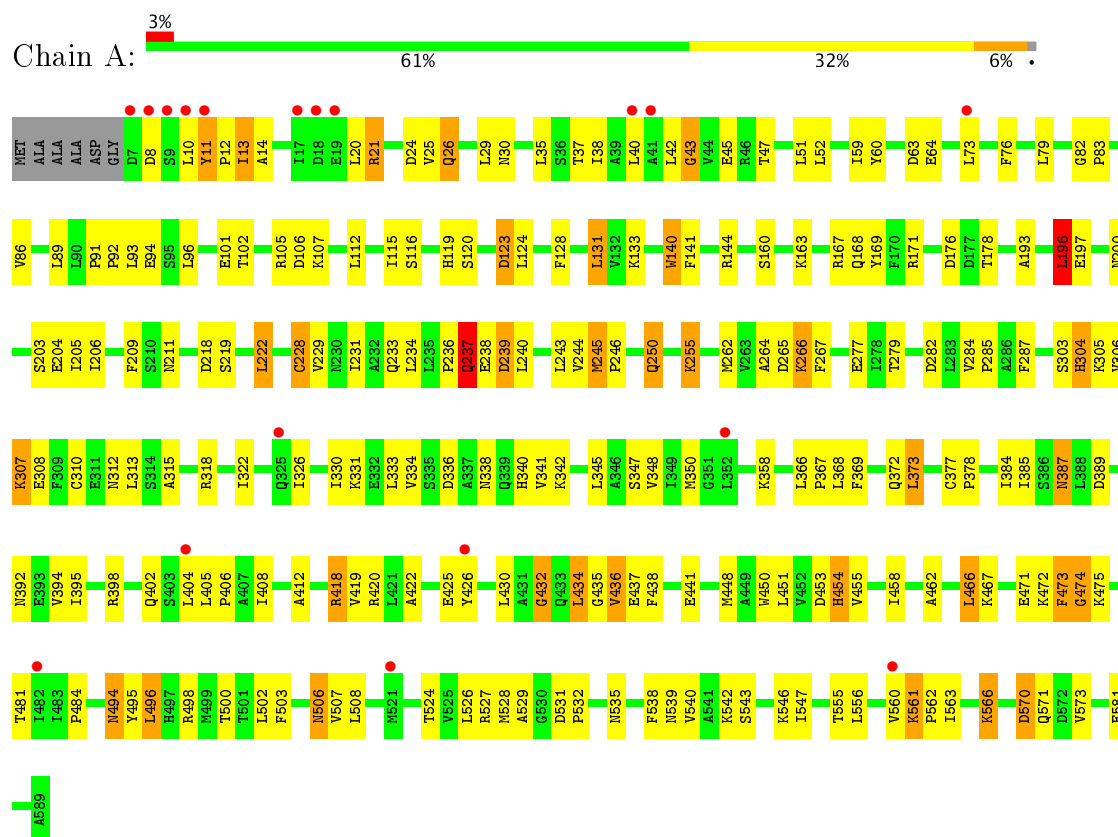
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mn	0	0
			2	2		
5	F	2	Total	Mn	0	0
			2	2		

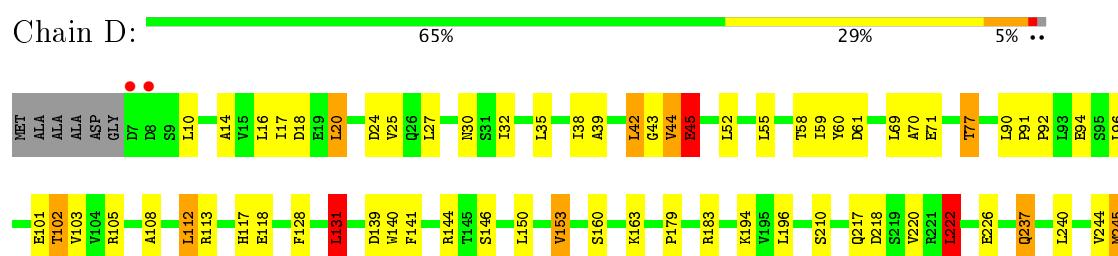
3 Residue-property plots

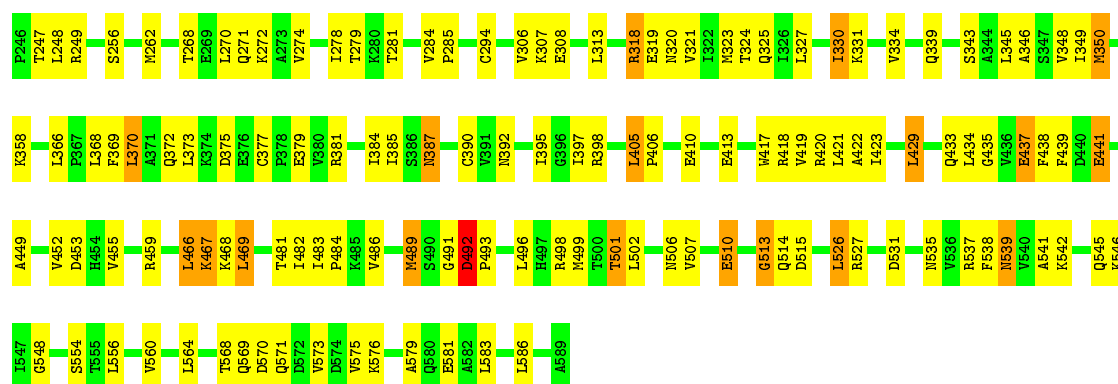
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



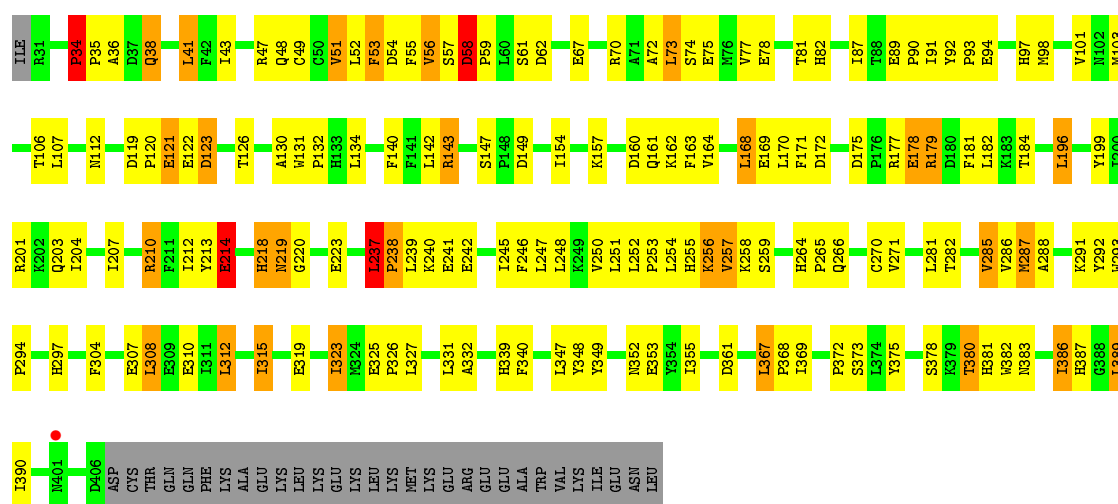
- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform





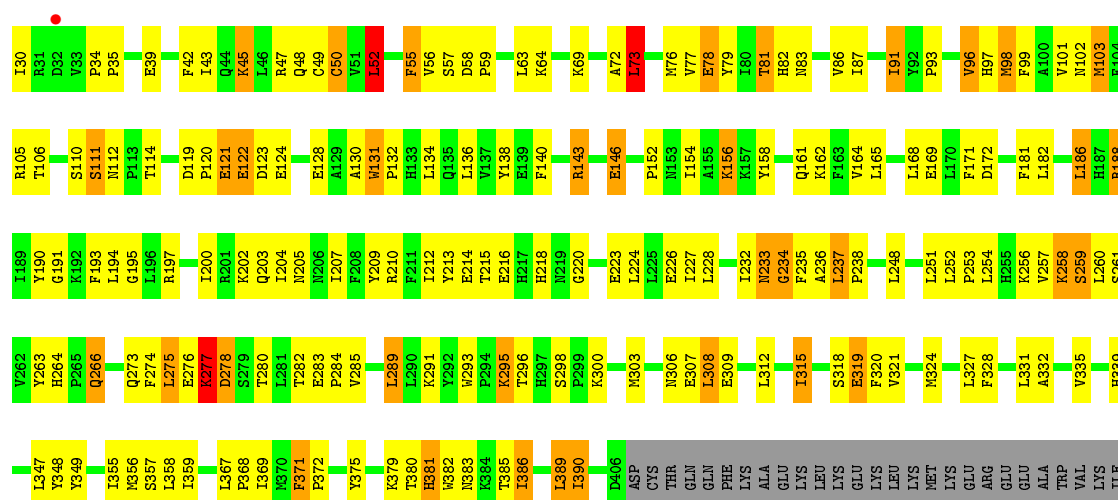
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

Chain B: 52% 32% 7% 8%



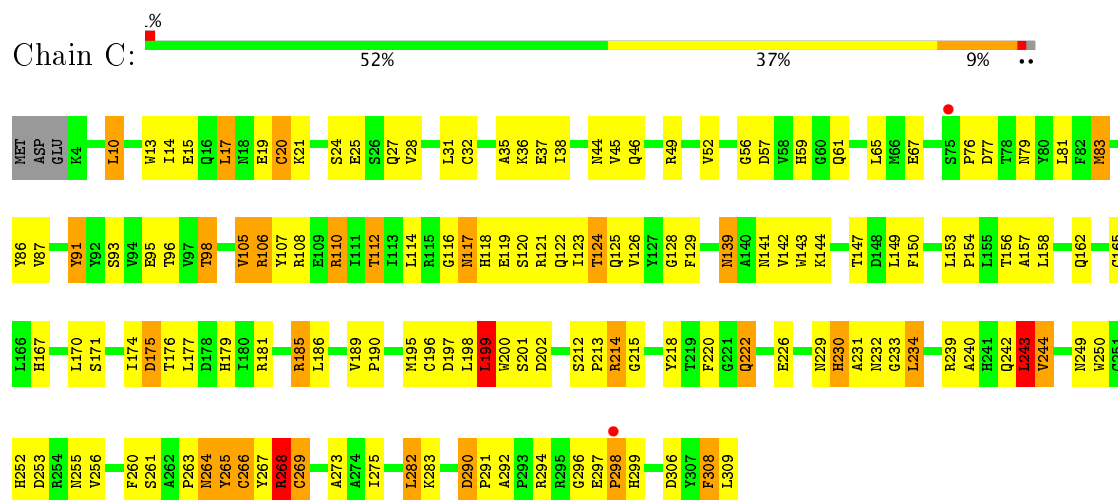
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

Chain E: 47% 36% 9% 7%

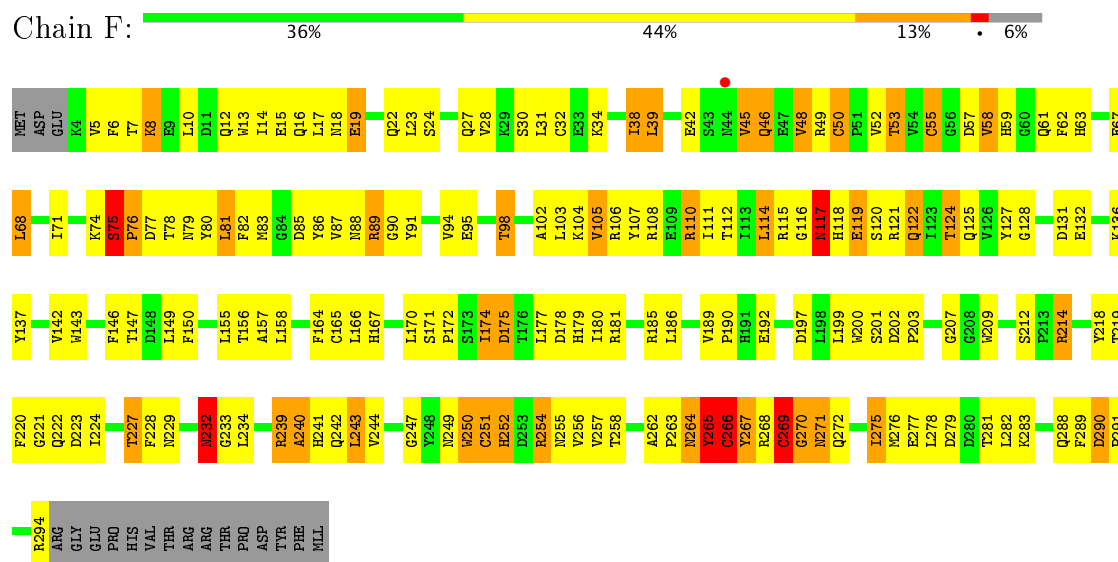


GLU
ASN
LEU

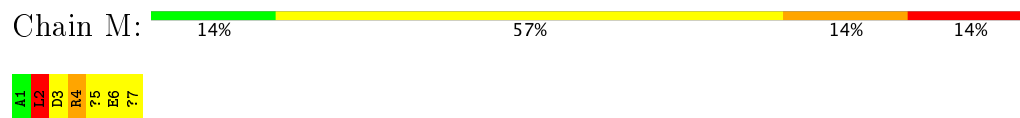
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



- Molecule 4: microcystin-LR



- Molecule 4: microcystin-LR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	265.30Å 265.30Å 265.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 49.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.50) 97.4 (49.27-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.316 0.229 , 0.273	Depositor DCC
R_{free} test set	3832 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	111.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19955	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: ACB, DAL, DAM, MN, MLL, 1ZN, FGA

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	0/4615	0.61	3/6266 (0.0%)
1	D	0.44	0/4615	0.63	2/6266 (0.0%)
2	B	0.46	0/3056	0.64	2/4170 (0.0%)
2	E	0.47	0/3073	0.64	2/4195 (0.0%)
3	C	0.44	0/2480	0.70	3/3371 (0.1%)
3	F	0.53	0/2393	0.75	1/3247 (0.0%)
4	M	0.69	0/17	0.98	0/19
4	N	1.49	0/17	1.81	0/19
All	All	0.45	0/20266	0.65	13/27553 (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	1
1	D	0	2
2	B	0	1
2	E	0	2
3	C	0	4
3	F	0	2
4	M	0	1
All	All	0	13

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	298	PRO	N-CA-CB	6.44	111.03	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	52	LEU	CA-CB-CG	6.18	129.51	115.30
2	B	34	PRO	N-CA-CB	5.86	110.33	103.30
1	A	434	LEU	CA-CB-CG	5.72	128.46	115.30
2	E	73	LEU	CA-CB-CG	5.63	128.25	115.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	LEU	Peptide
2	B	214	GLU	Peptide
3	C	233	GLY	Peptide
3	C	266	CYS	Peptide
3	C	296	GLY	Peptide

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	4541	0	4641	136	0
1	D	4541	0	4641	122	0
2	B	2974	0	2849	119	0
2	E	2987	0	2858	132	0
3	C	2430	0	2276	109	2
3	F	2336	0	2229	179	4
4	M	71	0	67	16	2
4	N	71	0	69	28	4
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	19955	0	19630	791	6

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 20.

The worst 5 of 791 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)
4:N:2:LEU:HA	4:N:3:ACB:C4	1.12	1.53
4:N:2:LEU:CA	4:N:3:ACB:H43	1.04	1.51
4:N:2:LEU:O	4:N:3:ACB:N	1.74	1.18
4:N:2:LEU:CA	4:N:3:ACB:C4	1.86	1.17
4:N:2:LEU:N	4:N:3:ACB:C4	2.09	1.12

The worst 5 of 6 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:C:175:ASP:OD1	4:M:4:ARG:NE[11_466]	1.57	0.63
3:F:175:ASP:OD2	4:N:4:ARG:NE[12_664]	1.61	0.59
3:F:175:ASP:OD2	4:N:3:ACB:OXT[12_664]	1.65	0.55
3:C:175:ASP:CG	4:M:4:ARG:NE[11_466]	2.01	0.19
3:F:175:ASP:CG	4:N:4:ARG:NE[12_664]	2.05	0.15

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	581/589 (99%)	502 (86%)	63 (11%)	16 (3%)	6	39
1	D	581/589 (99%)	505 (87%)	65 (11%)	11 (2%)	9	47
2	B	374/407 (92%)	300 (80%)	60 (16%)	14 (4%)	4	32
2	E	375/407 (92%)	307 (82%)	53 (14%)	15 (4%)	3	30
3	C	304/309 (98%)	253 (83%)	40 (13%)	11 (4%)	4	33
3	F	289/309 (94%)	231 (80%)	41 (14%)	17 (6%)	2	20
4	M	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2505/2617 (96%)	2099 (84%)	322 (13%)	84 (3%)	4	35

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	304	HIS
2	B	34	PRO
2	B	56	VAL
2	B	121	GLU

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	509/512 (99%)	448 (88%)	61 (12%)	6	28
1	D	509/512 (99%)	445 (87%)	64 (13%)	5	26
2	B	310/379 (82%)	254 (82%)	56 (18%)	2	11
2	E	311/379 (82%)	257 (83%)	54 (17%)	2	13
3	C	257/273 (94%)	211 (82%)	46 (18%)	2	11
3	F	253/273 (93%)	196 (78%)	57 (22%)	1	5
4	M	2/2 (100%)	0	2 (100%)	0	0
4	N	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	2153/2332 (92%)	1812 (84%)	341 (16%)	3	17

5 of 341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	264	ASN
1	D	327	LEU
3	F	158	LEU
3	C	282	LEU
1	D	77	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	179	HIS

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Mol	Chain	Res	Type
1	D	168	GLN
3	F	118	HIS
3	C	187	GLN
3	C	288	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 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
3	MLL	C	309	3	9,9,9	3.31	2 (22%)	11,11,11	2.22	2 (18%)
4	DAL	M	1	4	4,4,5	1.54	1 (25%)	1,4,6	0.01	0
4	ACB	M	3	4	4,8,9	1.24	0	3,10,12	2.55	2 (66%)
4	1ZN	M	5	4	22,23,24	1.93	1 (4%)	24,29,31	1.63	6 (25%)
4	FGA	M	6	4	3,8,9	2.00	1 (33%)	2,9,11	0.87	0
4	DAM	M	7	4	5,5,6	1.56	1 (20%)	3,5,7	3.10	2 (66%)
4	DAL	N	1	4	4,4,5	1.56	1 (25%)	1,4,6	0.56	0
4	ACB	N	3	4	4,8,9	1.25	0	3,10,12	2.37	1 (33%)
4	1ZN	N	5	4	22,23,24	2.10	1 (4%)	24,29,31	2.03	9 (37%)
4	FGA	N	6	4	3,8,9	2.01	1 (33%)	2,9,11	1.21	0
4	DAM	N	7	4	5,5,6	1.57	1 (20%)	3,5,7	4.29	2 (66%)

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
3	MLL	C	309	3	-	0/10/10/10	0/0/0/0
4	DAL	M	1	4	-	0/0/2/4	0/0/0/0
4	ACB	M	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	M	5	4	-	0/22/25/27	0/1/1/1
4	FGA	M	6	4	-	0/4/8/9	0/0/0/0
4	DAM	M	7	4	-	0/0/4/6	0/0/0/0
4	DAL	N	1	4	-	0/0/2/4	0/0/0/0
4	ACB	N	3	4	-	0/5/10/12	0/0/0/0
4	1ZN	N	5	4	-	0/22/25/27	0/1/1/1
4	FGA	N	6	4	-	0/4/8/9	0/0/0/0
4	DAM	N	7	4	-	0/0/4/6	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	5	1ZN	C15-C13	-9.08	1.26	1.45
4	M	5	1ZN	C15-C13	-8.45	1.27	1.45
4	M	6	FGA	OE2-CD	-3.41	1.24	1.42
4	N	6	FGA	OE2-CD	-3.37	1.24	1.42
4	N	1	DAL	CA-C	2.87	1.54	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	7	DAM	O-C-CA	-6.66	116.85	125.07
3	C	309	MLL	O9-C-O	-6.35	111.04	123.82
4	M	7	DAM	O-C-CA	-4.80	119.14	125.07
4	N	5	1ZN	C18-C17-C16	-4.69	106.17	113.01
4	N	3	ACB	CA-CB-CG	-3.37	106.29	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	309	MLL	5	0
4	M	3	ACB	3	0
4	M	5	1ZN	4	0
4	M	6	FGA	3	0
4	M	7	DAM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	1	DAL	1	0
4	N	3	ACB	15	1
4	N	5	1ZN	2	0
4	N	7	DAM	7	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	2:LEU	C	3:ACB	N	2.64

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	583/589 (98%)	0.07	18 (3%) 49 41	85, 114, 172, 203	0
1	D	583/589 (98%)	-0.16	2 (0%) 93 90	96, 113, 129, 144	0
2	B	376/407 (92%)	-0.43	1 (0%) 93 90	77, 90, 126, 152	0
2	E	377/407 (92%)	-0.38	1 (0%) 93 90	63, 76, 103, 139	0
3	C	305/309 (98%)	-0.25	2 (0%) 87 82	81, 93, 112, 139	0
3	F	291/309 (94%)	0.50	1 (0%) 93 90	131, 149, 159, 166	0
4	M	2/7 (28%)	-0.21	0 100 100	86, 86, 86, 91	0
4	N	2/7 (28%)	-0.04	0 100 100	80, 80, 80, 85	0
All	All	2519/2624 (95%)	-0.12	25 (0%) 82 75	63, 106, 153, 203	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	SER	4.6
1	A	8	ASP	4.5
1	A	17	ILE	4.4
1	D	7	ASP	4.2
1	A	11	TYR	3.9

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

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MLL	C	309	10/10	0.85	0.30	-	139,139,139,140	0
4	FGA	N	6	9/10	0.92	0.18	-	78,82,83,84	0
4	DAL	M	1	5/6	0.94	0.14	-	91,91,91,91	0
4	ACB	M	3	9/10	0.87	0.23	-	87,88,90,90	0
4	ACB	N	3	9/10	0.80	0.36	-	82,83,85,86	0
4	1ZN	N	5	23/24	0.92	0.34	-	63,66,76,77	0
4	DAM	M	7	6/7	0.81	0.32	-	93,93,93,93	0
4	DAL	N	1	5/6	0.93	0.19	-	84,84,84,84	0
4	DAM	N	7	6/7	0.88	0.20	-	84,84,84,85	0
4	1ZN	M	5	23/24	0.94	0.29	-	85,85,89,90	0
4	FGA	M	6	9/10	0.89	0.28	-	87,90,91,92	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	MN	C	310	1/1	0.99	0.27	1.84	119,119,119,119	0
5	MN	C	311	1/1	0.98	0.17	-0.92	63,63,63,63	0
5	MN	F	310	1/1	0.97	0.15	-2.46	86,86,86,86	0
5	MN	F	311	1/1	0.94	0.16	-2.94	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.