W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 01:42 PM EST

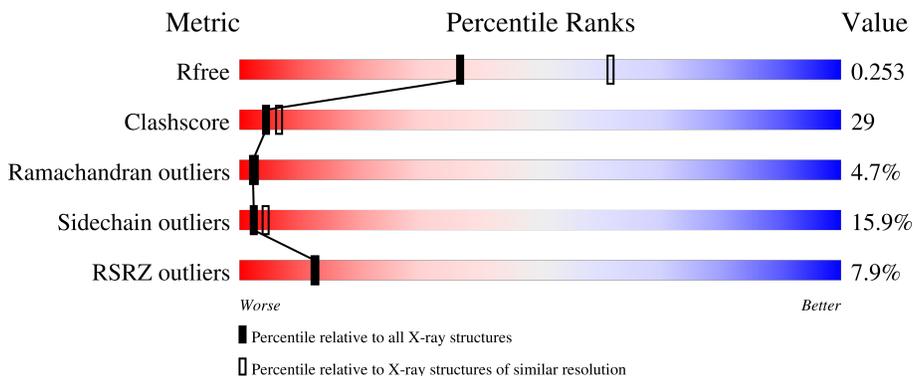|		
PDB ID	:	2ZBB
Title	:	P43 crystal of DctBp
Authors	:	Zhou, Y.F.; Nan, B.Y.; Liu, X.; Nan, J.; Liang, Y.H.; Panjikar, S.; Ma, Q.J.; Wang, Y.P.; Su, X.-D.
Deposited on	:	2007-10-18
Resolution	:	2.50 Å(reported)

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 2.50 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		29
Ramachandran outliers		4.7%
Sidechain outliers		15.9%
RSRZ outliers		7.9%

Worse ▬▬▬ *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	305	6% — 47% / 27% / 9% · 16%
1	B	305	9% — 45% / 22% / 12% / 5% 16%
1	C	305	8% — 47% / 30% / 6% · 16%
1	D	305	5% — 49% / 24% / 9% · 16%

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2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7852 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 C4-dicarboxylate transport sensor protein dctB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			
1	B	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			
1	C	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			
1	D	255	Total	C	N	O	S	0	0	0
			1952	1236	350	362	4			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP P13633
A	9	GLY	-	expression tag	UNP P13633
A	10	SER	-	expression tag	UNP P13633
A	11	SER	-	expression tag	UNP P13633
A	12	HIS	-	expression tag	UNP P13633
A	13	HIS	-	expression tag	UNP P13633
A	14	HIS	-	expression tag	UNP P13633
A	15	HIS	-	expression tag	UNP P13633
A	16	HIS	-	expression tag	UNP P13633
A	17	HIS	-	expression tag	UNP P13633
A	18	SER	-	expression tag	UNP P13633
A	19	SER	-	expression tag	UNP P13633
A	20	GLY	-	expression tag	UNP P13633
A	21	LEU	-	expression tag	UNP P13633
A	22	VAL	-	expression tag	UNP P13633
A	23	PRO	-	expression tag	UNP P13633
A	24	ARG	-	expression tag	UNP P13633
A	25	GLY	-	expression tag	UNP P13633
A	26	SER	-	expression tag	UNP P13633
A	27	HIS	-	expression tag	UNP P13633
A	28	MET	-	expression tag	UNP P13633

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Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ALA	-	expression tag	UNP P13633
A	30	SER	-	expression tag	UNP P13633
A	31	MET	-	expression tag	UNP P13633
A	32	THR	-	expression tag	UNP P13633
A	33	GLY	-	expression tag	UNP P13633
A	34	GLY	-	expression tag	UNP P13633
A	35	GLU	-	expression tag	UNP P13633
A	36	GLU	-	expression tag	UNP P13633
A	37	MET	-	expression tag	UNP P13633
A	38	GLY	-	expression tag	UNP P13633
A	39	ARG	-	expression tag	UNP P13633
A	40	GLY	-	expression tag	UNP P13633
A	41	SER	-	expression tag	UNP P13633
A	309	ASN	LYS	SEE REMARK 999	UNP P13633
B	8	MET	-	expression tag	UNP P13633
B	9	GLY	-	expression tag	UNP P13633
B	10	SER	-	expression tag	UNP P13633
B	11	SER	-	expression tag	UNP P13633
B	12	HIS	-	expression tag	UNP P13633
B	13	HIS	-	expression tag	UNP P13633
B	14	HIS	-	expression tag	UNP P13633
B	15	HIS	-	expression tag	UNP P13633
B	16	HIS	-	expression tag	UNP P13633
B	17	HIS	-	expression tag	UNP P13633
B	18	SER	-	expression tag	UNP P13633
B	19	SER	-	expression tag	UNP P13633
B	20	GLY	-	expression tag	UNP P13633
B	21	LEU	-	expression tag	UNP P13633
B	22	VAL	-	expression tag	UNP P13633
B	23	PRO	-	expression tag	UNP P13633
B	24	ARG	-	expression tag	UNP P13633
B	25	GLY	-	expression tag	UNP P13633
B	26	SER	-	expression tag	UNP P13633
B	27	HIS	-	expression tag	UNP P13633
B	28	MET	-	expression tag	UNP P13633
B	29	ALA	-	expression tag	UNP P13633
B	30	SER	-	expression tag	UNP P13633
B	31	MET	-	expression tag	UNP P13633
B	32	THR	-	expression tag	UNP P13633
B	33	GLY	-	expression tag	UNP P13633
B	34	GLY	-	expression tag	UNP P13633
B	35	GLU	-	expression tag	UNP P13633

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	GLU	-	expression tag	UNP P13633
B	37	MET	-	expression tag	UNP P13633
B	38	GLY	-	expression tag	UNP P13633
B	39	ARG	-	expression tag	UNP P13633
B	40	GLY	-	expression tag	UNP P13633
B	41	SER	-	expression tag	UNP P13633
B	309	ASN	LYS	SEE REMARK 999	UNP P13633
C	8	MET	-	expression tag	UNP P13633
C	9	GLY	-	expression tag	UNP P13633
C	10	SER	-	expression tag	UNP P13633
C	11	SER	-	expression tag	UNP P13633
C	12	HIS	-	expression tag	UNP P13633
C	13	HIS	-	expression tag	UNP P13633
C	14	HIS	-	expression tag	UNP P13633
C	15	HIS	-	expression tag	UNP P13633
C	16	HIS	-	expression tag	UNP P13633
C	17	HIS	-	expression tag	UNP P13633
C	18	SER	-	expression tag	UNP P13633
C	19	SER	-	expression tag	UNP P13633
C	20	GLY	-	expression tag	UNP P13633
C	21	LEU	-	expression tag	UNP P13633
C	22	VAL	-	expression tag	UNP P13633
C	23	PRO	-	expression tag	UNP P13633
C	24	ARG	-	expression tag	UNP P13633
C	25	GLY	-	expression tag	UNP P13633
C	26	SER	-	expression tag	UNP P13633
C	27	HIS	-	expression tag	UNP P13633
C	28	MET	-	expression tag	UNP P13633
C	29	ALA	-	expression tag	UNP P13633
C	30	SER	-	expression tag	UNP P13633
C	31	MET	-	expression tag	UNP P13633
C	32	THR	-	expression tag	UNP P13633
C	33	GLY	-	expression tag	UNP P13633
C	34	GLY	-	expression tag	UNP P13633
C	35	GLU	-	expression tag	UNP P13633
C	36	GLU	-	expression tag	UNP P13633
C	37	MET	-	expression tag	UNP P13633
C	38	GLY	-	expression tag	UNP P13633
C	39	ARG	-	expression tag	UNP P13633
C	40	GLY	-	expression tag	UNP P13633
C	41	SER	-	expression tag	UNP P13633
C	309	ASN	LYS	SEE REMARK 999	UNP P13633

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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	MET	-	expression tag	UNP P13633
D	9	GLY	-	expression tag	UNP P13633
D	10	SER	-	expression tag	UNP P13633
D	11	SER	-	expression tag	UNP P13633
D	12	HIS	-	expression tag	UNP P13633
D	13	HIS	-	expression tag	UNP P13633
D	14	HIS	-	expression tag	UNP P13633
D	15	HIS	-	expression tag	UNP P13633
D	16	HIS	-	expression tag	UNP P13633
D	17	HIS	-	expression tag	UNP P13633
D	18	SER	-	expression tag	UNP P13633
D	19	SER	-	expression tag	UNP P13633
D	20	GLY	-	expression tag	UNP P13633
D	21	LEU	-	expression tag	UNP P13633
D	22	VAL	-	expression tag	UNP P13633
D	23	PRO	-	expression tag	UNP P13633
D	24	ARG	-	expression tag	UNP P13633
D	25	GLY	-	expression tag	UNP P13633
D	26	SER	-	expression tag	UNP P13633
D	27	HIS	-	expression tag	UNP P13633
D	28	MET	-	expression tag	UNP P13633
D	29	ALA	-	expression tag	UNP P13633
D	30	SER	-	expression tag	UNP P13633
D	31	MET	-	expression tag	UNP P13633
D	32	THR	-	expression tag	UNP P13633
D	33	GLY	-	expression tag	UNP P13633
D	34	GLY	-	expression tag	UNP P13633
D	35	GLU	-	expression tag	UNP P13633
D	36	GLU	-	expression tag	UNP P13633
D	37	MET	-	expression tag	UNP P13633
D	38	GLY	-	expression tag	UNP P13633
D	39	ARG	-	expression tag	UNP P13633
D	40	GLY	-	expression tag	UNP P13633
D	41	SER	-	expression tag	UNP P13633
D	309	ASN	LYS	SEE REMARK 999	UNP P13633

- Molecule 2 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).
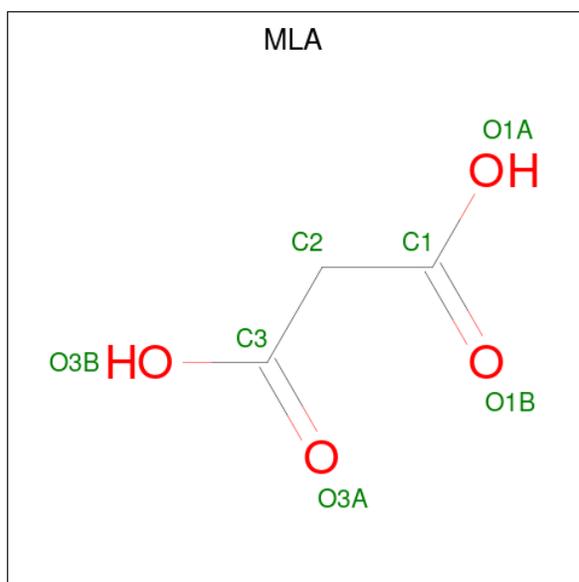
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 7	C 3	O 4	0	0
2	B	1	Total 7	C 3	O 4	0	0
2	C	1	Total 7	C 3	O 4	0	0
2	D	1	Total 7	C 3	O 4	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	6	Total 6	O 6	0	0
3	C	1	Total 1	O 1	0	0
3	D	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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.

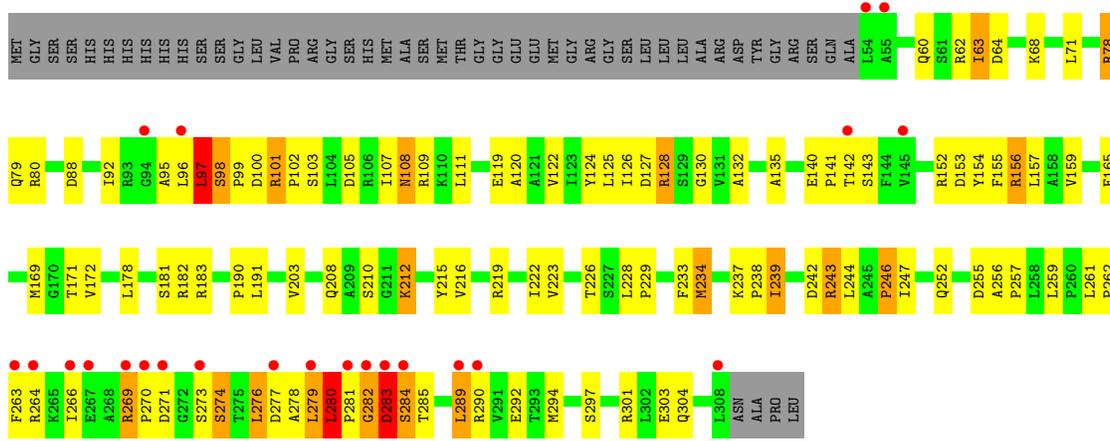- Molecule 1: C4-dicarboxylate transport sensor protein dctB
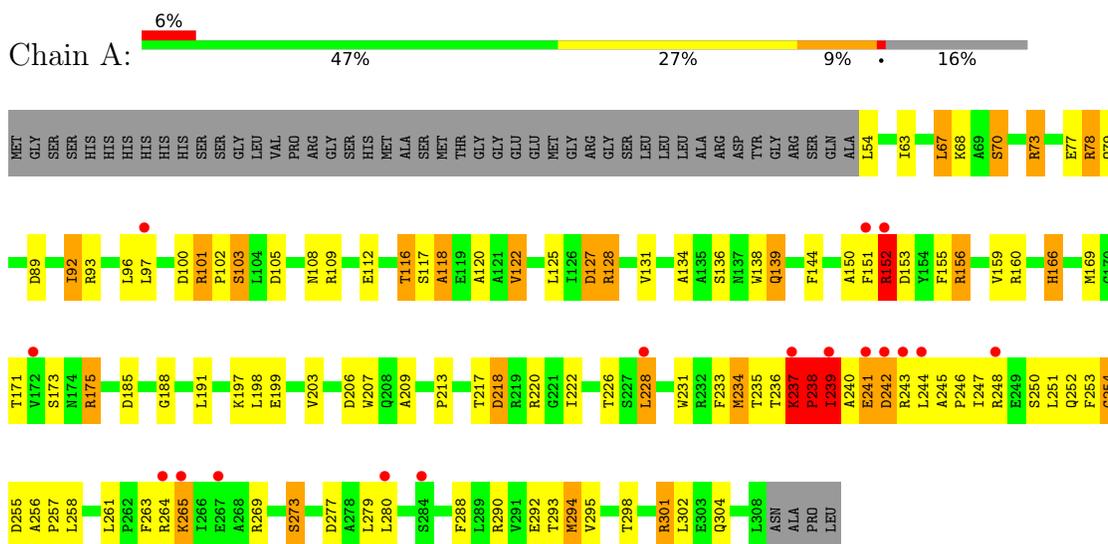
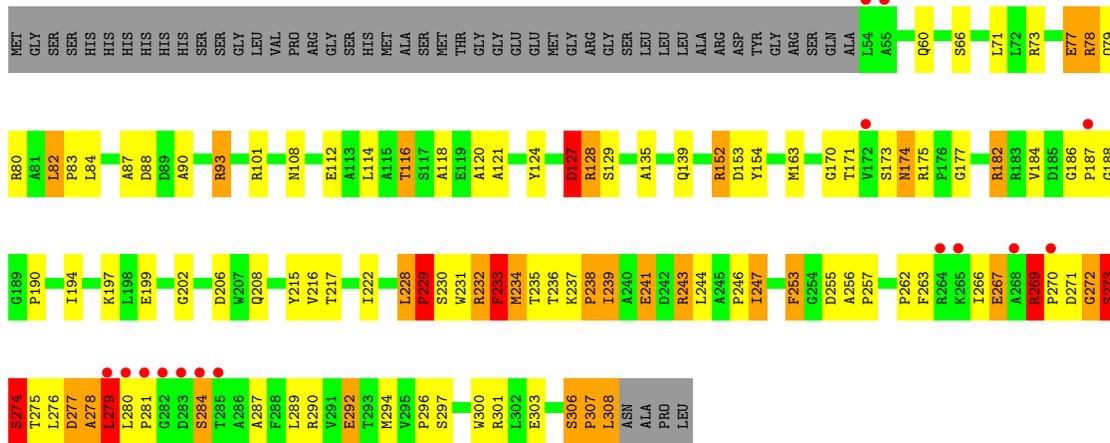- Molecule 1: C4-dicarboxylate transport sensor protein dctB
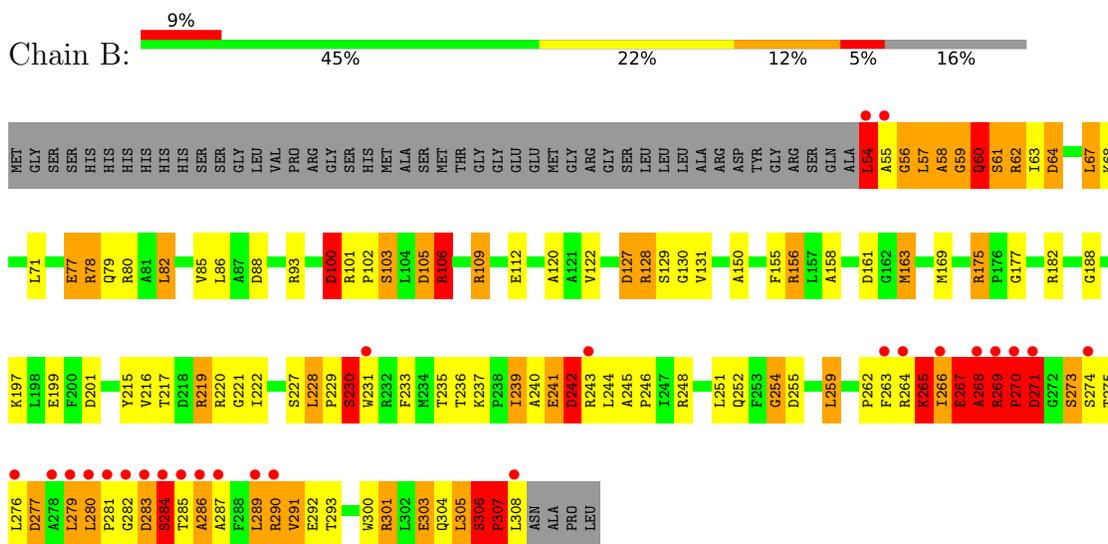
- Molecule 1: C4-dicarboxylate transport sensor protein dctB

• Molecule 1: C4-dicarboxylate transport sensor protein dctB

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	70.36Å 70.36Å 226.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 19.68 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.50) 99.3 (19.68-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.14 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.272 0.227 , 0.253	Depositor DCC
R_{free} test set	1880 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.7	EDS
L-test for twinning[2]	$<|L|>$ = 0.45, $<L^2>$ = 0.27	Xtriage
Estimated twinning fraction	0.093 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7852	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MLA

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	0.89	3/1992 (0.2%)	1.02	12/2710 (0.4%)
1	B	1.52	30/1992 (1.5%)	1.24	18/2710 (0.7%)
1	C	1.40	22/1992 (1.1%)	1.15	9/2710 (0.3%)
1	D	0.94	4/1992 (0.2%)	1.10	12/2710 (0.4%)
All	All	1.22	59/7968 (0.7%)	1.13	51/10840 (0.5%)

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	4	3
1	B	2	14
1	C	2	3
1	D	2	9
All	All	10	29

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	98	SER	CA-CB	17.51	1.79	1.52
1	B	289	LEU	C-O	16.45	1.54	1.23
1	B	306	SER	CA-CB	14.77	1.75	1.52
1	C	101	ARG	CZ-NH1	14.51	1.51	1.33
1	B	54	LEU	CB-CG	14.42	1.94	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	101	ARG	NE-CZ-NH2	-25.32	107.64	120.30
1	C	101	ARG	NH1-CZ-NH2	13.00	133.70	119.40
1	B	101	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	C	100	ASP	CB-CG-OD1	-12.18	107.34	118.30
1	B	54	LEU	CB-CG-CD2	-11.77	90.98	111.00

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	152	ARG	CA
1	A	237	LYS	CA
1	A	246	PRO	CA
1	A	264	ARG	CA
1	B	265	LYS	CA

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide
1	A	197	LYS	Peptide
1	A	237	LYS	Peptide
1	B	188	GLY	Peptide
1	B	56	GLY	Peptide,Mainchain

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	1952	0	1978	111	0
1	B	1952	0	1979	174	1
1	C	1952	0	1979	97	0
1	D	1952	0	1978	84	1
2	A	7	0	2	0	0
2	B	7	0	2	0	0
2	C	7	0	2	1	0
2	D	7	0	2	1	0
3	A	5	0	0	1	0
3	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	4	0	0	2	0
All	All	7852	0	7922	456	1

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 29.

The worst 5 of 456 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:SER:CA	1:B:306:SER:CB	1.75	1.61
1:C:97:LEU:CG	1:C:97:LEU:CD1	1.75	1.61
1:C:98:SER:CA	1:C:98:SER:CB	1.79	1.60
1:B:54:LEU:CB	1:B:54:LEU:CA	1.82	1.54
1:B:230:SER:HB3	1:B:231:TRP:CD1	1.45	1.50

All (1) 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)
1:B:161:ASP:OD1	1:D:241:GLU:OE2[3_554]	1.76	0.44

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	253/305 (83%)	225 (89%)	17 (7%)	11 (4%)	2	3
1	B	253/305 (83%)	216 (85%)	20 (8%)	17 (7%)	1	1
1	C	253/305 (83%)	226 (89%)	23 (9%)	4 (2%)	9	17
1	D	253/305 (83%)	216 (85%)	21 (8%)	16 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1012/1220 (83%)	883 (87%)	81 (8%)	48 (5%)	2 2

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	237	LYS
1	A	238	PRO
1	A	239	ILE
1	A	255	ASP

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	204/242 (84%)	177 (87%)	27 (13%)	4 7
1	B	204/242 (84%)	166 (81%)	38 (19%)	1 2
1	C	204/242 (84%)	173 (85%)	31 (15%)	3 5
1	D	204/242 (84%)	170 (83%)	34 (17%)	2 4
All	All	816/968 (84%)	686 (84%)	130 (16%)	2 4

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	228	LEU
1	D	253	PHE
1	B	175	ARG
1	B	163	MET
1	D	267	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	60	GLN
1	D	174	ASN
1	D	304	GLN
1	D	252	GLN
1	B	139	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	MLA	B	2	-	6,6,6	1.91	1 (16%)	7,7,7	1.36	1 (14%)
2	MLA	D	4	-	6,6,6	1.30	0	7,7,7	0.96	0
2	MLA	A	1	-	6,6,6	1.21	0	7,7,7	1.52	2 (28%)
2	MLA	C	3	-	6,6,6	1.15	0	7,7,7	1.28	0

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	MLA	B	2	-	-	0/4/4/4	-
2	MLA	D	4	-	-	2/4/4/4	-
2	MLA	A	1	-	-	4/4/4/4	-
2	MLA	C	3	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	MLA	C2-C3	3.76	1.56	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	MLA	O3A-C3-C2	-2.40	115.06	122.08
2	B	2	MLA	O1B-C1-C2	-2.05	116.10	122.08
2	A	1	MLA	O1B-C1-C2	-2.03	116.16	122.08

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	MLA	O1B-C1-C2-C3
2	D	4	MLA	O1A-C1-C2-C3
2	A	1	MLA	O1A-C1-C2-C3
2	A	1	MLA	C1-C2-C3-O3B
2	D	4	MLA	O1B-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	MLA	1	0
2	C	3	MLA	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	255/305 (83%)	0.22	17 (6%)	17	18	21, 46, 55, 63	21 (8%)
1	B	255/305 (83%)	0.47	26 (10%)	6	6	21, 46, 56, 64	4 (1%)
1	C	255/305 (83%)	0.40	23 (9%)	9	9	21, 47, 55, 60	12 (4%)
1	D	255/305 (83%)	0.30	15 (5%)	22	23	21, 47, 56, 62	14 (5%)
All	All	1020/1220 (83%)	0.35	81 (7%)	12	12	21, 46, 56, 64	51 (5%)

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	ASP	9.7
1	B	280	LEU	9.0
1	D	284	SER	7.0
1	B	289	LEU	5.8
1	C	282	GLY	5.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no 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, 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	MLA	A	1	7/7	0.93	0.12	46,48,49,54	0
2	MLA	B	2	7/7	0.94	0.10	39,41,44,46	0
2	MLA	D	4	7/7	0.94	0.11	43,47,51,52	0
2	MLA	C	3	7/7	0.96	0.15	38,44,47,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.