



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 06:09 PM JST

PDB ID : 8XAI  
Title : Crystal structure of Protease CPAVM1 in Bacillus subtilis LjM2  
Authors : Zhang, J.; Wang, C.Y.  
Deposited on : 2023-12-04  
Resolution : 1.83 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36.2  
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) : 2.36.2

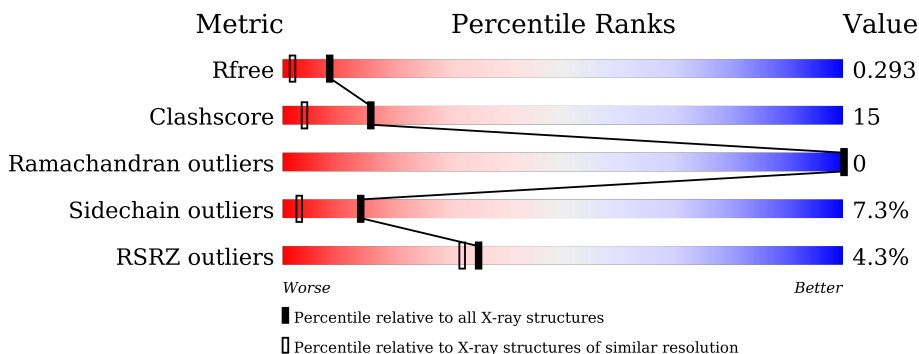
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	236	 4% 62% 22% • 14%
1	B	236	 3% 61% 20% • 14%
1	C	236	 4% 61% 22% •• 14%
1	D	236	 3% 56% 25% • 17%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6461 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 Lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	204	1544	969	263	311	1	0	1	0
1	B	202	1539	967	261	310	1	3	3	0
1	C	204	1550	973	263	313	1	0	3	0
1	D	197	1498	942	255	300	1	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	initiating methionine	UNP A0A6A8FLP5
A	40	ALA	VAL	conflict	UNP A0A6A8FLP5
B	16	MET	-	initiating methionine	UNP A0A6A8FLP5
B	40	ALA	VAL	conflict	UNP A0A6A8FLP5
C	16	MET	-	initiating methionine	UNP A0A6A8FLP5
C	40	ALA	VAL	conflict	UNP A0A6A8FLP5
D	16	MET	-	initiating methionine	UNP A0A6A8FLP5
D	40	ALA	VAL	conflict	UNP A0A6A8FLP5

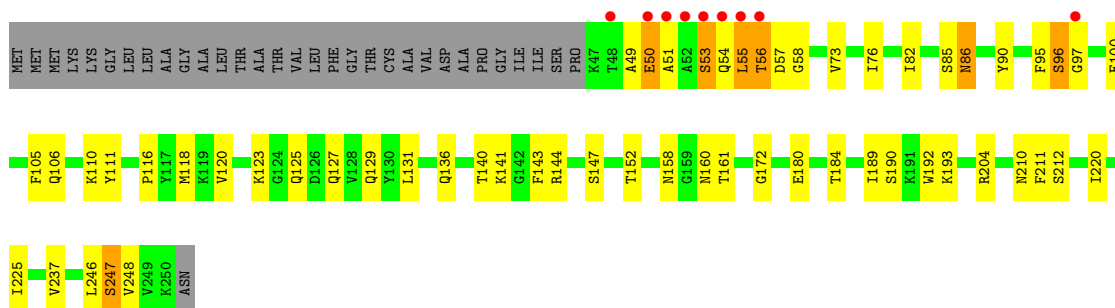
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		
2	B	81	Total	O	0	0
			81	81		
2	C	88	Total	O	0	0
			88	88		
2	D	87	Total	O	0	0
			87	87		

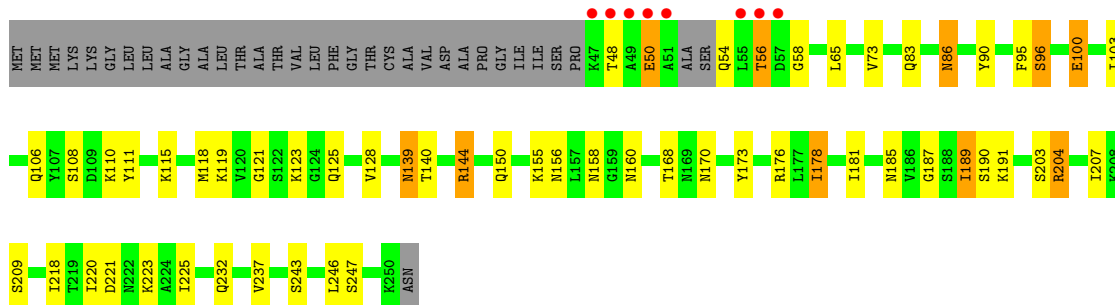
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

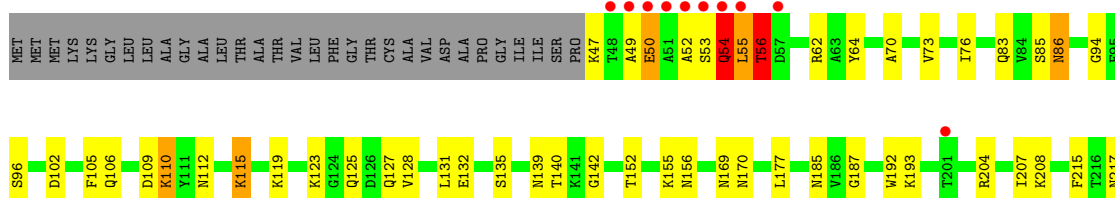
- Molecule 1: Lipoprotein

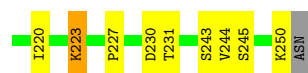


- Molecule 1: Lipoprotein

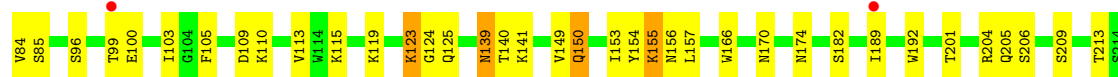
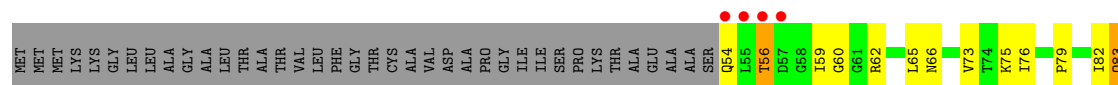


- Molecule 1: Lipoprotein





- Molecule 1: Lipoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.57Å 66.87Å 75.61Å 98.83° 90.16° 100.72°	Depositor
Resolution (Å)	37.87 – 1.83 37.87 – 1.83	Depositor EDS
% Data completeness (in resolution range)	95.0 (37.87-1.83) 95.0 (37.87-1.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 1.83Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.244 , 0.293 0.246 , 0.293	Depositor DCC
$R_{free}$ test set	3082 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtrriage
Anisotropy	0.284	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% 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 i

### 5.1 Standard geometry i

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	0.55	0/1574	0.85	4/2132 (0.2%)
1	B	0.54	1/1574 (0.1%)	0.80	3/2130 (0.1%)
1	C	0.55	0/1586	0.97	9/2148 (0.4%)
1	D	0.50	0/1528	0.89	7/2070 (0.3%)
All	All	0.54	1/6262 (0.0%)	0.88	23/8480 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	GLU	CD-OE2	-5.23	1.19	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	GLN	N-CA-CB	-11.02	90.77	110.60
1	A	54	GLN	N-CA-CB	-10.92	90.94	110.60
1	D	215	PHE	CB-CA-C	-10.78	88.85	110.40
1	C	53	SER	N-CA-C	-10.52	82.58	111.00
1	C	56	THR	N-CA-C	-10.26	83.29	111.00
1	D	99	THR	N-CA-C	9.76	137.35	111.00
1	C	54	GLN	N-CA-C	9.41	136.41	111.00
1	C	55	LEU	N-CA-C	-7.71	90.19	111.00
1	C	55	LEU	CB-CA-C	7.15	123.78	110.20
1	D	216	THR	N-CA-CB	-6.65	97.67	110.30
1	D	224	ALA	N-CA-CB	-6.60	100.86	110.10
1	A	54	GLN	N-CA-C	6.44	128.38	111.00
1	A	53	SER	N-CA-C	-6.36	93.83	111.00
1	C	243	SER	N-CA-CB	6.21	119.82	110.50
1	B	139	ASN	CB-CA-C	-6.20	98.00	110.40
1	D	99	THR	CB-CA-C	-6.18	94.92	111.60
1	B	139	ASN	N-CA-C	6.06	127.36	111.00
1	D	215	PHE	N-CA-C	-5.89	95.09	111.00
1	D	56	THR	N-CA-C	-5.85	95.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ASN	CB-CA-C	5.77	121.93	110.40
1	C	86	ASN	CB-CA-C	5.43	121.27	110.40
1	C	56	THR	N-CA-CB	5.07	119.93	110.30
1	B	140	THR	N-CA-CB	5.07	119.93	110.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	1544	0	1530	41	1
1	B	1539	0	1529	39	1
1	C	1550	0	1540	50	0
1	D	1498	0	1484	52	0
2	A	74	0	0	8	2
2	B	81	0	0	12	2
2	C	88	0	0	13	0
2	D	87	0	0	25	1
All	All	6461	0	6083	179	4

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 15.

All (179) 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:50:GLU:HG3	1:A:193:LYS:NZ	1.41	1.33
1:D:233:ASP:OD2	2:D:301:HOH:O	1.82	0.98
1:A:50:GLU:CG	1:A:193:LYS:NZ	2.30	0.94
1:D:205:GLN:NE2	2:D:302:HOH:O	2.00	0.94
1:C:83:GLN:NE2	1:C:85:SER:OG	2.01	0.93
1:A:50:GLU:HG3	1:A:193:LYS:HZ2	0.95	0.91
1:D:125:GLN:NE2	2:D:306:HOH:O	2.06	0.86
1:B:139:ASN:O	2:B:301:HOH:O	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:HB2	1:A:189:ILE:HG12	1.60	0.84
1:B:150:GLN:NE2	2:B:302:HOH:O	2.13	0.81
1:A:50:GLU:CG	1:A:193:LYS:HZ2	1.88	0.81
1:A:50:GLU:HG3	1:A:193:LYS:HZ3	1.42	0.80
1:C:170:ASN:ND2	2:C:307:HOH:O	2.15	0.79
1:C:250:LYS:O	2:C:302:HOH:O	2.00	0.78
1:A:136:GLN:OE1	2:A:301:HOH:O	2.01	0.77
1:C:110:LYS:HD2	1:C:110:LYS:H	1.47	0.77
1:C:125:GLN:NE2	2:C:308:HOH:O	2.17	0.77
1:D:236:LYS:HE2	1:D:238:THR:HG23	1.67	0.76
1:C:125:GLN:NE2	2:C:309:HOH:O	2.19	0.76
1:D:109:ASP:O	2:D:304:HOH:O	2.03	0.76
1:B:220:ILE:HD12	1:B:225:ILE:HG13	1.66	0.75
1:D:113:VAL:O	2:D:303:HOH:O	2.02	0.75
1:D:66:ASN:O	2:D:305:HOH:O	2.05	0.75
1:D:154:TYR:HB3	2:D:321:HOH:O	1.86	0.74
1:D:219:THR:HA	1:D:224:ALA:HA	1.68	0.74
1:D:232:GLN:NE2	2:D:309:HOH:O	2.19	0.73
1:D:219:THR:HB	1:D:223:LYS:O	1.89	0.73
1:C:155:LYS:NZ	1:C:187:GLY:O	2.22	0.72
1:D:115:LYS:NZ	2:D:312:HOH:O	2.23	0.72
1:C:131:LEU:O	2:C:304:HOH:O	2.08	0.71
1:C:125:GLN:O	1:C:128:VAL:HG12	1.93	0.69
1:A:51:ALA:HB2	1:A:100:GLU:OE1	1.94	0.67
1:A:97:GLY:HA3	1:A:190[B]:SER:OG	1.94	0.67
1:C:140:THR:HG21	1:D:157:LEU:HD11	1.77	0.67
1:D:83:GLN:O	2:D:307:HOH:O	2.12	0.66
1:B:160:ASN:HA	2:B:310:HOH:O	1.94	0.66
1:D:96:SER:HA	1:D:100:GLU:OE1	1.95	0.66
1:C:208:LYS:NZ	2:C:302:HOH:O	2.27	0.66
1:A:50:GLU:CG	1:A:193:LYS:HZ3	2.03	0.66
1:D:239:VAL:HG12	2:D:317:HOH:O	1.94	0.65
1:C:109:ASP:OD1	2:C:306:HOH:O	2.14	0.65
1:B:95:PHE:HB2	1:B:189:ILE:HG13	1.80	0.64
1:A:131:LEU:HD11	1:A:180:GLU:OE1	1.98	0.64
1:B:50:GLU:H	1:B:50:GLU:CD	2.00	0.63
1:D:125:GLN:HG3	2:D:316:HOH:O	1.97	0.63
1:D:250:LYS:HE2	2:D:302:HOH:O	1.97	0.62
1:C:49:ALA:O	1:C:62:ARG:NH1	2.33	0.62
1:A:95:PHE:HB2	1:A:189:ILE:CG1	2.28	0.61
1:D:54:GLN:OE1	1:D:56:THR:OG1	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLU:OE1	1:B:50:GLU:N	2.32	0.59
1:A:49:ALA:HB2	1:A:55:LEU:H	1.68	0.58
1:B:203:SER:N	2:B:305:HOH:O	2.22	0.58
1:A:96:SER:N	1:A:189:ILE:HD11	2.18	0.58
1:B:144:ARG:HD3	2:B:314:HOH:O	2.02	0.58
1:B:176:ARG:HD3	1:B:178:ILE:HD11	1.87	0.57
1:D:115:LYS:N	2:D:303:HOH:O	2.29	0.57
1:C:85:SER:HB2	1:C:208:LYS:HB2	1.86	0.57
1:D:110:LYS:O	2:D:308:HOH:O	2.17	0.57
1:A:118:MET:H	1:A:125:GLN:HE21	1.51	0.56
1:B:158:ASN:HA	2:B:342:HOH:O	2.05	0.56
1:A:76:ILE:HD12	1:A:105:PHE:HE2	1.71	0.56
1:C:110:LYS:HD3	2:C:321:HOH:O	2.06	0.56
1:B:110:LYS:HE3	1:B:111:TYR:CE1	2.42	0.55
1:C:155:LYS:HE2	2:C:315:HOH:O	2.06	0.55
1:D:150:GLN:HB3	1:D:166:TRP:HB3	1.89	0.55
1:C:50:GLU:OE1	1:C:193:LYS:NZ	2.40	0.55
1:D:209:SER:HB2	2:D:307:HOH:O	2.06	0.54
1:A:110:LYS:HE3	1:A:111:TYR:CE1	2.43	0.53
1:A:116:PRO:HG3	1:A:143:PHE:HE2	1.73	0.53
1:B:96:SER:OG	1:B:190[B]:SER:OG	2.26	0.53
1:C:54:GLN:O	1:C:55:LEU:C	2.47	0.52
1:A:118:MET:H	1:A:125:GLN:NE2	2.07	0.52
1:D:76:ILE:HD13	1:D:105:PHE:HE2	1.75	0.52
1:B:108:SER:HB2	1:B:115:LYS:HZ2	1.75	0.52
1:B:58:GLY:O	1:B:204:ARG:HD2	2.11	0.51
1:C:50:GLU:HG2	1:C:102:ASP:OD1	2.10	0.51
1:B:204:ARG:HA	1:B:207:ILE:HG13	1.92	0.51
1:C:47:LYS:HD3	1:C:55:LEU:HD23	1.93	0.51
1:D:225:ILE:HD11	2:D:305:HOH:O	2.10	0.50
1:B:103:ILE:HG12	1:B:118:MET:HG3	1.93	0.49
1:C:119:LYS:HD2	1:C:123:LYS:O	2.12	0.49
1:B:73:VAL:HG11	2:B:302:HOH:O	2.12	0.49
1:B:144:ARG:NH1	2:B:314:HOH:O	2.45	0.49
1:D:156:ASN:N	2:D:321:HOH:O	2.46	0.49
1:C:217:ASN:ND2	2:C:313:HOH:O	2.31	0.48
1:D:219:THR:CB	1:D:223:LYS:O	2.61	0.48
1:B:125:GLN:O	1:B:128:VAL:HG12	2.12	0.48
1:C:215:PHE:HB2	1:C:244:VAL:HG12	1.95	0.48
1:C:49:ALA:HB3	1:C:56:THR:HG23	1.95	0.48
1:C:227:PRO:HG2	1:C:244:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:HB	2:D:307:HOH:O	2.14	0.48
1:B:118:MET:HG2	1:B:181:ILE:CD1	2.44	0.47
1:B:118:MET:HG2	1:B:181:ILE:HD12	1.95	0.47
1:A:144:ARG:HG3	1:A:147:SER:HB3	1.95	0.47
1:B:50:GLU:HG2	1:B:100:GLU:OE1	2.14	0.47
1:D:65:LEU:HB2	1:D:192:TRP:HB2	1.95	0.47
1:B:155:LYS:HG3	1:B:156:ASN:N	2.29	0.47
1:D:241:GLY:N	2:D:317:HOH:O	2.41	0.47
1:A:237:VAL:HG22	1:A:246:LEU:HD23	1.96	0.47
1:C:70:ALA:HA	1:C:155:LYS:HG2	1.96	0.47
1:C:76:ILE:HD12	1:C:105:PHE:HE2	1.79	0.47
1:D:79:PRO:HD3	1:D:213:THR:HB	1.97	0.47
1:D:100:GLU:OE1	1:D:100:GLU:HA	2.15	0.47
1:C:217:ASN:HB2	2:C:313:HOH:O	2.14	0.46
1:C:127:GLN:HG2	1:D:174:ASN:O	2.16	0.46
1:C:170:ASN:N	1:C:170:ASN:OD1	2.48	0.46
1:A:120:VAL:HG21	1:A:161:THR:HG21	1.97	0.46
1:C:142:GLY:O	1:C:169:ASN:HA	2.16	0.46
1:B:155:LYS:NZ	1:B:187:GLY:O	2.44	0.46
1:B:158:ASN:HA	2:B:336:HOH:O	2.14	0.46
1:D:155:LYS:HG3	1:D:156:ASN:N	2.30	0.46
1:B:86:ASN:HB3	2:B:324:HOH:O	2.16	0.45
1:D:221:ASP:OD2	2:D:310:HOH:O	2.21	0.45
1:A:73:VAL:HG22	1:A:152:THR:HG23	1.98	0.45
1:A:158:ASN:ND2	2:A:303:HOH:O	2.21	0.45
1:B:185:ASN:OD1	2:B:303:HOH:O	2.21	0.45
1:B:243:SER:OG	2:B:304:HOH:O	2.21	0.45
1:D:238:THR:OG1	1:D:245:SER:HB2	2.16	0.45
1:C:132:GLU:O	1:C:177:LEU:HD12	2.17	0.45
1:A:82:ILE:HD12	1:A:211:PHE:CG	2.52	0.45
1:A:172:GLY:HA3	1:C:185:ASN:OD1	2.17	0.45
1:B:168:THR:HA	1:B:173:TYR:O	2.16	0.45
1:C:73:VAL:HG22	1:C:152:THR:HG23	1.99	0.45
1:B:56:THR:C	1:B:58:GLY:H	2.19	0.45
1:C:230:ASP:OD2	1:C:231:THR:HG23	2.17	0.45
1:D:123:LYS:HG3	2:D:339:HOH:O	2.17	0.45
1:A:210:ASN:HA	1:A:248:VAL:O	2.16	0.44
1:C:83:GLN:HE22	1:C:85:SER:HG	1.51	0.44
1:B:65:LEU:HD22	1:B:218:ILE:HG21	1.98	0.44
1:A:141:LYS:HD3	2:A:328:HOH:O	2.16	0.44
1:D:219:THR:CA	1:D:223:LYS:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:GLN:O	1:B:209:SER:HA	2.18	0.44
1:D:65:LEU:HB3	1:D:225:ILE:HG21	1.99	0.44
1:A:184:THR:HG23	2:A:305:HOH:O	2.17	0.44
1:A:192:TRP:CE2	2:A:307:HOH:O	2.70	0.43
1:C:110:LYS:HD2	1:C:110:LYS:N	2.26	0.43
1:C:110:LYS:H	1:C:110:LYS:CD	2.14	0.43
1:C:86:ASN:HB3	1:C:207:ILE:HA	1.99	0.43
1:C:54:GLN:O	1:C:56:THR:N	2.52	0.43
1:C:50:GLU:H	1:C:50:GLU:HG3	1.23	0.43
1:C:192:TRP:CD1	1:C:220:ILE:HD13	2.53	0.43
1:C:110:LYS:CD	2:C:321:HOH:O	2.65	0.43
1:A:51:ALA:CB	1:A:100:GLU:OE1	2.65	0.43
1:A:204:ARG:NH2	2:A:309:HOH:O	2.51	0.43
1:C:128:VAL:O	1:C:128:VAL:HG13	2.19	0.43
1:D:219:THR:HA	1:D:223:LYS:O	2.19	0.43
1:A:56:THR:O	1:A:58:GLY:N	2.48	0.42
1:B:221:ASP:O	1:B:223:LYS:HE2	2.19	0.42
1:C:94:GLY:O	1:C:193:LYS:HG2	2.18	0.42
1:D:170:ASN:OD1	2:D:311:HOH:O	2.22	0.42
1:C:155:LYS:HG3	1:C:156:ASN:N	2.34	0.42
1:D:59:ILE:HG21	1:D:250:LYS:HD2	2.01	0.42
1:A:90:TYR:CE2	1:A:106:GLN:HB2	2.54	0.42
1:B:119:LYS:HE2	1:B:121:GLY:O	2.19	0.42
1:D:60:GLY:N	1:D:233:ASP:O	2.50	0.42
1:D:115:LYS:HD3	1:D:141:LYS:O	2.19	0.42
1:A:111:TYR:CE1	1:A:140:THR:HG23	2.55	0.42
1:A:160:ASN:HA	2:A:305:HOH:O	2.20	0.41
1:D:103:ILE:HD12	1:D:153:ILE:HG21	2.01	0.41
1:A:212:SER:HB3	1:A:247:SER:HB2	2.01	0.41
1:B:237:VAL:HG22	1:B:246:LEU:HD23	2.02	0.41
1:C:52:ALA:HB2	1:C:64:TYR:OH	2.20	0.41
1:D:115:LYS:HG2	2:D:303:HOH:O	2.21	0.41
1:D:139:ASN:HB2	1:D:140:THR:H	1.62	0.41
1:A:220:ILE:HD12	1:A:225:ILE:HG13	2.02	0.41
1:D:75:LYS:HA	1:D:150:GLN:HA	2.02	0.41
1:A:129:GLN:NE2	1:A:131:LEU:HD21	2.36	0.41
1:C:135:SER:OG	2:C:301:HOH:O	1.81	0.41
1:D:82:ILE:HG21	2:D:342:HOH:O	2.21	0.41
1:D:119:LYS:HD2	1:D:124:GLY:HA2	2.03	0.41
1:A:189:ILE:HA	1:A:189:ILE:HD12	1.74	0.41
1:C:115:LYS:HE3	1:C:139:ASN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ILE:HB	1:D:233:ASP:O	2.21	0.40
1:B:232:GLN:HG2	1:B:237:VAL:HG23	2.02	0.40
1:C:223:LYS:HA	1:C:223:LYS:HD2	1.93	0.40
1:A:118:MET:HG2	2:A:350:HOH:O	2.21	0.40
1:B:90:TYR:CE1	1:B:106:GLN:HB2	2.57	0.40
1:D:189:ILE:HD13	1:D:189:ILE:HA	1.83	0.40

All (4) 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:A:127:GLN:NE2	1:B:173:TYR:OH[1_655]	1.99	0.21
2:B:308:HOH:O	2:B:365:HOH:O[1_455]	2.12	0.08
2:A:319:HOH:O	2:D:366:HOH:O[1_655]	2.17	0.03
2:A:308:HOH:O	2:B:352:HOH:O[1_665]	2.18	0.02

## 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	203/236 (86%)	193 (95%)	10 (5%)	0	100	100
1	B	201/236 (85%)	189 (94%)	12 (6%)	0	100	100
1	C	205/236 (87%)	189 (92%)	16 (8%)	0	100	100
1	D	196/236 (83%)	182 (93%)	14 (7%)	0	100	100
All	All	805/944 (85%)	753 (94%)	52 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	170/192 (88%)	160 (94%)	10 (6%)	19	5
1	B	171/192 (89%)	157 (92%)	14 (8%)	11	2
1	C	172/192 (90%)	161 (94%)	11 (6%)	17	4
1	D	166/192 (86%)	152 (92%)	14 (8%)	11	2
All	All	679/768 (88%)	630 (93%)	49 (7%)	14	3

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	53	SER
1	A	55	LEU
1	A	56	THR
1	A	57	ASP
1	A	85	SER
1	A	86	ASN
1	A	96	SER
1	A	123	LYS
1	A	247	SER
1	B	48	THR
1	B	50	GLU
1	B	54	GLN
1	B	56	THR
1	B	86	ASN
1	B	96	SER
1	B	123	LYS
1	B	144	ARG
1	B	170	ASN
1	B	178	ILE
1	B	189	ILE
1	B	191	LYS
1	B	204	ARG
1	B	247	SER

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Mol	Chain	Res	Type
1	C	50	GLU
1	C	54	GLN
1	C	56	THR
1	C	96	SER
1	C	106	GLN
1	C	110	LYS
1	C	112	ASN
1	C	115	LYS
1	C	204	ARG
1	C	223	LYS
1	C	245	SER
1	D	62	ARG
1	D	73	VAL
1	D	83	GLN
1	D	85	SER
1	D	123	LYS
1	D	139	ASN
1	D	149	VAL
1	D	150	GLN
1	D	155	LYS
1	D	182	SER
1	D	201	THR
1	D	204	ARG
1	D	206	SER
1	D	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	136	GLN
1	B	106	GLN
1	B	150	GLN
1	B	174	ASN
1	B	185	ASN
1	C	83	GLN
1	C	106	GLN
1	C	150	GLN
1	D	139	ASN
1	D	170	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 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	204/236 (86%)	0.21	9 (4%) 34 31	10, 15, 34, 50	0
1	B	202/236 (85%)	0.19	8 (3%) 38 35	11, 15, 30, 58	0
1	C	204/236 (86%)	0.17	10 (4%) 29 27	12, 16, 36, 51	0
1	D	197/236 (83%)	0.20	8 (4%) 37 34	13, 18, 34, 55	0
All	All	807/944 (85%)	0.19	35 (4%) 35 32	10, 16, 35, 58	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	ALA	9.1
1	B	55	LEU	7.7
1	C	53	SER	7.4
1	B	48	THR	6.5
1	A	55	LEU	6.5
1	D	56	THR	6.1
1	C	54	GLN	5.9
1	C	55	LEU	5.7
1	A	52	ALA	5.3
1	D	55	LEU	5.1
1	B	51	ALA	4.8
1	C	51	ALA	4.7
1	A	48	THR	4.6
1	C	49	ALA	4.5
1	B	56	THR	4.1
1	A	53	SER	3.9
1	A	51	ALA	3.8
1	A	97	GLY	3.7
1	C	52	ALA	3.6
1	B	47	LYS	3.5
1	D	54	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	48	THR	3.1
1	D	224	ALA	3.1
1	A	56	THR	3.1
1	A	50	GLU	3.0
1	B	50	GLU	3.0
1	D	189	ILE	2.6
1	D	223	LYS	2.6
1	C	57	ASP	2.5
1	C	50	GLU	2.4
1	B	57	ASP	2.4
1	D	99	THR	2.3
1	D	57	ASP	2.3
1	A	54	GLN	2.3
1	C	201	THR	2.2

## 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 monosaccharides 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.