



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:30 pm GMT

PDB ID : 3E4P  
Title : Crystal structure of malonate occupied DctB  
Authors : Zhou, Y.F.; Nan, J.; Nan, B.Y.; Liang, Y.H.; Panjikar, S.; Su, X.D.  
Deposited on : 2008-08-12  
Resolution : 2.30 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

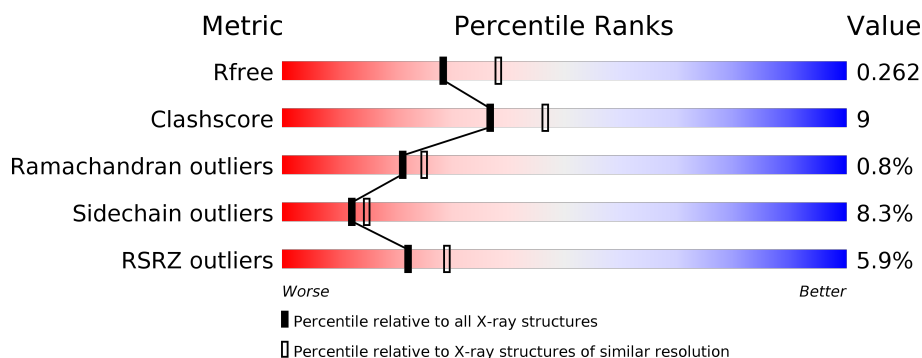
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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  $\geq 3$ , 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	305	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	305	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>13%</div> <div>5%</div> <div>•</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3984 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	254	Total	C	N	O	S	3	0	0
			1945	1232	349	360	4			
1	B	253	Total	C	N	O	S	0	0	0
			1909	1207	344	354	4			

There are 72 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
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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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	174	LYS	ASN	SEE REMARK 999	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
B	36	GLU	-	EXPRESSION TAG	UNP P13633
B	37	MET	-	EXPRESSION TAG	UNP P13633
B	38	GLY	-	EXPRESSION TAG	UNP P13633

*Continued on next page...*

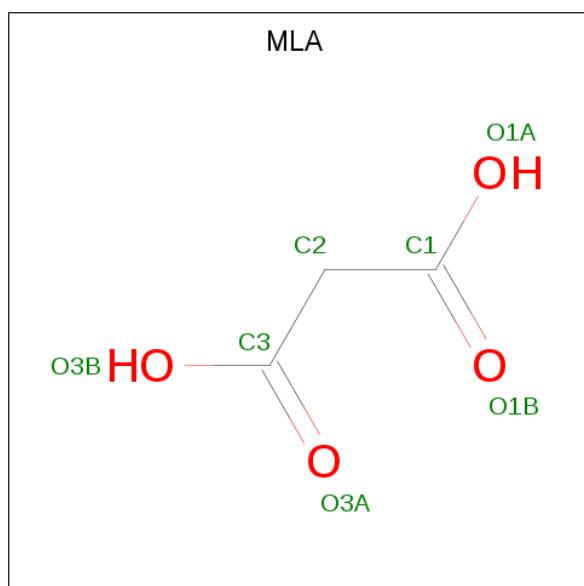
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	ARG	-	EXPRESSION TAG	UNP P13633
B	40	GLY	-	EXPRESSION TAG	UNP P13633
B	41	SER	-	EXPRESSION TAG	UNP P13633
B	174	LYS	ASN	SEE REMARK 999	UNP P13633
B	309	ASN	LYS	SEE REMARK 999	UNP P13633

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Sr 2 2	0	0
2	A	1	Total Sr 1 1	0	0

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 3 4	0	0
3	B	1	Total C O 7 3 4	0	0

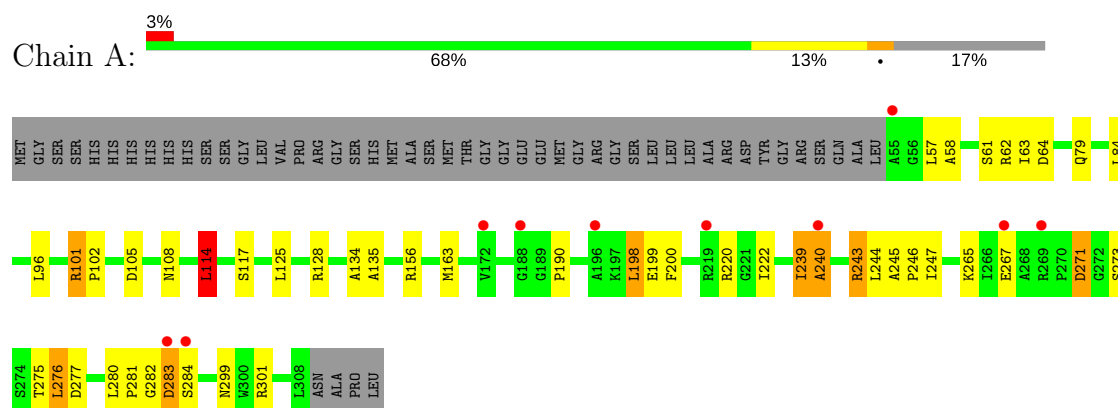
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	58	Total 58	O 58	0	0

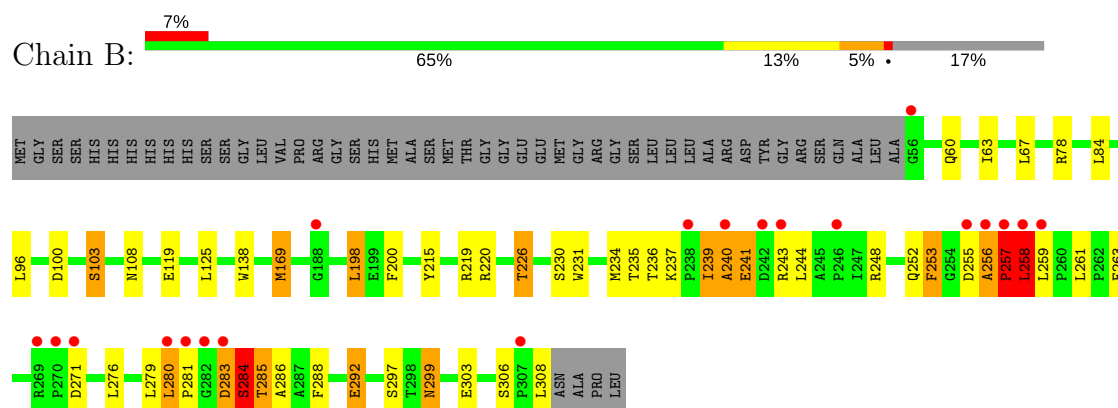
### 3 Residue-property plots [i](#)

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: C4-dicarboxylate transport sensor protein dctB



- Molecule 1: C4-dicarboxylate transport sensor protein dctB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.98Å 39.10Å 111.54Å 90.00° 94.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 28.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.30) 97.6 (28.57-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.196 , 0.262 0.204 , 0.262	Depositor DCC
$R_{free}$ test set	1142 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SR, 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	0.67	0/1985	0.81	3/2699 (0.1%)
1	B	0.68	0/1949	0.82	3/2649 (0.1%)
All	All	0.68	0/3934	0.82	6/5348 (0.1%)

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	1	7
1	B	1	7
All	All	2	14

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	280	LEU	C-N-CD	14.07	157.96	128.40
1	A	276	LEU	CA-CB-CG	9.82	137.90	115.30
1	B	280	LEU	C-N-CA	-7.65	89.86	122.00
1	B	280	LEU	N-CA-C	7.36	130.88	111.00
1	A	283	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	114	LEU	CA-CB-CG	5.11	127.05	115.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	240	ALA	CA
1	B	256	ALA	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	ILE	Peptide
1	A	240	ALA	Peptide
1	A	271	ASP	Peptide
1	A	275	THR	Peptide
1	A	281	PRO	Peptide
1	A	282	GLY	Peptide
1	A	283	ASP	Peptide
1	B	256	ALA	Peptide
1	B	257	PRO	Peptide
1	B	258	LEU	Peptide
1	B	271	ASP	Peptide
1	B	279	LEU	Peptide
1	B	283	ASP	Peptide
1	B	284	SER	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	1945	0	1975	29	0
1	B	1909	0	1913	38	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	7	0	2	0	0
3	B	7	0	2	0	0
4	A	55	0	0	2	0
4	B	58	0	0	1	0
All	All	3984	0	3892	66	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 9.

All (66) 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:239:ILE:HG22	1:A:240:ALA:CB	1.69	1.23

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:CG2	1:A:240:ALA:HB3	1.68	1.22
1:B:256:ALA:CB	1:B:257:PRO:HD2	1.82	1.09
1:B:261:LEU:O	4:B:645:HOH:O	1.72	1.06
1:A:101:ARG:NH1	1:A:105:ASP:OD1	2.01	0.94
1:B:256:ALA:HB1	1:B:257:PRO:HD2	1.47	0.93
1:B:256:ALA:CB	1:B:257:PRO:CD	2.46	0.92
1:B:256:ALA:HB2	1:B:257:PRO:HD2	1.54	0.87
1:A:265:LYS:HD2	1:A:277:ASP:OD2	1.78	0.83
1:B:256:ALA:HB2	1:B:257:PRO:CD	2.09	0.78
1:B:215:TYR:HB3	1:B:226:THR:HG23	1.64	0.78
1:A:128:ARG:HD2	1:A:190:PRO:O	1.86	0.75
1:A:101:ARG:O	1:A:101:ARG:HD3	1.87	0.75
1:A:245:ALA:HB3	1:A:246:PRO:HD3	1.69	0.73
1:A:79:GLN:HG3	1:A:198:LEU:HG	1.70	0.73
1:A:243:ARG:O	1:A:247:ILE:HD12	1.90	0.71
1:B:239:ILE:HG13	1:B:240:ALA:N	2.05	0.71
1:A:267:GLU:OE1	4:A:720:HOH:O	2.11	0.68
1:B:169:MET:O	1:B:252:GLN:NE2	2.27	0.67
1:B:299:ASN:HD22	1:B:299:ASN:C	1.98	0.66
1:A:79:GLN:CG	1:A:198:LEU:HG	2.25	0.66
1:B:286:ALA:HB3	1:B:288:PHE:CE2	2.33	0.64
1:A:58:ALA:O	1:A:62:ARG:HG3	1.99	0.61
1:B:258:LEU:H	1:B:258:LEU:HD23	1.67	0.60
1:B:239:ILE:O	1:B:240:ALA:HB2	2.02	0.59
1:B:244:LEU:O	1:B:248:ARG:HG3	2.03	0.58
1:B:256:ALA:O	1:B:257:PRO:O	2.21	0.58
1:B:239:ILE:HG23	1:B:240:ALA:H	1.69	0.57
1:B:292:GLU:HG3	1:B:303:GLU:HG2	1.86	0.56
1:B:256:ALA:O	1:B:257:PRO:C	2.46	0.55
1:A:108:ASN:ND2	1:A:135:ALA:H	2.07	0.53
1:B:256:ALA:HB1	1:B:257:PRO:CD	2.22	0.53
1:B:258:LEU:N	1:B:258:LEU:HD23	2.25	0.52
1:A:240:ALA:HB1	1:A:244:LEU:HG	1.93	0.51
1:B:100:ASP:OD1	1:B:103:SER:HB3	2.12	0.50
1:A:271:ASP:HB3	1:A:273:SER:H	1.77	0.50
1:A:198:LEU:HD13	1:A:200:PHE:CZ	2.48	0.49
1:A:96:LEU:HD11	1:A:125:LEU:HD11	1.95	0.49
1:A:239:ILE:HG22	1:A:240:ALA:HB3	0.75	0.48
1:A:61:SER:HB3	4:A:732:HOH:O	2.13	0.48
1:B:253:PHE:CD1	1:B:253:PHE:C	2.87	0.48
1:B:280:LEU:O	1:B:281:PRO:C	2.43	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HB3	1:B:138:TRP:CD1	2.50	0.47
1:B:96:LEU:HD11	1:B:125:LEU:HD11	1.97	0.46
1:B:241:GLU:HA	1:B:244:LEU:HD12	1.98	0.45
1:A:198:LEU:HD13	1:A:200:PHE:CE1	2.50	0.45
1:A:63:ILE:HG13	1:A:64:ASP:N	2.32	0.45
1:B:241:GLU:C	1:B:243:ARG:H	2.20	0.44
1:A:198:LEU:HD22	1:A:199:GLU:O	2.17	0.44
1:B:253:PHE:C	1:B:253:PHE:HD1	2.22	0.44
1:A:114:LEU:HD12	1:B:84:LEU:HG	2.00	0.43
1:B:219:ARG:O	1:B:237:LYS:NZ	2.50	0.43
1:B:78:ARG:NH2	1:B:119:GLU:OE2	2.42	0.43
1:A:220:ARG:HB2	1:A:222:ILE:HD12	2.01	0.43
1:A:271:ASP:CB	1:A:273:SER:H	2.31	0.43
1:B:231:TRP:CE3	1:B:261:LEU:HD22	2.54	0.43
1:B:263:PHE:CD2	1:B:276:LEU:HD11	2.53	0.43
1:B:60:GLN:HA	1:B:63:ILE:HD12	2.01	0.42
1:A:108:ASN:HD21	1:A:134:ALA:HA	1.85	0.41
1:A:101:ARG:HD3	1:A:101:ARG:C	2.37	0.41
1:B:284:SER:HB3	1:B:285:THR:H	1.57	0.41
1:B:198:LEU:HD13	1:B:200:PHE:CZ	2.56	0.41
1:B:234:MET:SD	1:B:259:LEU:HB2	2.61	0.41
1:B:236:THR:HG22	1:B:261:LEU:HD12	2.04	0.40
1:A:101:ARG:N	1:A:102:PRO:CD	2.84	0.40
1:A:79:GLN:HG2	1:A:198:LEU:HG	2.02	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	252/305 (83%)	241 (96%)	11 (4%)	0	<a href="#">100</a> <a href="#">100</a>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	251/305 (82%)	235 (94%)	12 (5%)	4 (2%)	11	10
All	All	503/610 (82%)	476 (95%)	23 (5%)	4 (1%)	21	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	PRO
1	B	283	ASP
1	B	240	ALA
1	B	239	ILE

### 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	203/242 (84%)	189 (93%)	14 (7%)	17	22
1	B	196/242 (81%)	177 (90%)	19 (10%)	9	10
All	All	399/484 (82%)	366 (92%)	33 (8%)	12	15

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	84	LEU
1	A	101	ARG
1	A	114	LEU
1	A	117	SER
1	A	156	ARG
1	A	163	MET
1	A	198	LEU
1	A	243	ARG
1	A	276	LEU
1	A	280	LEU
1	A	284	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	299	ASN
1	A	301	ARG
1	B	67	LEU
1	B	103	SER
1	B	169	MET
1	B	198	LEU
1	B	220	ARG
1	B	226	THR
1	B	230	SER
1	B	235	THR
1	B	241	GLU
1	B	253	PHE
1	B	255	ASP
1	B	258	LEU
1	B	284	SER
1	B	285	THR
1	B	292	GLU
1	B	297	SER
1	B	299	ASN
1	B	306	SER
1	B	308	LEU

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

Mol	Chain	Res	Type
1	A	79	GLN
1	A	108	ASN
1	A	299	ASN
1	B	299	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	MLA	A	701	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLA	B	601	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLA	A	701	-	-	0/0/4/4	0/0/0/0
3	MLA	B	601	-	-	0/0/4/4	0/0/0/0

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	254/305 (83%)	0.13	10 (3%) 39 46	21, 31, 46, 53	2 (0%)
1	B	253/305 (82%)	0.09	20 (7%) 12 17	22, 31, 50, 57	0
All	All	507/610 (83%)	0.11	30 (5%) 22 29	21, 31, 48, 57	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	6.3
1	B	281	PRO	4.8
1	B	258	LEU	4.7
1	B	270	PRO	4.6
1	A	240	ALA	4.4
1	A	188	GLY	4.1
1	B	188	GLY	3.5
1	B	255	ASP	3.5
1	B	240	ALA	3.4
1	B	56	GLY	3.3
1	A	269	ARG	3.3
1	B	269	ARG	3.2
1	B	271	ASP	3.2
1	B	280	LEU	3.0
1	B	257	PRO	3.0
1	B	242	ASP	2.8
1	A	55	ALA	2.7
1	B	282	GLY	2.7
1	A	172	VAL	2.6
1	B	238	PRO	2.6
1	B	246	PRO	2.4
1	A	219	ARG	2.4
1	A	196	ALA	2.3
1	B	307	PRO	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	243	ARG	2.2
1	A	284	SER	2.2
1	B	256	ALA	2.2
1	B	259	LEU	2.1
1	B	283	ASP	2.1
1	A	267	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	MLA	A	701	7/7	0.94	0.09	25,26,30,30	0
2	SR	A	502	1/1	0.97	0.11	43,43,43,43	1
2	SR	B	503	1/1	0.98	0.11	38,38,38,38	1
3	MLA	B	601	7/7	0.98	0.07	21,23,24,25	0
2	SR	B	501	1/1	0.99	0.02	54,54,54,54	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.