



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:23 pm BST

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)

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

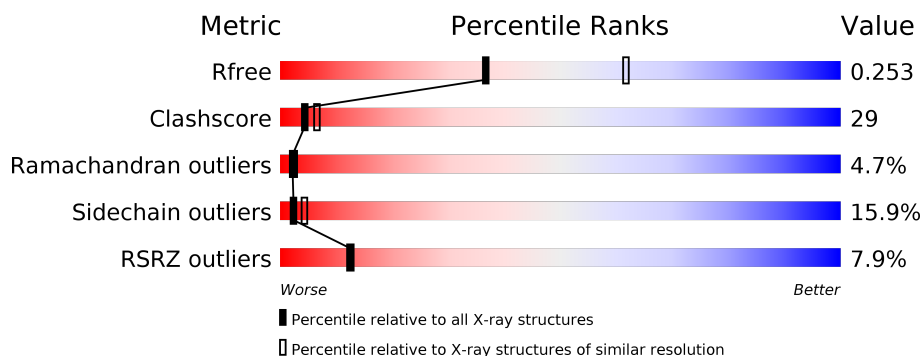
1 Overall quality at a glance

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	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 on 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	305	<div> <div>6%</div> <div> <div>47%</div> <div>27%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	305	<div> <div>9%</div> <div> <div>45%</div> <div>22%</div> <div>12%</div> <div>5%</div> <div>16%</div> </div> </div>
1	C	305	<div> <div>8%</div> <div> <div>47%</div> <div>30%</div> <div>6%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	305	<div> <div>5%</div> <div> <div>49%</div> <div>24%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>

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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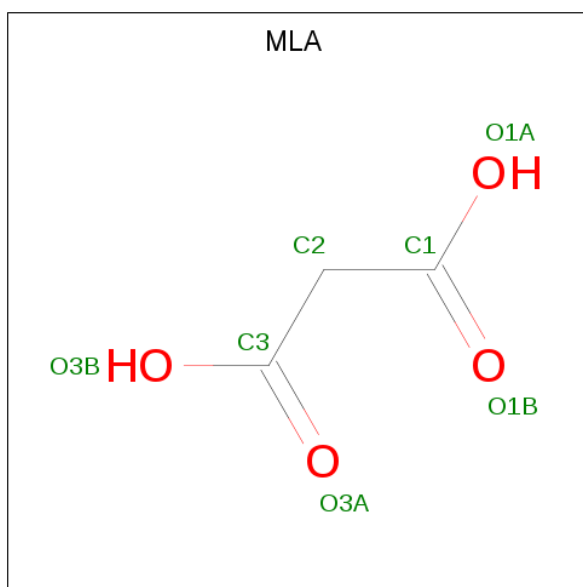
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	GLU	-	EXPRESSION TAG	UNP P13633
B	37	MET	-	EXPRESSION TAG	UNP P13633
B	38	GLY	-	EXPRESSION TAG	UNP P13633
B	39	ARG	-	EXPRESSION TAG	UNP P13633
B	40	GLY	-	EXPRESSION TAG	UNP P13633
B	41	SER	-	EXPRESSION TAG	UNP P13633
B	309	ASN	LYS	SEE REMARK 999	UNP 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: C₃H₄O₄).



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

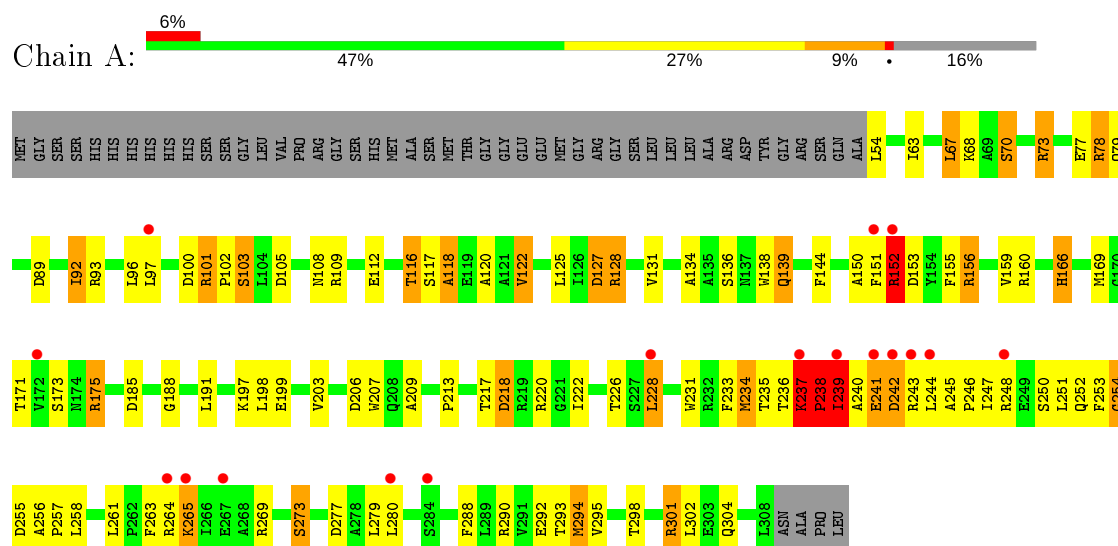
- Molecule 3 is water.

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

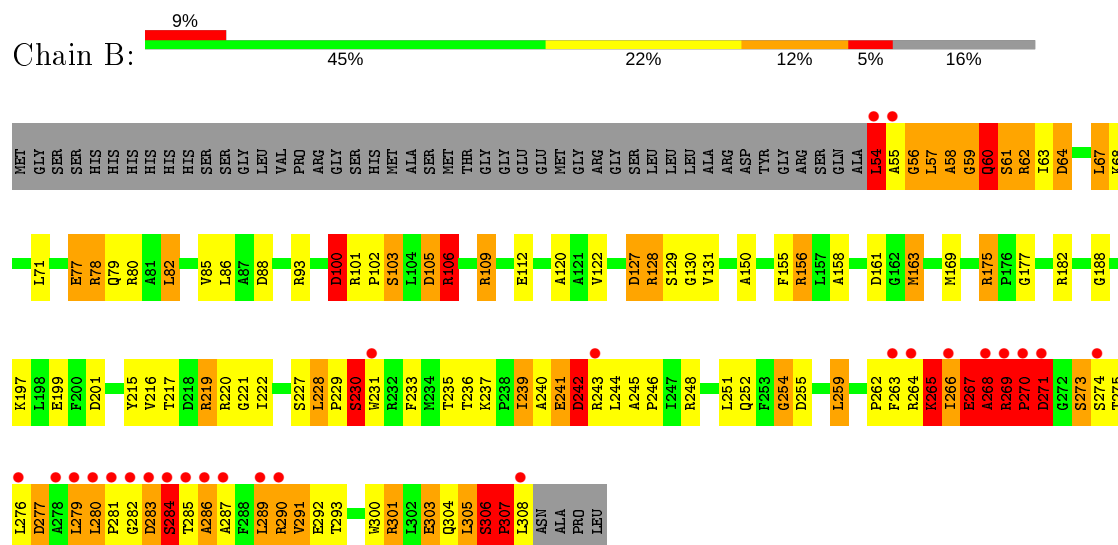
3 Residue-property plots [i](#)

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

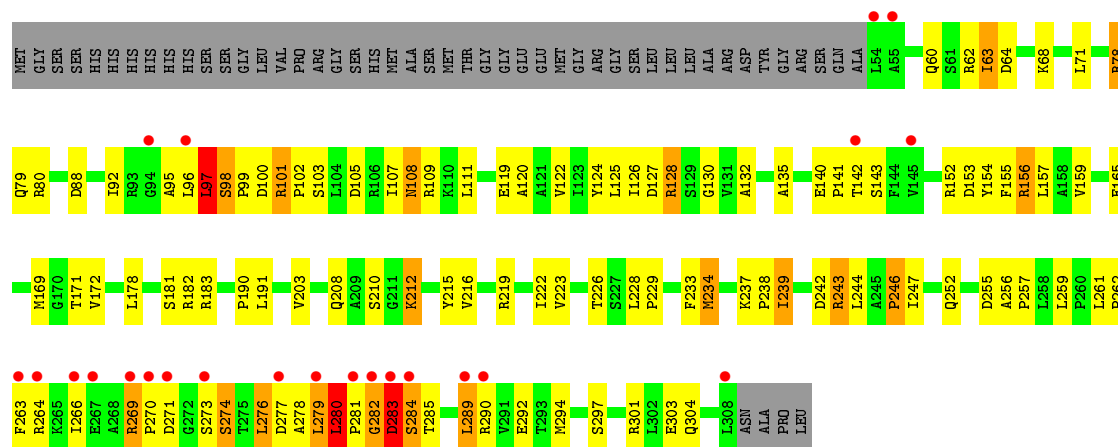


- Molecule 1: C4-dicarboxylate transport sensor protein dctB

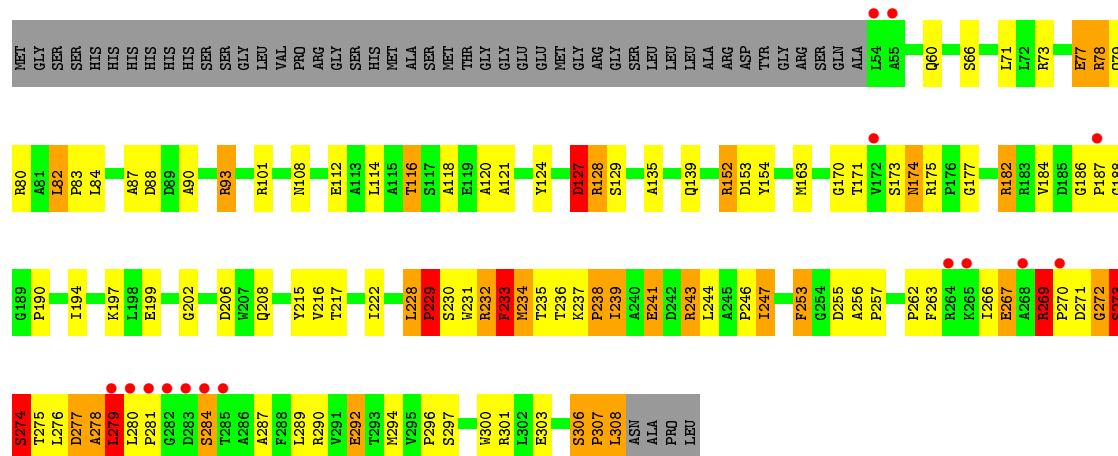


- Molecule 1: C4-dicarboxylate transport sensor protein dctB





• Molecule 1: C4-dicarboxylate transport sensor protein dctB



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	70.36 Å 70.36 Å 226.92 Å 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
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.50 Å)	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	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

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:
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

All (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
1	C	99	PRO	N-CD	13.36	1.66	1.47
1	C	101	ARG	NE-CZ	12.67	1.49	1.33
1	B	54	LEU	CA-CB	12.43	1.82	1.53
1	B	259	LEU	CB-CG	12.24	1.88	1.52
1	B	109	ARG	CZ-NH1	12.09	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	PRO	N-CD	11.64	1.64	1.47
1	B	54	LEU	C-N	11.01	1.59	1.34
1	C	143	SER	CA-CB	10.86	1.69	1.52
1	B	54	LEU	CG-CD1	10.45	1.90	1.51
1	B	277	ASP	C-N	10.46	1.58	1.34
1	B	103	SER	CB-OG	10.32	1.55	1.42
1	C	101	ARG	CZ-NH2	10.05	1.46	1.33
1	B	305	LEU	C-O	10.02	1.42	1.23
1	C	98	SER	CB-OG	10.00	1.55	1.42
1	C	100	ASP	CG-OD2	9.89	1.48	1.25
1	B	307	PRO	N-CD	9.77	1.61	1.47
1	B	305	LEU	C-N	9.52	1.55	1.34
1	A	160	ARG	CZ-NH1	9.28	1.45	1.33
1	D	272	GLY	CA-C	8.94	1.66	1.51
1	C	95	ALA	C-O	8.91	1.40	1.23
1	B	59	GLY	C-N	8.86	1.54	1.34
1	D	279	LEU	C-O	8.25	1.39	1.23
1	B	303	GLU	CD-OE1	8.07	1.34	1.25
1	B	60	GLN	CD-NE2	7.89	1.52	1.32
1	C	98	SER	C-N	7.42	1.48	1.34
1	A	239	ILE	C-O	7.39	1.37	1.23
1	C	97	LEU	C-O	7.26	1.37	1.23
1	C	143	SER	CB-OG	7.18	1.51	1.42
1	B	59	GLY	C-O	7.15	1.35	1.23
1	C	100	ASP	CB-CG	7.06	1.66	1.51
1	C	100	ASP	CA-CB	6.83	1.69	1.53
1	B	306	SER	CB-OG	6.81	1.51	1.42
1	D	139	GLN	CG-CD	6.71	1.66	1.51
1	B	306	SER	CA-C	6.50	1.69	1.52
1	B	60	GLN	C-O	-6.48	1.11	1.23
1	C	97	LEU	CG-CD1	6.45	1.75	1.51
1	C	140	GLU	N-CA	6.13	1.58	1.46
1	C	98	SER	C-O	6.10	1.34	1.23
1	C	101	ARG	CD-NE	6.01	1.56	1.46
1	B	109	ARG	NE-CZ	5.97	1.40	1.33
1	B	303	GLU	CD-OE2	5.87	1.32	1.25
1	B	61	SER	C-O	5.67	1.34	1.23
1	D	127	ASP	CB-CG	-5.58	1.40	1.51
1	C	100	ASP	N-CA	5.47	1.57	1.46
1	B	100	ASP	CG-OD2	5.45	1.37	1.25
1	B	64	ASP	CB-CG	5.45	1.63	1.51
1	B	277	ASP	C-O	5.39	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	ALA	CA-C	5.31	1.66	1.52
1	B	307	PRO	CG-CD	5.22	1.67	1.50
1	B	61	SER	CB-OG	5.18	1.49	1.42
1	C	97	LEU	CG-CD2	5.14	1.70	1.51
1	B	58	ALA	C-N	5.09	1.42	1.33
1	A	239	ILE	C-N	-5.06	1.22	1.34
1	C	212	LYS	CE-NZ	5.05	1.61	1.49

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	D	232	ARG	N-CA-C	-11.66	79.51	111.00
1	B	101	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	B	54	LEU	CA-CB-CG	-10.48	91.19	115.30
1	B	109	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	D	247	ILE	N-CA-C	-8.74	87.41	111.00
1	B	228	LEU	N-CA-C	8.38	133.63	111.00
1	A	160	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	D	127	ASP	CB-CG-OD1	-7.69	111.38	118.30
1	C	101	ARG	NE-CZ-NH1	-7.43	116.58	120.30
1	A	198	LEU	N-CA-C	-7.26	91.39	111.00
1	B	307	PRO	N-CD-CG	-7.05	92.63	103.20
1	A	118	ALA	N-CA-C	-6.86	92.47	111.00
1	B	100	ASP	CB-CG-OD1	6.86	124.47	118.30
1	B	163	MET	CG-SD-CE	-6.65	89.55	100.20
1	A	67	LEU	CA-CB-CG	6.54	130.34	115.30
1	B	259	LEU	CD1-CG-CD2	6.51	130.05	110.50
1	D	278	ALA	C-N-CA	6.51	137.98	121.70
1	C	101	ARG	CD-NE-CZ	-6.49	114.51	123.60
1	A	218	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	73	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	218	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	233	PHE	N-CA-C	-6.29	94.03	111.00
1	D	233	PHE	CB-CA-C	-6.14	98.11	110.40
1	B	259	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	A	238	PRO	C-N-CA	6.03	136.77	121.70
1	B	254	GLY	N-CA-C	6.02	128.14	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	GLY	N-CA-C	-5.91	98.33	113.10
1	B	289	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	73	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	289	LEU	CD1-CG-CD2	5.65	127.45	110.50
1	D	153	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	106	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	82	LEU	CB-CG-CD1	5.33	120.05	111.00
1	D	182	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	273	SER	N-CA-C	5.32	125.37	111.00
1	B	277	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	271	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	229	PRO	N-CA-C	5.19	125.59	112.10
1	D	277	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	277	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	141	PRO	N-CD-CG	-5.11	95.53	103.20
1	C	280	LEU	CA-CB-CG	5.08	126.98	115.30
1	D	234	MET	N-CA-C	5.04	124.61	111.00
1	B	67	LEU	CA-CB-CG	-5.02	103.76	115.30
1	A	118	ALA	C-N-CA	-5.01	109.18	121.70
1	C	109	ARG	NE-CZ-NH2	-5.00	117.80	120.30

All (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
1	B	269	ARG	CA
1	C	283	ASP	CA
1	C	284	SER	CA
1	D	238	PRO	CA
1	D	241	GLU	CA

All (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

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Mol	Chain	Res	Type	Group
1	B	227	SER	Peptide
1	B	230	SER	Peptide
1	B	237	LYS	Peptide
1	B	241	GLU	Peptide
1	B	242	ASP	Peptide
1	B	265	LYS	Peptide
1	B	267	GLU	Peptide
1	B	268	ALA	Peptide
1	B	269	ARG	Peptide
1	B	270	PRO	Peptide
1	B	271	ASP	Peptide
1	B	56	GLY	Mainchain,Peptide
1	C	281	PRO	Peptide
1	C	282	GLY	Peptide
1	C	284	SER	Peptide
1	D	229	PRO	Peptide
1	D	231	TRP	Peptide
1	D	232	ARG	Peptide
1	D	233	PHE	Peptide
1	D	246	PRO	Peptide
1	D	269	ARG	Peptide
1	D	273	SER	Peptide
1	D	278	ALA	Peptide
1	D	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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	0	0
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.

All (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
1:B:259:LEU:CB	1:B:259:LEU:CG	1.88	1.48
1:B:54:LEU:CG	1:B:54:LEU:CD1	1.90	1.48
1:B:54:LEU:CB	1:B:54:LEU:CG	1.94	1.46
1:B:230:SER:CB	1:B:231:TRP:HD1	1.35	1.35
1:D:235:THR:HG21	1:D:239:ILE:CD1	1.59	1.33
1:C:283:ASP:HA	1:C:284:SER:CB	1.52	1.33
1:C:283:ASP:CA	1:C:284:SER:HB2	1.63	1.29
1:D:235:THR:CG2	1:D:239:ILE:HD11	1.67	1.24
1:A:152:ARG:O	1:A:156:ARG:HD3	1.33	1.22
1:D:267:GLU:O	1:D:275:THR:HG22	1.34	1.21
1:A:238:PRO:O	1:A:239:ILE:HG23	1.41	1.21
1:B:266:ILE:CD1	1:B:267:GLU:H	1.52	1.20
1:B:228:LEU:HD22	1:B:280:LEU:CD2	1.73	1.19
1:C:279:LEU:HD12	1:C:279:LEU:N	1.57	1.17
1:B:268:ALA:CA	1:B:269:ARG:HG3	1.75	1.16
1:D:262:PRO:CB	1:D:279:LEU:HD12	1.75	1.16
1:A:264:ARG:CG	1:A:265:LYS:H	1.55	1.14
1:B:276:LEU:HD12	1:B:290:ARG:HB2	1.19	1.14
1:A:301:ARG:HH11	1:A:301:ARG:CB	1.62	1.13
1:B:276:LEU:CD1	1:B:290:ARG:HB2	1.80	1.11
1:B:228:LEU:HD22	1:B:280:LEU:HD22	1.17	1.09
1:A:100:ASP:OD2	1:A:103:SER:HB2	1.51	1.08
1:A:264:ARG:HG3	1:A:265:LYS:N	1.63	1.07
1:B:219:ARG:HH11	1:B:219:ARG:HG3	0.97	1.07
1:B:266:ILE:HD12	1:B:267:GLU:H	0.98	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ILE:HD12	1:B:267:GLU:N	1.70	1.07
1:B:262:PRO:HB3	1:B:279:LEU:HD12	1.37	1.06
1:D:243:ARG:HH11	1:D:243:ARG:HG2	0.91	1.06
1:C:269:ARG:HB2	1:C:273:SER:OG	1.54	1.06
1:B:268:ALA:CB	1:B:269:ARG:HG3	1.87	1.04
1:B:262:PRO:CB	1:B:279:LEU:HD12	1.88	1.03
1:B:231:TRP:CZ3	1:B:263:PHE:HE2	1.76	1.02
1:B:268:ALA:HA	1:B:269:ARG:HG3	1.33	1.02
1:D:262:PRO:HB2	1:D:279:LEU:CD1	1.89	1.01
1:C:279:LEU:H	1:C:279:LEU:HD12	1.12	1.00
1:D:243:ARG:CG	1:D:243:ARG:HH11	1.72	0.99
1:A:68:LYS:HE2	1:A:304:GLN:HE21	1.23	0.98
1:B:265:LYS:C	1:B:266:ILE:HG23	1.84	0.98
1:C:264:ARG:HD2	1:C:277:ASP:HB2	1.44	0.98
1:B:219:ARG:HG3	1:B:219:ARG:NH1	1.76	0.97
1:B:282:GLY:O	1:B:283:ASP:CG	2.03	0.96
1:A:236:THR:O	1:A:237:LYS:HB2	1.65	0.96
1:A:228:LEU:HD13	1:A:231:TRP:CE3	2.00	0.96
1:B:102:PRO:O	1:B:106:ARG:HG3	1.65	0.96
1:B:228:LEU:CD2	1:B:280:LEU:HD22	1.93	0.96
1:A:152:ARG:O	1:A:156:ARG:CD	2.14	0.95
1:A:151:PHE:CZ	1:A:152:ARG:CZ	2.50	0.95
1:A:264:ARG:HG3	1:A:265:LYS:H	0.78	0.94
1:C:154:TYR:OH	2:C:3:MLA:O3B	1.85	0.94
1:B:231:TRP:HZ3	1:B:263:PHE:HE2	1.02	0.93
1:D:243:ARG:HG2	1:D:243:ARG:NH1	1.57	0.93
1:A:301:ARG:HH11	1:A:301:ARG:HB2	1.31	0.93
1:B:231:TRP:CZ3	1:B:263:PHE:CE2	2.59	0.91
1:B:230:SER:CB	1:B:231:TRP:CD1	2.24	0.91
1:B:266:ILE:CG1	1:B:267:GLU:H	1.78	0.90
1:B:282:GLY:O	1:B:283:ASP:OD1	1.91	0.88
1:B:265:LYS:H	1:B:266:ILE:CG2	1.86	0.88
1:D:292:GLU:HG3	1:D:303:GLU:HG2	1.56	0.88
1:A:188:GLY:HA2	1:D:175:ARG:NH1	1.89	0.86
1:A:263:PHE:O	1:A:264:ARG:HB2	1.75	0.86
1:A:301:ARG:HB3	1:A:301:ARG:NH1	1.91	0.86
1:B:269:ARG:HB2	1:B:270:PRO:O	1.75	0.86
1:C:279:LEU:CD1	1:C:279:LEU:N	2.33	0.86
1:B:156:ARG:HH11	1:B:156:ARG:HG3	1.37	0.85
1:B:268:ALA:HB1	1:B:269:ARG:HG3	1.58	0.85
1:B:54:LEU:CB	1:B:54:LEU:CD2	2.54	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:PRO:HB2	1:D:279:LEU:HD12	0.93	0.85
1:A:301:ARG:HH11	1:A:301:ARG:HB3	1.38	0.85
1:A:301:ARG:CB	1:A:301:ARG:NH1	2.39	0.85
1:A:228:LEU:HD13	1:A:231:TRP:CZ3	2.12	0.84
1:A:151:PHE:CZ	1:A:152:ARG:NH1	2.45	0.84
1:C:283:ASP:CA	1:C:284:SER:CB	2.30	0.83
1:D:154:TYR:OH	2:D:4:MLA:O1A	1.96	0.83
1:B:230:SER:HB3	1:B:231:TRP:HD1	0.67	0.83
1:B:265:LYS:H	1:B:266:ILE:HG23	1.44	0.83
1:B:262:PRO:HB3	1:B:279:LEU:CD1	2.08	0.82
1:C:269:ARG:CB	1:C:273:SER:OG	2.27	0.82
1:C:279:LEU:CD1	1:C:279:LEU:H	1.92	0.82
1:A:139:GLN:CD	1:A:139:GLN:H	1.83	0.81
1:B:231:TRP:HZ3	1:B:263:PHE:CE2	1.93	0.81
1:A:263:PHE:O	1:A:264:ARG:CB	2.28	0.81
1:A:237:LYS:O	1:A:237:LYS:HG2	1.79	0.80
1:A:248:ARG:HB3	1:A:254:GLY:HA2	1.63	0.80
1:C:264:ARG:O	1:C:266:ILE:HG23	1.81	0.80
1:A:173:SER:HB2	1:A:175:ARG:HG3	1.64	0.80
1:A:235:THR:HG21	1:A:239:ILE:HD13	1.62	0.80
1:B:276:LEU:CD1	1:B:290:ARG:CB	2.60	0.79
1:A:138:TRP:CD1	1:A:139:GLN:NE2	2.50	0.79
1:D:228:LEU:HG	1:D:281:PRO:HG2	1.64	0.79
1:B:54:LEU:HD12	1:B:54:LEU:N	1.97	0.79
1:B:264:ARG:O	1:B:265:LYS:HG3	1.83	0.79
1:A:151:PHE:CE2	1:A:152:ARG:NH1	2.50	0.79
1:C:234:MET:HE2	1:C:259:LEU:H	1.47	0.79
1:B:61:SER:HB3	1:B:291:VAL:CG2	2.13	0.78
1:C:97:LEU:CB	1:C:97:LEU:CD1	2.62	0.78
1:B:268:ALA:HB1	1:B:269:ARG:HD3	1.66	0.77
1:D:253:PHE:HD1	1:D:256:ALA:HB2	1.47	0.77
1:B:219:ARG:HH11	1:B:219:ARG:CG	1.90	0.77
1:A:241:GLU:O	1:A:244:LEU:HG	1.85	0.76
1:A:245:ALA:HB3	1:A:246:PRO:HD3	1.66	0.76
1:B:268:ALA:HA	1:B:269:ARG:CG	2.14	0.76
1:C:78:ARG:HA	1:D:78:ARG:HB2	1.67	0.76
1:B:262:PRO:HB2	1:B:279:LEU:HD12	1.67	0.75
1:B:266:ILE:CG1	1:B:267:GLU:N	2.45	0.75
1:D:241:GLU:CB	1:D:244:LEU:HD12	2.16	0.75
1:C:78:ARG:HA	1:D:78:ARG:CB	2.17	0.75
1:B:266:ILE:CD1	1:B:267:GLU:N	2.38	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PHE:HZ	1:A:152:ARG:CZ	1.99	0.74
1:B:264:ARG:C	1:B:265:LYS:HG3	2.06	0.74
1:C:68:LYS:NZ	1:C:304:GLN:HE21	1.86	0.74
1:B:268:ALA:HB1	1:B:269:ARG:CD	2.18	0.74
1:C:153:ASP:HB3	1:C:157:LEU:HD12	1.68	0.73
1:B:259:LEU:CB	1:B:259:LEU:CD1	2.67	0.73
1:B:263:PHE:O	1:B:263:PHE:CD1	2.42	0.73
1:D:73:ARG:HD2	1:D:296:PRO:HB2	1.69	0.73
1:B:268:ALA:HB1	1:B:269:ARG:CG	2.19	0.72
1:D:241:GLU:HB2	1:D:244:LEU:HD12	1.69	0.72
1:C:274:SER:O	1:C:289:LEU:HD22	1.90	0.71
1:B:54:LEU:CG	1:B:54:LEU:CA	2.69	0.71
1:C:269:ARG:HB2	1:C:273:SER:HG	1.55	0.71
1:B:306:SER:N	1:B:306:SER:CB	2.53	0.71
1:A:175:ARG:HH11	1:A:199:GLU:CD	1.92	0.71
1:B:265:LYS:O	1:B:266:ILE:HG23	1.91	0.71
1:B:56:GLY:C	1:B:58:ALA:H	1.95	0.70
1:A:108:ASN:HD21	1:A:134:ALA:HA	1.55	0.70
1:B:285:THR:HG22	1:B:285:THR:O	1.92	0.70
1:B:59:GLY:HA2	1:B:62:ARG:NH1	2.06	0.69
1:C:234:MET:CE	1:C:259:LEU:H	2.05	0.69
1:C:68:LYS:HZ3	1:C:304:GLN:HE21	1.39	0.69
1:A:238:PRO:O	1:A:239:ILE:CG2	2.32	0.69
1:A:153:ASP:HB2	1:A:166:HIS:CE1	2.28	0.68
1:B:265:LYS:N	1:B:266:ILE:HG23	2.09	0.68
1:B:228:LEU:HD22	1:B:280:LEU:HD23	1.74	0.68
1:B:276:LEU:HD11	1:B:290:ARG:CB	2.23	0.68
1:A:173:SER:CB	1:A:175:ARG:HG3	2.23	0.68
1:A:68:LYS:CE	1:A:304:GLN:HE21	2.01	0.68
1:D:279:LEU:O	1:D:280:LEU:C	2.32	0.68
1:A:175:ARG:NH1	1:A:199:GLU:CD	2.47	0.68
1:B:217:THR:HG21	1:B:236:THR:CG2	2.24	0.68
1:B:217:THR:HG21	1:B:236:THR:HG23	1.75	0.67
1:C:152:ARG:O	1:C:156:ARG:HG2	1.95	0.67
1:B:248:ARG:HB3	1:B:254:GLY:HA2	1.77	0.67
1:B:259:LEU:CG	1:B:259:LEU:CA	2.71	0.67
1:B:265:LYS:C	1:B:266:ILE:CG2	2.57	0.67
1:C:78:ARG:NH1	1:D:77:GLU:HG2	2.09	0.67
1:D:90:ALA:HA	1:D:93:ARG:HG2	1.76	0.66
1:D:253:PHE:CD1	1:D:256:ALA:HB2	2.29	0.66
1:A:152:ARG:NH2	1:A:171:THR:OG1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:HD2	1:C:190:PRO:HB3	1.77	0.66
1:D:77:GLU:HG3	3:D:316:HOH:O	1.96	0.65
1:B:242:ASP:N	1:B:242:ASP:OD1	2.30	0.65
1:A:236:THR:O	1:A:237:LYS:CB	2.43	0.64
1:A:264:ARG:CG	1:A:265:LYS:N	2.30	0.64
1:C:234:MET:HE1	1:C:257:PRO:HB2	1.79	0.64
1:A:151:PHE:HZ	1:A:152:ARG:NH2	1.95	0.64
1:A:78:ARG:HG2	3:A:314:HOH:O	1.97	0.64
1:C:292:GLU:HG2	1:C:303:GLU:HG2	1.80	0.64
1:B:229:PRO:O	1:B:231:TRP:N	2.31	0.64
1:C:269:ARG:HG2	1:C:270:PRO:HD2	1.79	0.64
1:C:233:PHE:HB2	1:C:257:PRO:HD2	1.80	0.63
1:D:235:THR:HG21	1:D:239:ILE:HD11	0.75	0.63
1:D:77:GLU:CG	3:D:316:HOH:O	2.47	0.63
1:A:245:ALA:CB	1:A:246:PRO:HD3	2.29	0.63
1:A:269:ARG:HD3	1:A:273:SER:OG	1.99	0.63
1:B:61:SER:HB3	1:B:291:VAL:HG21	1.81	0.63
1:C:169:MET:HE1	1:C:233:PHE:CE2	2.34	0.63
1:B:230:SER:OG	1:B:231:TRP:CD1	2.51	0.62
1:B:217:THR:OG1	1:B:301:ARG:HG2	1.99	0.62
1:B:61:SER:HB3	1:B:291:VAL:HG22	1.80	0.62
1:D:292:GLU:CG	1:D:303:GLU:HG2	2.26	0.62
1:B:265:LYS:N	1:B:266:ILE:CG2	2.60	0.62
1:A:280:LEU:HD13	1:A:288:PHE:CZ	2.35	0.62
1:B:263:PHE:O	1:B:263:PHE:HD1	1.81	0.62
1:B:259:LEU:CD2	1:B:259:LEU:CB	2.73	0.61
1:A:70:SER:OG	1:A:73:ARG:NH2	2.33	0.61
1:B:264:ARG:C	1:B:265:LYS:CG	2.69	0.61
1:D:73:ARG:CD	1:D:296:PRO:HB2	2.30	0.61
1:B:276:LEU:HD11	1:B:290:ARG:HB2	1.75	0.61
1:B:231:TRP:CH2	1:B:263:PHE:CD2	2.88	0.61
1:C:92:ILE:HD13	1:C:107:ILE:HD12	1.82	0.61
1:B:266:ILE:HD12	1:B:267:GLU:CA	2.32	0.60
1:C:169:MET:O	1:C:252:GLN:NE2	2.35	0.60
1:B:262:PRO:CB	1:B:279:LEU:CD1	2.73	0.60
1:A:188:GLY:HA2	1:D:175:ARG:CZ	2.31	0.60
1:A:254:GLY:O	1:A:256:ALA:N	2.35	0.60
1:B:266:ILE:O	1:B:275:THR:HG22	2.03	0.59
1:B:231:TRP:CH2	1:B:263:PHE:CE2	2.90	0.59
1:D:170:GLY:O	1:D:174:ASN:HA	2.03	0.59
1:D:241:GLU:HB3	1:D:244:LEU:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:HB3	1:A:109:ARG:NH2	2.17	0.59
1:A:78:ARG:HA	1:B:78:ARG:HB2	1.84	0.59
1:A:151:PHE:O	1:A:152:ARG:O	2.20	0.58
1:C:234:MET:CE	1:C:257:PRO:HB2	2.33	0.58
1:B:105:ASP:HB3	1:B:109:ARG:HH22	1.69	0.58
1:D:253:PHE:HD1	1:D:256:ALA:CB	2.15	0.58
1:C:283:ASP:HA	1:C:284:SER:HB2	0.69	0.58
1:C:105:ASP:HA	1:C:108:ASN:HB2	1.86	0.58
1:A:175:ARG:NH1	1:A:199:GLU:OE1	2.37	0.58
1:A:155:PHE:O	1:A:159:VAL:HG23	2.04	0.57
1:B:216:VAL:HG13	1:B:300:TRP:HB3	1.85	0.57
1:C:126:ILE:HA	1:C:132:ALA:HA	1.86	0.57
1:B:265:LYS:H	1:B:266:ILE:HG22	1.65	0.57
1:B:82:LEU:O	1:B:86:LEU:HG	2.04	0.57
1:C:234:MET:HE2	1:C:259:LEU:N	2.17	0.57
1:B:276:LEU:HD11	1:B:290:ARG:CG	2.35	0.57
1:B:169:MET:HE1	1:B:233:PHE:CZ	2.40	0.57
1:D:152:ARG:HG3	1:D:154:TYR:CE2	2.41	0.56
1:B:228:LEU:O	1:B:231:TRP:HB2	2.05	0.56
1:C:243:ARG:O	1:C:247:ILE:HG13	2.06	0.56
1:D:82:LEU:HB2	1:D:83:PRO:HD3	1.88	0.56
1:B:231:TRP:HH2	1:B:263:PHE:CD2	2.24	0.56
1:B:68:LYS:NZ	1:B:304:GLN:HE21	2.04	0.56
1:A:243:ARG:O	1:A:247:ILE:HG13	2.06	0.55
1:A:93:ARG:NH1	1:A:185:ASP:O	2.38	0.55
1:D:108:ASN:ND2	1:D:135:ALA:H	2.04	0.55
1:A:112:GLU:O	1:A:116:THR:HG23	2.06	0.55
1:A:261:LEU:HD13	1:A:263:PHE:CE1	2.41	0.55
1:B:54:LEU:CB	1:B:54:LEU:C	2.73	0.55
1:B:156:ARG:HH11	1:B:156:ARG:CG	2.13	0.55
1:B:231:TRP:HH2	1:B:263:PHE:HD2	1.55	0.55
1:B:54:LEU:CD2	1:B:54:LEU:CD1	2.84	0.55
1:C:101:ARG:HG2	1:C:105:ASP:OD1	2.06	0.55
1:A:218:ASP:OD2	1:A:220:ARG:NH2	2.34	0.55
1:B:105:ASP:OD1	1:B:105:ASP:N	2.36	0.55
1:B:239:ILE:HD11	1:B:244:LEU:HD23	1.88	0.55
1:C:216:VAL:HG13	1:C:301:ARG:O	2.07	0.54
1:B:155:PHE:O	1:B:158:ALA:HB3	2.06	0.54
1:C:108:ASN:HD21	1:C:135:ALA:H	1.55	0.54
1:C:101:ARG:HB3	1:C:102:PRO:HD3	1.90	0.54
1:C:165:GLU:HG2	1:C:178:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ARG:O	1:D:83:PRO:HD2	2.07	0.54
1:B:105:ASP:HB3	1:B:109:ARG:NH2	2.23	0.54
1:B:273:SER:O	1:B:274:SER:HB3	2.08	0.54
1:A:152:ARG:HD3	1:A:252:GLN:CD	2.29	0.53
1:B:301:ARG:NH1	1:B:301:ARG:HB2	2.23	0.53
1:D:127:ASP:HB3	1:D:129:SER:H	1.72	0.53
1:A:151:PHE:C	1:A:152:ARG:O	2.47	0.53
1:B:283:ASP:O	1:B:285:THR:N	2.42	0.53
1:B:265:LYS:CA	1:B:266:ILE:HG23	2.37	0.53
1:A:78:ARG:NH1	1:B:77:GLU:HG2	2.24	0.53
1:B:268:ALA:CA	1:B:269:ARG:CG	2.69	0.53
1:B:306:SER:C	1:B:306:SER:CB	2.76	0.53
1:B:54:LEU:N	1:B:54:LEU:CD1	2.71	0.53
1:C:264:ARG:HD2	1:C:277:ASP:CB	2.30	0.53
1:B:77:GLU:OE2	1:B:80:ARG:HD2	2.09	0.53
1:B:175:ARG:NH1	1:B:199:GLU:OE1	2.42	0.53
1:A:213:PRO:HB3	1:A:228:LEU:HD11	1.91	0.52
1:A:228:LEU:CD1	1:A:231:TRP:CZ3	2.89	0.52
1:B:259:LEU:HA	1:B:259:LEU:HD23	1.91	0.52
1:C:79:GLN:NE2	1:C:120:ALA:HB2	2.24	0.52
1:A:96:LEU:HD11	1:A:125:LEU:HD11	1.92	0.52
1:D:241:GLU:CB	1:D:244:LEU:CD1	2.85	0.52
1:A:108:ASN:HB3	1:A:138:TRP:CD1	2.44	0.52
1:C:234:MET:HG3	1:C:259:LEU:O	2.10	0.52
1:B:266:ILE:HG13	1:B:267:GLU:N	2.23	0.52
1:B:276:LEU:HD11	1:B:290:ARG:HE	1.74	0.52
1:B:68:LYS:NZ	1:B:304:GLN:NE2	2.58	0.52
1:A:117:SER:C	1:A:118:ALA:O	2.47	0.51
1:D:152:ARG:CG	1:D:154:TYR:CE2	2.92	0.51
1:D:217:THR:HA	1:D:222:ILE:O	2.11	0.51
1:B:220:ARG:HB2	1:B:222:ILE:HD12	1.92	0.51
1:B:56:GLY:C	1:B:58:ALA:N	2.62	0.51
1:B:169:MET:HE1	1:B:233:PHE:HZ	1.76	0.51
1:B:106:ARG:HB3	1:B:106:ARG:HH11	1.76	0.51
1:C:63:ILE:HG12	1:C:64:ASP:N	2.25	0.51
1:C:68:LYS:NZ	1:C:304:GLN:NE2	2.56	0.51
1:C:274:SER:O	1:C:289:LEU:CD2	2.57	0.51
1:D:186:GLY:O	1:D:188:GLY:N	2.41	0.51
1:D:279:LEU:O	1:D:280:LEU:O	2.28	0.51
1:A:246:PRO:O	1:A:250:SER:N	2.37	0.51
1:C:126:ILE:HG21	1:C:130:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ARG:HH11	1:C:156:ARG:HG3	1.76	0.51
1:C:237:LYS:HB2	1:C:238:PRO:HD2	1.93	0.50
1:B:269:ARG:HH21	1:B:270:PRO:HA	1.75	0.50
1:D:84:LEU:HA	1:D:182:ARG:HD2	1.93	0.50
1:A:280:LEU:HD13	1:A:288:PHE:HZ	1.76	0.50
1:B:231:TRP:CH2	1:B:263:PHE:HD2	2.29	0.50
1:B:277:ASP:OD1	1:B:287:ALA:HA	2.11	0.50
1:C:126:ILE:CG2	1:C:130:GLY:HA2	2.41	0.50
1:C:101:ARG:O	1:C:105:ASP:OD1	2.30	0.50
1:C:266:ILE:O	1:C:266:ILE:HG13	2.12	0.50
1:A:79:GLN:NE2	1:A:120:ALA:HB2	2.26	0.50
1:A:217:THR:HA	1:A:222:ILE:O	2.12	0.50
1:C:234:MET:CE	1:C:234:MET:HA	2.41	0.50
1:C:290:ARG:HA	1:C:304:GLN:O	2.11	0.50
1:A:188:GLY:HA2	1:D:175:ARG:HH12	1.76	0.50
1:C:80:ARG:NH2	1:C:165:GLU:OE2	2.38	0.49
1:C:79:GLN:HA	1:C:79:GLN:OE1	2.11	0.49
1:C:128:ARG:HB3	1:C:191:LEU:O	2.12	0.49
1:D:79:GLN:NE2	1:D:120:ALA:HB2	2.28	0.49
1:A:169:MET:CE	1:A:233:PHE:CE2	2.95	0.49
1:B:240:ALA:O	1:B:241:GLU:C	2.51	0.49
1:C:280:LEU:O	1:C:282:GLY:HA2	2.12	0.49
1:C:78:ARG:HA	1:D:78:ARG:HB3	1.92	0.49
1:B:292:GLU:HG3	1:B:301:ARG:HD3	1.93	0.49
1:D:269:ARG:HD3	1:D:272:GLY:HA2	1.93	0.49
1:D:292:GLU:HG2	1:D:301:ARG:HD3	1.94	0.49
1:A:169:MET:HE1	1:A:233:PHE:CZ	2.48	0.49
1:D:108:ASN:HD22	1:D:135:ALA:H	1.59	0.49
1:D:112:GLU:O	1:D:116:THR:HG23	2.12	0.49
1:C:243:ARG:HA	1:C:246:PRO:HG2	1.94	0.49
1:C:183:ARG:HD2	1:C:190:PRO:CB	2.42	0.49
1:D:262:PRO:CB	1:D:279:LEU:CD1	2.68	0.49
1:B:219:ARG:NH1	1:B:219:ARG:CG	2.59	0.48
1:A:234:MET:CE	1:A:257:PRO:HB2	2.43	0.48
1:C:234:MET:HE2	1:C:234:MET:HA	1.93	0.48
1:C:126:ILE:HG22	1:C:127:ASP:O	2.13	0.48
1:D:79:GLN:HA	1:D:82:LEU:CD2	2.44	0.48
1:D:237:LYS:HA	1:D:238:PRO:HD3	1.41	0.48
1:A:173:SER:HB2	1:A:175:ARG:CG	2.38	0.48
1:B:177:GLY:HA3	1:B:197:LYS:HE2	1.95	0.48
1:C:215:TYR:OH	1:C:303:GLU:OE1	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:PHE:O	1:D:255:ASP:N	2.47	0.48
1:D:128:ARG:HH21	1:D:190:PRO:HG2	1.79	0.47
1:B:105:ASP:CB	1:B:109:ARG:NH2	2.77	0.47
1:B:264:ARG:HB3	1:B:265:LYS:HG2	1.95	0.47
1:D:121:ALA:HB2	1:D:199:GLU:HG3	1.96	0.47
1:D:306:SER:O	1:D:307:PRO:O	2.31	0.47
1:A:217:THR:OG1	1:A:301:ARG:HG3	2.15	0.47
1:A:108:ASN:HB3	1:A:138:TRP:CG	2.50	0.47
1:A:237:LYS:CG	1:A:237:LYS:O	2.57	0.47
1:D:294:MET:O	1:D:296:PRO:HD3	2.15	0.47
1:A:68:LYS:HD3	1:A:207:TRP:CD1	2.50	0.47
1:A:169:MET:HE3	1:A:233:PHE:CE2	2.50	0.47
1:B:105:ASP:OD2	1:C:297:SER:HB3	2.15	0.47
1:B:130:GLY:HA3	1:B:150:ALA:HB2	1.97	0.47
1:D:287:ALA:HB1	1:D:308:LEU:HD23	1.97	0.46
1:B:282:GLY:O	1:B:283:ASP:CB	2.62	0.46
1:B:63:ILE:HD12	1:B:63:ILE:C	2.36	0.46
1:D:173:SER:O	1:D:174:ASN:ND2	2.48	0.46
1:C:283:ASP:CA	1:C:284:SER:HB3	2.37	0.46
1:B:60:GLN:HG3	1:B:64:ASP:OD2	2.16	0.46
1:C:278:ALA:C	1:C:279:LEU:HD12	2.32	0.46
1:A:68:LYS:HE2	1:A:304:GLN:NE2	2.08	0.46
1:C:107:ILE:O	1:C:111:LEU:HG	2.15	0.46
1:A:127:ASP:HB2	1:A:131:VAL:O	2.16	0.46
1:A:240:ALA:O	1:A:241:GLU:C	2.55	0.46
1:B:169:MET:HB2	1:B:169:MET:HE3	1.86	0.46
1:D:177:GLY:HA3	1:D:197:LYS:HE2	1.98	0.46
1:A:97:LEU:HD23	1:A:191:LEU:HD21	1.99	0.45
1:C:98:SER:CB	1:C:98:SER:C	2.75	0.45
1:A:152:ARG:HD3	1:A:252:GLN:NE2	2.32	0.45
1:A:292:GLU:HG2	1:A:293:THR:N	2.31	0.45
1:C:128:ARG:HE	1:C:128:ARG:HB2	1.48	0.45
1:B:240:ALA:O	1:B:242:ASP:N	2.50	0.45
1:B:274:SER:OG	1:B:290:ARG:NE	2.49	0.45
1:A:251:LEU:O	1:A:252:GLN:HB2	2.16	0.45
1:B:217:THR:HA	1:B:222:ILE:O	2.16	0.45
1:B:301:ARG:HH11	1:B:301:ARG:HB2	1.81	0.45
1:C:262:PRO:O	1:C:263:PHE:HD1	1.99	0.45
1:D:253:PHE:HB3	1:D:256:ALA:HB2	1.98	0.45
1:B:276:LEU:O	1:B:277:ASP:OD1	2.34	0.45
1:B:285:THR:O	1:B:286:ALA:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:GLN:HE22	1:C:120:ALA:HB2	1.80	0.45
1:D:217:THR:HG21	1:D:236:THR:HG23	1.99	0.45
1:D:228:LEU:HD21	1:D:281:PRO:HD2	1.99	0.45
1:B:301:ARG:HD2	1:B:303:GLU:OE2	2.17	0.45
1:D:306:SER:HA	1:D:307:PRO:HD2	1.90	0.45
1:A:151:PHE:CZ	1:A:152:ARG:NH2	2.74	0.45
1:B:216:VAL:CG1	1:B:300:TRP:HB3	2.47	0.45
1:C:284:SER:OG	1:C:285:THR:N	2.50	0.45
1:A:290:ARG:HA	1:A:304:GLN:O	2.17	0.44
1:B:217:THR:HG21	1:B:236:THR:HG21	1.98	0.44
1:B:239:ILE:O	1:B:239:ILE:HG13	2.17	0.44
1:A:139:GLN:N	1:A:139:GLN:CD	2.59	0.44
1:C:222:ILE:HD11	1:C:247:ILE:HD13	1.99	0.44
1:D:217:THR:HG21	1:D:236:THR:CG2	2.46	0.44
1:A:89:ASP:HB3	1:A:92:ILE:HG13	1.99	0.44
1:B:68:LYS:HZ3	1:B:304:GLN:HE21	1.66	0.44
1:D:73:ARG:HH11	1:D:296:PRO:HG2	1.82	0.44
1:A:108:ASN:ND2	1:A:134:ALA:HA	2.29	0.44
1:D:269:ARG:H	1:D:274:SER:H	1.64	0.44
1:B:279:LEU:O	1:B:280:LEU:HB2	2.18	0.44
1:A:100:ASP:OD2	1:A:103:SER:CB	2.44	0.44
1:B:251:LEU:O	1:B:252:GLN:HB2	2.16	0.44
1:A:169:MET:HE3	1:A:233:PHE:HE2	1.83	0.43
1:B:283:ASP:O	1:B:284:SER:C	2.56	0.43
1:D:87:ALA:HA	1:D:184:VAL:HG22	2.00	0.43
1:D:186:GLY:C	1:D:188:GLY:H	2.20	0.43
1:B:269:ARG:O	1:B:271:ASP:HB2	2.17	0.43
1:B:100:ASP:O	1:B:103:SER:HB2	2.18	0.43
1:C:98:SER:CA	1:C:98:SER:OG	2.59	0.43
1:A:138:TRP:NE1	1:A:139:GLN:NE2	2.65	0.43
1:D:274:SER:HB3	1:D:290:ARG:HB3	1.99	0.43
1:A:73:ARG:HH11	1:A:73:ARG:HG2	1.83	0.43
1:B:228:LEU:HA	1:B:229:PRO:HD3	1.77	0.43
1:C:96:LEU:HD11	1:C:125:LEU:HD11	2.00	0.43
1:C:210:SER:C	1:C:212:LYS:H	2.21	0.43
1:D:216:VAL:HA	1:D:301:ARG:O	2.18	0.43
1:C:239:ILE:HD11	1:C:244:LEU:CD1	2.49	0.43
1:B:127:ASP:HB2	1:B:131:VAL:O	2.19	0.43
1:D:280:LEU:HD12	1:D:280:LEU:HA	1.84	0.43
1:C:228:LEU:HA	1:C:229:PRO:HD2	1.89	0.43
1:D:215:TYR:HH	1:D:263:PHE:HE1	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ALA:HA	1:A:155:PHE:CD2	2.54	0.42
1:B:266:ILE:O	1:B:267:GLU:O	2.38	0.42
1:B:59:GLY:HA2	1:B:62:ARG:HH12	1.80	0.42
1:C:169:MET:HB2	1:C:169:MET:HE3	1.56	0.42
1:C:283:ASP:N	1:C:284:SER:HB3	2.33	0.42
1:D:273:SER:O	1:D:274:SER:HB2	2.18	0.42
1:B:306:SER:HA	1:B:307:PRO:HD2	1.79	0.42
1:C:155:PHE:O	1:C:159:VAL:HG23	2.18	0.42
1:D:216:VAL:HG13	1:D:300:TRP:HB3	2.01	0.42
1:A:152:ARG:HD3	1:A:252:GLN:OE1	2.20	0.42
1:A:233:PHE:O	1:A:258:LEU:HD23	2.20	0.42
1:B:128:ARG:HG3	1:B:128:ARG:O	2.20	0.42
1:B:169:MET:CA	1:B:169:MET:HE2	2.50	0.42
1:C:108:ASN:ND2	1:C:135:ALA:H	2.15	0.42
1:A:240:ALA:O	1:A:242:ASP:N	2.53	0.42
1:A:302:LEU:C	1:A:302:LEU:HD23	2.40	0.42
1:A:151:PHE:HZ	1:A:152:ARG:NH1	2.06	0.42
1:B:265:LYS:N	1:B:266:ILE:HG22	2.31	0.42
1:B:276:LEU:HD11	1:B:290:ARG:NE	2.34	0.42
1:D:202:GLY:O	1:D:206:ASP:OD1	2.37	0.42
1:A:173:SER:OG	1:A:175:ARG:HG3	2.19	0.42
1:A:97:LEU:HD23	1:A:191:LEU:CD2	2.50	0.42
1:B:271:ASP:HB3	1:B:273:SER:OG	2.19	0.42
1:B:289:LEU:HD23	1:B:308:LEU:HD11	2.01	0.42
1:D:253:PHE:CD1	1:D:256:ALA:CA	3.03	0.42
1:B:79:GLN:NE2	1:B:120:ALA:HB2	2.35	0.42
1:B:276:LEU:HD11	1:B:290:ARG:HG3	2.01	0.42
1:C:156:ARG:NH1	1:C:156:ARG:HG3	2.35	0.41
1:A:295:VAL:O	1:A:298:THR:OG1	2.30	0.41
1:D:79:GLN:HE22	1:D:120:ALA:HB2	1.85	0.41
1:A:101:ARG:HB3	1:A:102:PRO:CD	2.50	0.41
1:A:231:TRP:O	1:A:234:MET:HB2	2.19	0.41
1:B:68:LYS:HZ3	1:B:304:GLN:NE2	2.18	0.41
1:C:108:ASN:HA	1:C:108:ASN:HD22	1.52	0.41
1:C:239:ILE:HD11	1:C:244:LEU:HD13	2.02	0.41
1:C:261:LEU:HD13	1:C:263:PHE:CE2	2.55	0.41
1:B:169:MET:CE	1:B:233:PHE:CZ	3.03	0.41
1:C:181:SER:O	1:C:182:ARG:HG3	2.21	0.41
1:C:283:ASP:N	1:C:284:SER:CB	2.82	0.41
1:D:276:LEU:HD12	1:D:277:ASP:N	2.36	0.41
1:A:206:ASP:O	1:A:209:ALA:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ARG:NH1	1:B:156:ARG:HG3	2.16	0.41
1:B:275:THR:C	1:B:276:LEU:HG	2.41	0.41
1:D:253:PHE:HD1	1:D:256:ALA:CA	2.34	0.41
1:B:215:TYR:OH	1:B:303:GLU:OE1	2.29	0.41
1:B:289:LEU:O	1:B:305:LEU:HA	2.21	0.41
1:A:122:VAL:HG21	1:A:144:PHE:CE2	2.56	0.40
1:B:266:ILE:HD12	1:B:267:GLU:HA	2.03	0.40
1:C:215:TYR:HB2	1:C:223:VAL:HG13	2.03	0.40
1:A:294:MET:CE	1:A:301:ARG:HH12	2.35	0.40
1:C:255:ASP:O	1:C:256:ALA:C	2.60	0.40
1:B:245:ALA:N	1:B:246:PRO:HD2	2.36	0.40
1:D:121:ALA:CB	1:D:199:GLU:HG3	2.51	0.40
1:D:279:LEU:C	1:D:280:LEU:O	2.60	0.40
1:D:78:ARG:NH1	1:D:118:ALA:HA	2.36	0.40
1:C:263:PHE:CD1	1:C:276:LEU:HD13	2.57	0.40
1:B:221:GLY:O	1:B:235:THR:HA	2.22	0.40

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 [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	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

All (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
1	B	230	SER
1	B	255	ASP
1	B	265	LYS
1	B	266	ILE
1	B	268	ALA
1	B	269	ARG
1	B	270	PRO
1	B	279	LEU
1	B	283	ASP
1	C	283	ASP
1	D	230	SER
1	D	233	PHE
1	D	234	MET
1	D	269	ARG
1	D	270	PRO
1	D	273	SER
1	D	274	SER
1	D	279	LEU
1	D	307	PRO
1	A	128	ARG
1	A	241	GLU
1	B	267	GLU
1	B	280	LEU
1	B	281	PRO
1	B	284	SER
1	B	286	ALA
1	A	136	SER
1	B	271	ASP
1	B	307	PRO
1	C	97	LEU
1	C	142	THR
1	A	265	LYS

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Mol	Chain	Res	Type
1	A	273	SER
1	D	127	ASP
1	D	238	PRO
1	B	57	LEU
1	A	92	ILE
1	C	242	ASP
1	D	239	ILE
1	D	257	PRO
1	D	284	SER
1	D	229	PRO
1	D	187	PRO

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

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	63	ILE
1	A	67	LEU
1	A	70	SER
1	A	77	GLU
1	A	78	ARG
1	A	101	ARG
1	A	103	SER
1	A	116	THR
1	A	122	VAL

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Mol	Chain	Res	Type
1	A	127	ASP
1	A	128	ARG
1	A	139	GLN
1	A	152	ARG
1	A	156	ARG
1	A	166	HIS
1	A	175	ARG
1	A	203	VAL
1	A	226	THR
1	A	228	LEU
1	A	234	MET
1	A	237	LYS
1	A	242	ASP
1	A	253	PHE
1	A	279	LEU
1	A	294	MET
1	A	301	ARG
1	B	54	LEU
1	B	57	LEU
1	B	60	GLN
1	B	62	ARG
1	B	67	LEU
1	B	71	LEU
1	B	77	GLU
1	B	78	ARG
1	B	85	VAL
1	B	88	ASP
1	B	93	ARG
1	B	100	ASP
1	B	105	ASP
1	B	106	ARG
1	B	112	GLU
1	B	122	VAL
1	B	127	ASP
1	B	128	ARG
1	B	129	SER
1	B	156	ARG
1	B	163	MET
1	B	175	ARG
1	B	182	ARG
1	B	201	ASP
1	B	219	ARG

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Mol	Chain	Res	Type
1	B	239	ILE
1	B	242	ASP
1	B	243	ARG
1	B	267	GLU
1	B	269	ARG
1	B	271	ASP
1	B	273	SER
1	B	284	SER
1	B	290	ARG
1	B	291	VAL
1	B	293	THR
1	B	301	ARG
1	B	306	SER
1	C	60	GLN
1	C	62	ARG
1	C	63	ILE
1	C	71	LEU
1	C	78	ARG
1	C	88	ASP
1	C	103	SER
1	C	108	ASN
1	C	119	GLU
1	C	122	VAL
1	C	124	TYR
1	C	128	ARG
1	C	156	ARG
1	C	171	THR
1	C	172	VAL
1	C	203	VAL
1	C	208	GLN
1	C	219	ARG
1	C	226	THR
1	C	234	MET
1	C	239	ILE
1	C	243	ARG
1	C	246	PRO
1	C	269	ARG
1	C	274	SER
1	C	276	LEU
1	C	279	LEU
1	C	280	LEU
1	C	283	ASP

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Mol	Chain	Res	Type
1	C	289	LEU
1	C	294	MET
1	D	60	GLN
1	D	66	SER
1	D	71	LEU
1	D	77	GLU
1	D	78	ARG
1	D	82	LEU
1	D	88	ASP
1	D	93	ARG
1	D	101	ARG
1	D	114	LEU
1	D	116	THR
1	D	124	TYR
1	D	128	ARG
1	D	152	ARG
1	D	163	MET
1	D	171	THR
1	D	174	ASN
1	D	194	ILE
1	D	208	GLN
1	D	228	LEU
1	D	241	GLU
1	D	243	ARG
1	D	247	ILE
1	D	253	PHE
1	D	266	ILE
1	D	267	GLU
1	D	271	ASP
1	D	273	SER
1	D	274	SER
1	D	289	LEU
1	D	292	GLU
1	D	297	SER
1	D	306	SER
1	D	308	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	A	166	HIS
1	A	304	GLN
1	B	79	GLN
1	B	108	ASN
1	B	139	GLN
1	B	252	GLN
1	B	299	ASN
1	B	304	GLN
1	C	108	ASN
1	C	208	GLN
1	C	299	ASN
1	C	304	GLN
1	D	60	GLN
1	D	79	GLN
1	D	108	ASN
1	D	174	ASN
1	D	252	GLN
1	D	304	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

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	A	1	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	B	2	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	D	4	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLA	C	3	-	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
2	MLA	A	1	-	-	0/0/4/4	-
2	MLA	B	2	-	-	0/0/4/4	-
2	MLA	D	4	-	-	0/0/4/4	-
2	MLA	C	3	-	-	0/0/4/4	-

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.

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 [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	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, 47, 56, 64	51 (5%)

All (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
1	B	279	LEU	5.5
1	C	54	LEU	5.2
1	B	281	PRO	5.2
1	B	283	ASP	5.0
1	C	264	ARG	5.0
1	B	268	ALA	4.9
1	B	55	ALA	4.8
1	D	279	LEU	4.7
1	C	271	ASP	4.5
1	B	264	ARG	4.5
1	B	278	ALA	4.3
1	B	290	ARG	4.3
1	C	263	PHE	4.3
1	A	239	ILE	4.3
1	B	276	LEU	4.2
1	B	54	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	281	PRO	4.0
1	B	282	GLY	4.0
1	B	287	ALA	3.8
1	D	283	ASP	3.8
1	D	265	LYS	3.7
1	D	264	ARG	3.7
1	D	268	ALA	3.7
1	B	308	LEU	3.7
1	D	282	GLY	3.6
1	C	281	PRO	3.5
1	D	285	THR	3.5
1	B	231	TRP	3.5
1	B	270	PRO	3.3
1	A	237	LYS	3.2
1	B	286	ALA	3.2
1	B	284	SER	3.2
1	A	242	ASP	3.2
1	A	151	PHE	3.2
1	B	266	ILE	3.2
1	C	284	SER	3.1
1	C	273	SER	3.1
1	A	241	GLU	3.1
1	A	152	ARG	3.0
1	C	145	VAL	3.0
1	D	187	PRO	3.0
1	C	266	ILE	2.9
1	A	244	LEU	2.8
1	A	97	LEU	2.7
1	C	277	ASP	2.7
1	D	172	VAL	2.7
1	A	172	VAL	2.7
1	D	270	PRO	2.7
1	D	54	LEU	2.7
1	A	243	ARG	2.6
1	C	55	ALA	2.6
1	B	271	ASP	2.6
1	C	267	GLU	2.6
1	C	96	LEU	2.5
1	A	284	SER	2.5
1	A	267	GLU	2.5
1	A	265	LYS	2.4
1	C	290	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	279	LEU	2.4
1	B	269	ARG	2.4
1	C	270	PRO	2.4
1	C	94	GLY	2.4
1	B	285	THR	2.4
1	A	228	LEU	2.3
1	C	269	ARG	2.3
1	C	289	LEU	2.3
1	A	248	ARG	2.3
1	B	243	ARG	2.2
1	A	280	LEU	2.2
1	B	274	SER	2.2
1	B	263	PHE	2.1
1	C	308	LEU	2.1
1	D	280	LEU	2.0
1	A	264	ARG	2.0
1	C	142	THR	2.0
1	D	55	ALA	2.0

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, 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 [i](#)

There are no such residues in this entry.