



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:29 pm BST

PDB ID : 6JZN  
Title : Structure of the intermembrane space region of PARC6-PDV1  
Authors : Feng, Y.; Liu, Z.  
Deposited on : 2019-05-02  
Resolution : 2.89 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.

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

MolProbity	:	4.02b-467
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

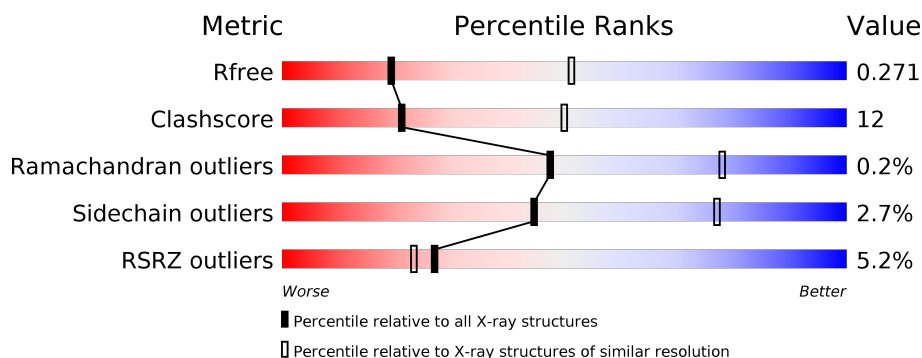
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	149	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>••</div> <div>13%</div> </div> </div>
1	B	149	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	149	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	149	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>19%</div> <div>••</div> <div>13%</div> </div> </div>
2	E	10	<div> <div>10%</div> <div> <div></div> <div>70%</div> <div>10%</div> <div>10%</div> <div>10%</div> </div> </div>
2	F	10	<div> <div>10%</div> <div> <div></div> <div>70%</div> <div>20%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	10	
2	H	10	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4583 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 Plastid division protein CDP1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	133	Total	C	N	O	S	0	0	0
			1085	691	176	214	4			
1	B	134	Total	C	N	O	S	0	0	0
			1089	694	177	214	4			
1	D	129	Total	C	N	O	S	0	0	0
			1053	672	172	205	4			
1	A	130	Total	C	N	O	S	0	0	0
			1068	681	173	210	4			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	671	MET	-	expression tag	UNP Q8VY16
C	672	GLY	-	expression tag	UNP Q8VY16
C	673	SER	-	expression tag	UNP Q8VY16
C	674	SER	-	expression tag	UNP Q8VY16
C	675	HIS	-	expression tag	UNP Q8VY16
C	676	HIS	-	expression tag	UNP Q8VY16
C	677	HIS	-	expression tag	UNP Q8VY16
C	678	HIS	-	expression tag	UNP Q8VY16
C	679	HIS	-	expression tag	UNP Q8VY16
C	680	HIS	-	expression tag	UNP Q8VY16
C	681	SER	-	expression tag	UNP Q8VY16
C	682	GLN	-	expression tag	UNP Q8VY16
C	683	ASP	-	expression tag	UNP Q8VY16
C	684	PRO	-	expression tag	UNP Q8VY16
B	671	MET	-	expression tag	UNP Q8VY16
B	672	GLY	-	expression tag	UNP Q8VY16
B	673	SER	-	expression tag	UNP Q8VY16
B	674	SER	-	expression tag	UNP Q8VY16
B	675	HIS	-	expression tag	UNP Q8VY16
B	676	HIS	-	expression tag	UNP Q8VY16
B	677	HIS	-	expression tag	UNP Q8VY16

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Chain	Residue	Modelled	Actual	Comment	Reference
B	678	HIS	-	expression tag	UNP Q8VY16
B	679	HIS	-	expression tag	UNP Q8VY16
B	680	HIS	-	expression tag	UNP Q8VY16
B	681	SER	-	expression tag	UNP Q8VY16
B	682	GLN	-	expression tag	UNP Q8VY16
B	683	ASP	-	expression tag	UNP Q8VY16
B	684	PRO	-	expression tag	UNP Q8VY16
D	671	MET	-	expression tag	UNP Q8VY16
D	672	GLY	-	expression tag	UNP Q8VY16
D	673	SER	-	expression tag	UNP Q8VY16
D	674	SER	-	expression tag	UNP Q8VY16
D	675	HIS	-	expression tag	UNP Q8VY16
D	676	HIS	-	expression tag	UNP Q8VY16
D	677	HIS	-	expression tag	UNP Q8VY16
D	678	HIS	-	expression tag	UNP Q8VY16
D	679	HIS	-	expression tag	UNP Q8VY16
D	680	HIS	-	expression tag	UNP Q8VY16
D	681	SER	-	expression tag	UNP Q8VY16
D	682	GLN	-	expression tag	UNP Q8VY16
D	683	ASP	-	expression tag	UNP Q8VY16
D	684	PRO	-	expression tag	UNP Q8VY16
A	671	MET	-	expression tag	UNP Q8VY16
A	672	GLY	-	expression tag	UNP Q8VY16
A	673	SER	-	expression tag	UNP Q8VY16
A	674	SER	-	expression tag	UNP Q8VY16
A	675	HIS	-	expression tag	UNP Q8VY16
A	676	HIS	-	expression tag	UNP Q8VY16
A	677	HIS	-	expression tag	UNP Q8VY16
A	678	HIS	-	expression tag	UNP Q8VY16
A	679	HIS	-	expression tag	UNP Q8VY16
A	680	HIS	-	expression tag	UNP Q8VY16
A	681	SER	-	expression tag	UNP Q8VY16
A	682	GLN	-	expression tag	UNP Q8VY16
A	683	ASP	-	expression tag	UNP Q8VY16
A	684	PRO	-	expression tag	UNP Q8VY16

- Molecule 2 is a protein called Peptide from Plastid division protein PDV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total 70	C 42	N 14	O 12	S 2	0	0	0
2	F	9	Total 70	C 42	N 14	O 12	S 2	0	0	0

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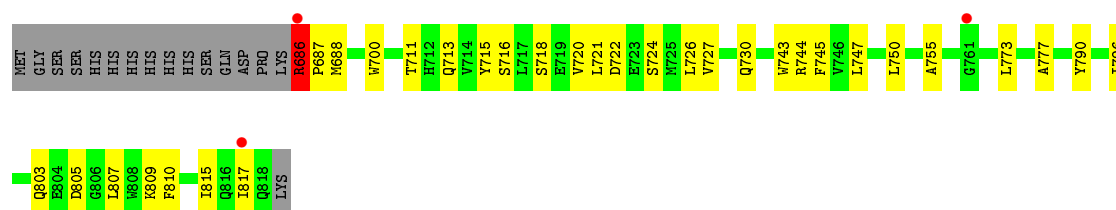
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	10	Total	C	N	O	S	0	0	0
			78	46	15	15	2			
2	E	9	Total	C	N	O	S	0	0	0
			70	42	14	12	2			

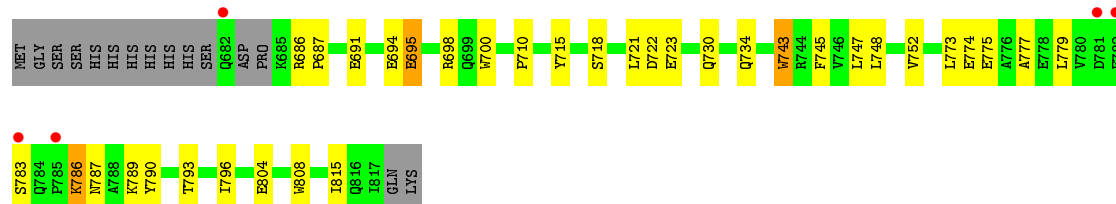
### 3 Residue-property plots [i](#)

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.

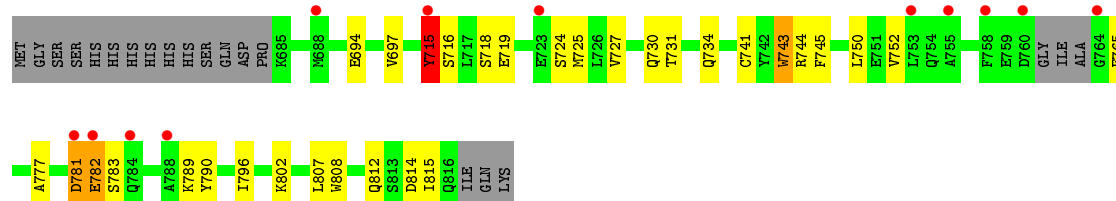
- Molecule 1: Plastid division protein CDP1, chloroplastic



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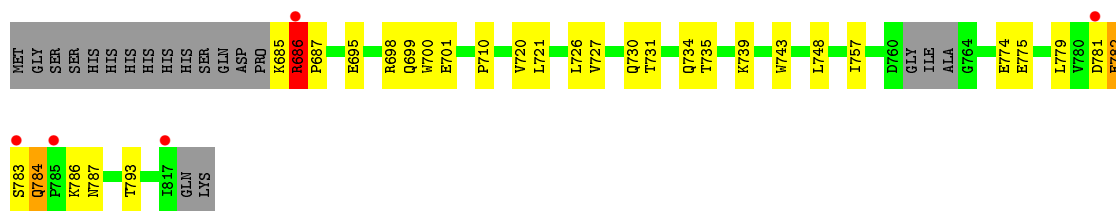


- Molecule 1: Plastid division protein CDP1, chloroplastic



- Molecule 1: Plastid division protein CDP1, chloroplastic

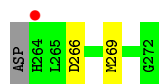




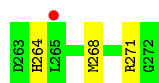
- Molecule 2: Peptide from Plastid division protein PDV1



- Molecule 2: Peptide from Plastid division protein PDV1



- Molecule 2: Peptide from Plastid division protein PDV1



- Molecule 2: Peptide from Plastid division protein PDV1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.45Å 95.83Å 196.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.89 49.14 – 2.89	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.14-2.89) 95.0 (49.14-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.223 , 0.272 0.223 , 0.271	Depositor DCC
$R_{free}$ test set	959 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4583	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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

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	0.54	2/1089 (0.2%)	0.90	7/1473 (0.5%)
1	B	0.36	0/1110	0.64	2/1501 (0.1%)
1	C	0.35	0/1107	0.72	4/1500 (0.3%)
1	D	0.41	1/1074 (0.1%)	0.80	4/1453 (0.3%)
2	E	1.61	0/70	1.02	1/90 (1.1%)
2	F	1.26	0/70	1.15	0/90
2	G	0.97	0/70	0.79	0/90
2	H	1.66	0/78	0.85	0/101
All	All	0.54	3/4668 (0.1%)	0.78	18/6298 (0.3%)

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	D	0	2
2	H	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	685	LYS	C-N	8.68	1.54	1.34
1	A	782	GLU	CB-CG	6.61	1.64	1.52
1	D	782	GLU	CB-CG	5.45	1.62	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	ARG	NE-CZ-NH1	-17.10	111.75	120.30
1	D	715	TYR	CB-CG-CD2	-10.60	114.64	121.00
1	C	686	ARG	NE-CZ-NH1	9.83	125.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	686	ARG	CG-CD-NE	9.57	131.91	111.80
1	C	686	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	686	ARG	CA-CB-CG	-7.31	97.32	113.40
1	D	782	GLU	CA-CB-CG	7.26	129.37	113.40
1	A	686	ARG	CD-NE-CZ	-6.84	114.03	123.60
1	D	715	TYR	CB-CA-C	-6.53	97.33	110.40
1	B	695	GLU	N-CA-CB	-6.41	99.07	110.60
1	B	783	SER	C-N-CA	6.40	137.71	121.70
1	C	686	ARG	CD-NE-CZ	6.34	132.47	123.60
1	A	686	ARG	NH1-CZ-NH2	5.85	125.83	119.40
2	E	264	HIS	N-CA-C	-5.75	95.47	111.00
1	A	783	SER	C-N-CA	5.73	136.03	121.70
1	A	782	GLU	CA-CB-CG	5.53	125.56	113.40
1	D	781	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	784	GLN	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	715	TYR	Sidechain
1	D	782	GLU	Mainchain
2	H	264	HIS	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	1068	0	1035	25	0
1	B	1089	0	1055	24	0
1	C	1085	0	1050	32	0
1	D	1053	0	1018	26	0
2	E	70	0	69	2	0
2	F	70	0	69	1	0
2	G	70	0	69	18	0
2	H	78	0	73	1	0
All	All	4583	0	4438	109	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 12.

All (109) 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:695:GLU:O	1:A:699:GLN:OE1	1.79	1.00
1:D:715:TYR:HD1	1:D:716:SER:N	1.75	0.84
2:F:266:ASP:O	2:F:269:MET:HG3	1.81	0.81
1:B:786:LYS:HD3	1:B:787:ASN:H	1.47	0.78
1:A:686:ARG:HG3	1:A:687:PRO:HD2	1.66	0.76
1:D:715:TYR:CD1	1:D:716:SER:N	2.54	0.75
1:C:817:ILE:HB	2:G:271:ARG:NH1	2.03	0.74
1:B:774:GLU:HB2	1:B:793:THR:HG22	1.70	0.74
2:G:268:MET:HE3	2:G:271:ARG:HH21	1.53	0.73
1:D:715:TYR:CD1	1:D:716:SER:OG	2.42	0.73
2:G:268:MET:CE	2:G:271:ARG:HH21	2.02	0.72
1:C:817:ILE:HD12	2:G:271:ARG:NH2	2.04	0.72
1:A:730:GLN:O	1:A:734:GLN:HG3	1.90	0.72
1:C:711:THR:HG21	1:C:713:GLN:HE21	1.54	0.71
1:C:817:ILE:HB	2:G:271:ARG:HH12	1.57	0.70
1:B:804:GLU:N	1:B:804:GLU:OE2	2.23	0.70
1:A:686:ARG:HG3	1:A:687:PRO:CD	2.22	0.70
1:B:730:GLN:O	1:B:734:GLN:HG3	1.93	0.69
1:D:715:TYR:CE1	1:D:716:SER:OG	2.46	0.68
1:C:745:PHE:O	1:D:744:ARG:NH1	2.26	0.68
1:C:747:LEU:O	1:D:789:LYS:NZ	2.27	0.68
1:A:781:ASP:OD1	1:A:784:GLN:NE2	2.27	0.67
2:G:268:MET:HE3	2:G:271:ARG:NH2	2.10	0.66
1:A:739:LYS:HZ1	2:E:264:HIS:N	1.94	0.66
2:G:268:MET:CE	2:G:271:ARG:NH2	2.58	0.65
1:D:715:TYR:O	1:D:718:SER:OG	2.15	0.64
1:B:691:GLU:O	1:B:695:GLU:HG3	1.98	0.64
1:B:694:GLU:HG3	1:B:752:VAL:HG23	1.81	0.63
1:B:796:ILE:HD12	1:B:815:ILE:HG13	1.79	0.62
1:C:726:LEU:O	1:C:730:GLN:HB2	1.99	0.62
1:C:817:ILE:HD12	2:G:271:ARG:HH22	1.63	0.62
1:C:817:ILE:HD12	2:G:271:ARG:CZ	2.29	0.61
1:C:796:ILE:HD12	1:C:815:ILE:HG12	1.81	0.61
1:B:698:ARG:HD3	1:A:786:LYS:HG2	1.82	0.61
1:D:730:GLN:O	1:D:734:GLN:HG2	2.02	0.60
2:G:264:HIS:CG	2:G:265:LEU:H	2.20	0.60
1:C:817:ILE:HD12	2:G:271:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:LEU:HD13	1:C:773:LEU:HD21	1.85	0.58
1:D:715:TYR:HD1	1:D:716:SER:HG	1.41	0.58
1:A:726:LEU:O	1:A:730:GLN:HB2	2.04	0.57
1:C:711:THR:CG2	1:C:713:GLN:HG3	2.34	0.57
1:D:796:ILE:HD12	1:D:815:ILE:HG13	1.85	0.57
1:C:807:LEU:HD22	1:C:809:LYS:HZ3	1.70	0.57
1:C:688:MET:HE3	1:C:755:ALA:HB1	1.87	0.56
1:C:722:ASP:HA	1:C:726:LEU:HD22	1.88	0.56
1:D:741:CYS:HB3	1:D:781:ASP:HA	1.88	0.56
1:D:725:MET:HB2	1:D:812:GLN:HA	1.87	0.55
1:C:715:TYR:O	1:C:718:SER:OG	2.24	0.55
1:C:724:SER:O	1:C:727:VAL:HG12	2.07	0.54
1:D:727:VAL:O	1:D:731:THR:HG23	2.08	0.54
1:D:802:LYS:HG3	1:D:808:TRP:CE2	2.44	0.53
1:D:783:SER:OG	1:D:783:SER:O	2.27	0.52
2:H:268:MET:CE	2:H:271:ARG:NH2	2.73	0.52
1:A:727:VAL:O	1:A:731:THR:HG23	2.10	0.52
1:C:744:ARG:NH2	1:D:745:PHE:O	2.37	0.52
1:C:777:ALA:HB3	1:C:790:TYR:CE2	2.46	0.51
1:D:765:GLU:OE1	1:D:802:LYS:HD3	2.11	0.51
1:A:779:LEU:O	1:A:787:ASN:HB3	2.11	0.51
1:A:786:LYS:HG3	1:A:787:ASN:H	1.77	0.50
1:B:747:LEU:HD11	1:B:773:LEU:HD22	1.92	0.50
1:C:750:LEU:HD13	1:C:773:LEU:CD2	2.42	0.50
1:B:691:GLU:O	1:B:695:GLU:HB2	2.12	0.50
2:G:268:MET:O	2:G:271:ARG:HG3	2.12	0.49
1:D:802:LYS:HG3	1:D:808:TRP:CD2	2.48	0.49
1:A:700:TRP:CZ3	1:A:721:LEU:HD11	2.48	0.49
1:B:779:LEU:O	1:B:787:ASN:HB3	2.13	0.49
1:D:715:TYR:HD1	1:D:716:SER:CA	2.26	0.49
2:G:268:MET:HE2	2:G:271:ARG:NH2	2.28	0.48
1:C:711:THR:HG23	1:C:713:GLN:HG3	1.95	0.47
1:C:721:LEU:HD23	1:C:810:PHE:HB2	1.96	0.47
1:C:686:ARG:HD3	1:C:687:PRO:O	2.14	0.47
2:G:264:HIS:CG	2:G:265:LEU:N	2.81	0.47
1:B:789:LYS:HE3	1:B:789:LYS:HB2	1.66	0.47
1:D:697:VAL:HG12	1:D:750:LEU:HD11	1.96	0.47
1:A:686:ARG:O	1:A:757:ILE:N	2.47	0.46
1:A:701:GLU:OE1	2:E:272:GLY:OXT	2.34	0.46
1:B:722:ASP:OD1	1:B:723:GLU:N	2.47	0.45
1:C:790:TYR:HD2	2:G:267:VAL:HG22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:817:ILE:HD12	2:G:271:ARG:HH12	1.80	0.45
1:A:720:VAL:HG23	1:A:721:LEU:HG	1.98	0.45
1:A:781:ASP:OD2	1:A:782:GLU:N	2.50	0.45
1:C:807:LEU:HD22	1:C:809:LYS:NZ	2.31	0.45
1:B:710:PRO:HG2	1:A:710:PRO:HG2	1.99	0.44
1:C:790:TYR:CD2	2:G:267:VAL:HG22	2.53	0.44
1:A:686:ARG:HG3	1:A:687:PRO:N	2.32	0.44
1:B:698:ARG:HD3	1:A:786:LYS:CG	2.48	0.44
1:D:716:SER:HA	1:D:719:GLU:HG2	1.97	0.44
1:B:748:LEU:HB2	1:B:774:GLU:HG2	2.00	0.44
1:D:807:LEU:HA	1:D:807:LEU:HD23	1.84	0.44
1:B:743:TRP:HB3	1:B:745:PHE:CE2	2.53	0.44
1:B:777:ALA:HB3	1:B:790:TYR:CE2	2.53	0.43
1:D:715:TYR:HD1	1:D:716:SER:OG	1.90	0.43
1:B:715:TYR:O	1:B:718:SER:OG	2.36	0.42
1:B:698:ARG:HD3	1:A:786:LYS:CB	2.49	0.42
1:C:700:TRP:CZ3	1:C:721:LEU:HD11	2.54	0.42
1:B:789:LYS:NZ	1:A:748:LEU:O	2.45	0.42
1:D:777:ALA:HB3	1:D:790:TYR:CE2	2.54	0.42
1:C:720:VAL:O	1:C:810:PHE:N	2.52	0.42
1:B:700:TRP:CZ3	1:B:721:LEU:HD11	2.55	0.41
1:B:686:ARG:HG3	1:B:687:PRO:HD2	2.02	0.41
1:D:694:GLU:HG2	1:D:752:VAL:HG23	2.01	0.41
1:C:803:GLN:HB2	1:C:805:ASP:OD1	2.21	0.41
1:A:786:LYS:HD3	1:A:786:LYS:HA	1.69	0.41
1:D:743:TRP:HB3	1:D:745:PHE:CE2	2.56	0.40
1:A:774:GLU:HB2	1:A:793:THR:HG23	2.02	0.40
1:C:720:VAL:HG23	1:C:721:LEU:HG	2.03	0.40
1:B:786:LYS:HE3	1:A:698:ARG:HD3	2.03	0.40
1:A:735:THR:HG22	1:A:739:LYS:HD2	2.03	0.40
2:G:268:MET:HE2	2:G:271:ARG:HH21	1.80	0.40

There are no symmetry-related clashes.

## 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	126/149 (85%)	124 (98%)	2 (2%)	0	100	100
1	B	131/149 (88%)	128 (98%)	3 (2%)	0	100	100
1	C	131/149 (88%)	129 (98%)	2 (2%)	0	100	100
1	D	125/149 (84%)	120 (96%)	4 (3%)	1 (1%)	19	51
2	E	7/10 (70%)	7 (100%)	0	0	100	100
2	F	7/10 (70%)	7 (100%)	0	0	100	100
2	G	7/10 (70%)	7 (100%)	0	0	100	100
2	H	8/10 (80%)	8 (100%)	0	0	100	100
All	All	542/636 (85%)	530 (98%)	11 (2%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	724	SER

### 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	114/130 (88%)	111 (97%)	3 (3%)	46	77
1	B	115/130 (88%)	111 (96%)	4 (4%)	36	70
1	C	115/130 (88%)	112 (97%)	3 (3%)	46	77
1	D	111/130 (85%)	108 (97%)	3 (3%)	44	77
2	E	7/8 (88%)	7 (100%)	0	100	100
2	F	7/8 (88%)	7 (100%)	0	100	100
2	G	7/8 (88%)	7 (100%)	0	100	100
2	H	8/8 (100%)	8 (100%)	0	100	100
All	All	484/552 (88%)	471 (97%)	13 (3%)	44	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	686	ARG
1	C	716	SER
1	C	743	TRP
1	B	743	TRP
1	B	775	GLU
1	B	786	LYS
1	B	808	TRP
1	D	715	TYR
1	D	743	TRP
1	D	814	ASP
1	A	686	ARG
1	A	743	TRP
1	A	775	GLU

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

Mol	Chain	Res	Type
1	C	713	GLN
1	B	816	GLN
1	D	812	GLN
2	F	264	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.



## 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, 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	130/149 (87%)	0.40	5 (3%) 40 36	27, 41, 79, 96	0
1	B	134/149 (89%)	0.37	5 (3%) 41 37	25, 41, 71, 88	0
1	C	133/149 (89%)	0.30	3 (2%) 60 58	25, 43, 72, 96	0
1	D	129/149 (86%)	0.59	12 (9%) 8 6	29, 47, 80, 109	0
2	E	9/10 (90%)	0.58	1 (11%) 5 4	32, 38, 52, 84	0
2	F	9/10 (90%)	1.15	1 (11%) 5 4	29, 42, 59, 90	0
2	G	9/10 (90%)	0.69	1 (11%) 5 4	31, 36, 49, 74	0
2	H	10/10 (100%)	0.62	1 (10%) 7 5	38, 46, 80, 85	0
All	All	563/636 (88%)	0.43	29 (5%) 27 23	25, 43, 75, 109	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	264	HIS	5.3
1	A	783	SER	4.1
1	D	760	ASP	3.8
1	B	785	PRO	3.7
1	B	682	GLN	3.4
1	A	686	ARG	3.1
2	G	264	HIS	3.1
1	D	781	ASP	3.0
2	E	264	HIS	3.0
1	D	715	TYR	3.0
1	C	686	ARG	2.8
1	D	758	PHE	2.8
1	D	723	GLU	2.8
1	C	817	ILE	2.7
1	B	782	GLU	2.7
1	B	783	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	265	LEU	2.5
1	D	755	ALA	2.3
1	D	753	LEU	2.3
1	D	782	GLU	2.3
1	D	784	GLN	2.3
1	D	788	ALA	2.2
1	D	764	GLY	2.2
1	B	781	ASP	2.2
1	A	817	ILE	2.1
1	D	688	MET	2.1
1	C	761	GLY	2.0
1	A	785	PRO	2.0
1	A	781	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.