



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2016 – 01:25 PM EDT

PDB ID : 5EHD  
Title : Crystal structure of human nucleophosmin-core in complex with cytochrome c  
Authors : Bernardo-Garcia, N.; Hermoso, J.A.; Gonzalez-Arzola, K.; Diaz-Moreno, I.;  
De la Rosa, M.A.  
Deposited on : 2015-10-28  
Resolution : 2.55 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

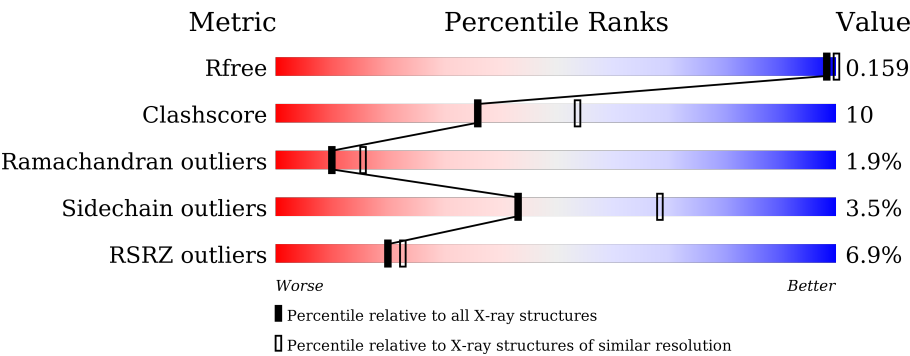
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	116	<div><div>8%</div><div><div></div><div>63%</div><div>25%</div><div>•</div><div>9%</div></div></div>
1	B	116	<div><div>12%</div><div><div></div><div>63%</div><div>24%</div><div>•</div><div>9%</div></div></div>
1	C	116	<div><div>10%</div><div><div></div><div>63%</div><div>27%</div><div>•</div><div>8%</div></div></div>
1	D	116	<div><div>7%</div><div><div></div><div>57%</div><div>33%</div><div>•</div><div>9%</div></div></div>
1	E	116	<div><div>9%</div><div><div></div><div>64%</div><div>26%</div><div>•</div><div>9%</div></div></div>
1	F	116	<div><div>5%</div><div><div></div><div>63%</div><div>28%</div><div>•</div><div>8%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	116	
1	H	116	
1	I	116	
1	J	116	
1	a	116	
1	b	116	
1	c	116	
1	d	116	
1	e	116	
1	f	116	
1	g	116	
1	h	116	
1	i	116	
1	j	116	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16452 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 Nucleophosmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			807	511	137	155	4			
1	B	105	Total	C	N	O	S	0	0	0
			800	506	136	154	4			
1	C	107	Total	C	N	O	S	0	0	0
			818	517	141	156	4			
1	D	105	Total	C	N	O	S	0	0	0
			800	506	136	154	4			
1	E	106	Total	C	N	O	S	0	0	0
			807	511	137	155	4			
1	F	107	Total	C	N	O	S	0	0	0
			818	517	141	156	4			
1	G	106	Total	C	N	O	S	0	0	0
			807	511	137	155	4			
1	H	107	Total	C	N	O	S	0	0	0
			818	517	141	156	4			
1	I	107	Total	C	N	O	S	0	0	0
			818	517	141	156	4			
1	J	107	Total	C	N	O	S	0	0	0
			816	516	138	158	4			
1	a	106	Total	C	N	O	S	0	0	0
			807	511	137	155	4			
1	b	105	Total	C	N	O	S	0	0	0
			800	506	136	154	4			
1	c	106	Total	C	N	O	S	0	0	0
			807	511	137	155	4			
1	d	107	Total	C	N	O	S	0	0	0
			818	517	141	156	4			
1	e	107	Total	C	N	O	S	0	0	0
			818	517	141	156	4			
1	f	106	Total	C	N	O	S	0	0	0
			807	511	137	155	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	g	106	Total	C	N	O	S	0	0	0
			807	511	137	155	4			
1	h	106	Total	C	N	O	S	0	0	0
			811	512	140	155	4			
1	i	107	Total	C	N	O	S	0	0	0
			818	517	141	156	4			
1	j	106	Total	C	N	O	S	0	0	0
			811	512	140	155	4			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cl	0	0
			1	1		
2	b	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	f	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	7	Total	O	0	0
			7	7		
3	C	1	Total	O	0	0
			1	1		
3	D	6	Total	O	0	0
			6	6		
3	E	9	Total	O	0	0
			9	9		
3	F	20	Total	O	0	0
			20	20		
3	G	14	Total	O	0	0
			14	14		
3	H	15	Total	O	0	0
			15	15		
3	I	17	Total	O	0	0
			17	17		

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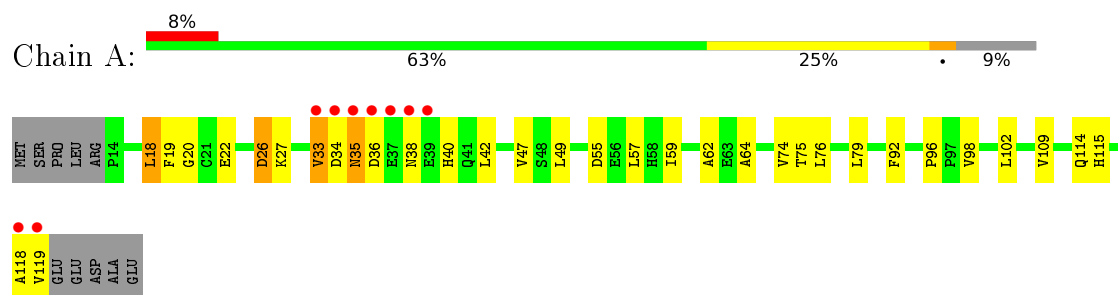
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	12	Total 12	O 12	0	0
3	a	8	Total 8	O 8	0	0
3	b	5	Total 5	O 5	0	0
3	c	8	Total 8	O 8	0	0
3	d	16	Total 16	O 16	0	0
3	e	14	Total 14	O 14	0	0
3	f	12	Total 12	O 12	0	0
3	g	18	Total 18	O 18	0	0
3	h	12	Total 12	O 12	0	0
3	i	16	Total 16	O 16	0	0
3	j	19	Total 19	O 19	0	0

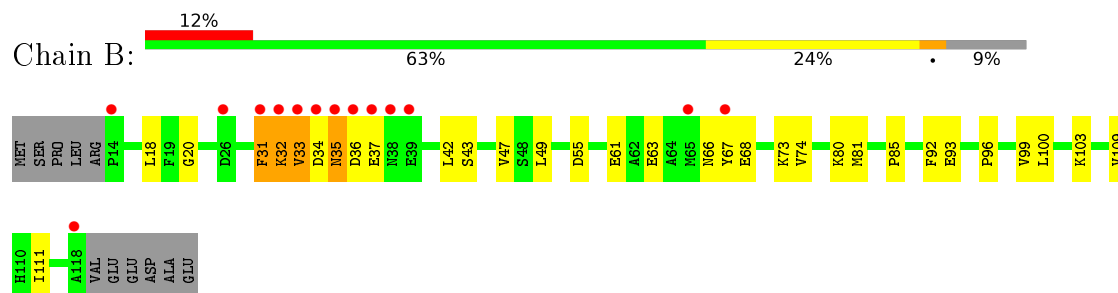
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

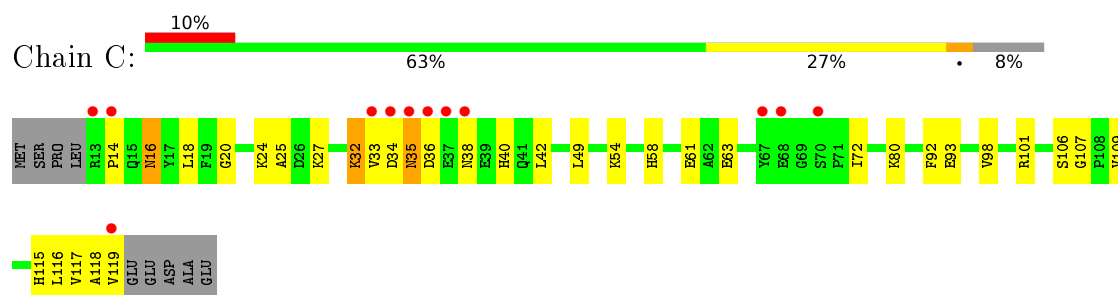
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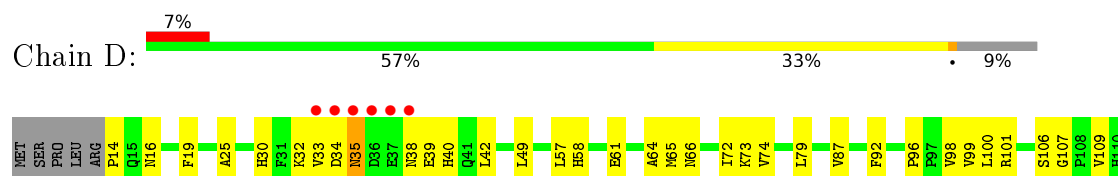
#### • Molecule 1: Nucleophosmin



#### • Molecule 1: Nucleophosmin

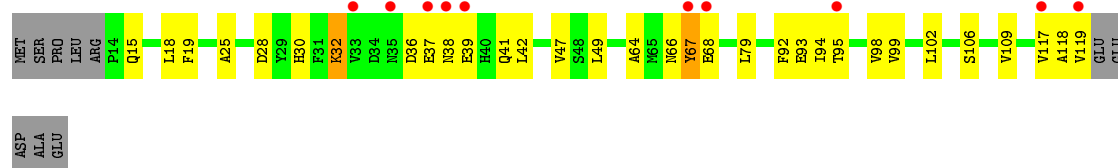


#### • Molecule 1: Nucleophosmin

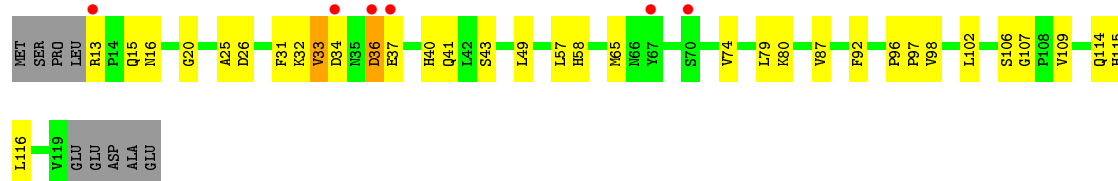




• Molecule 1: Nucleophosmin



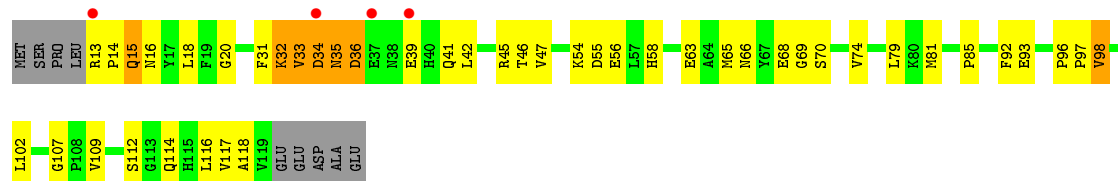
• Molecule 1: Nucleophosmin



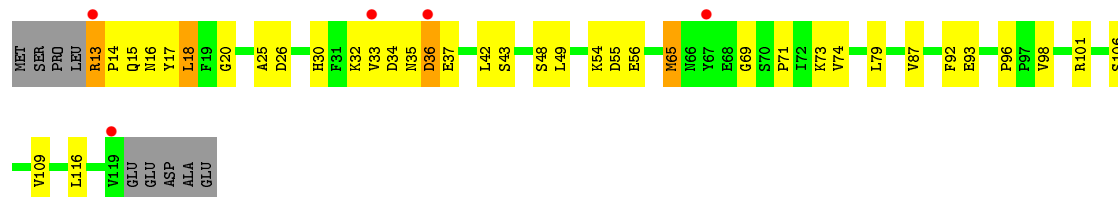
• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin

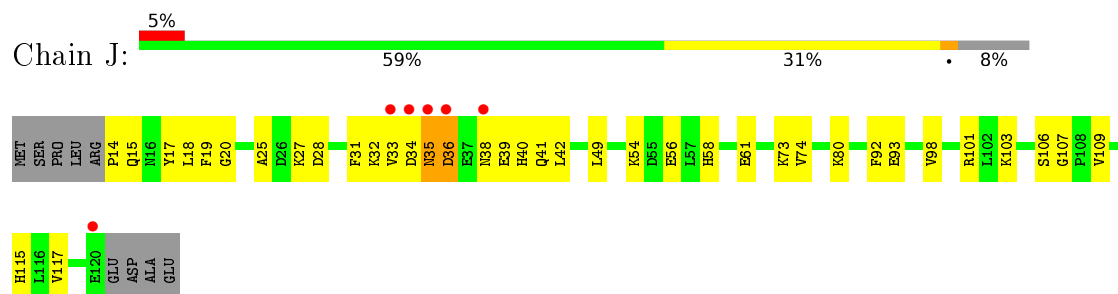


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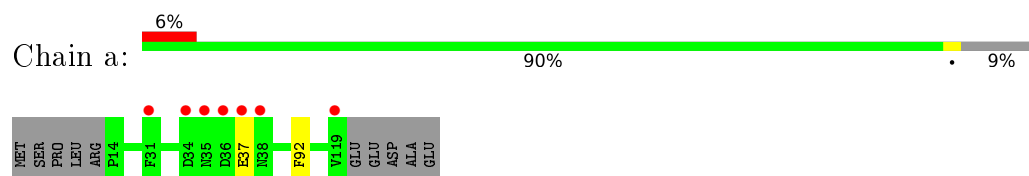




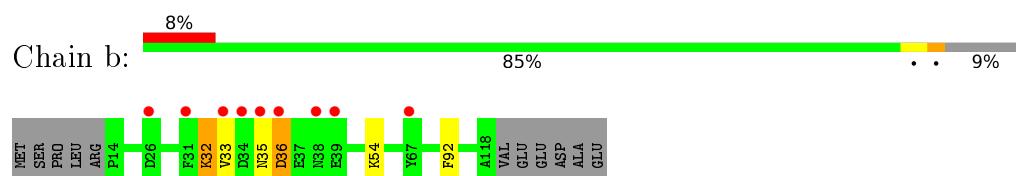
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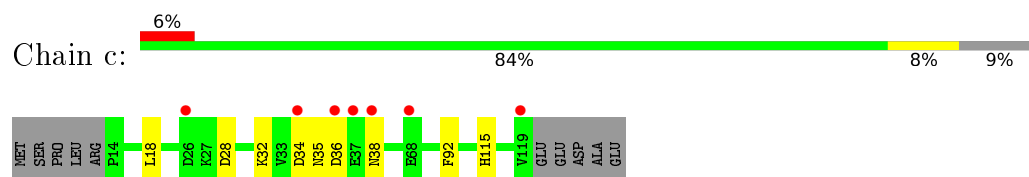
## • Molecule 1: Nucleophosmin



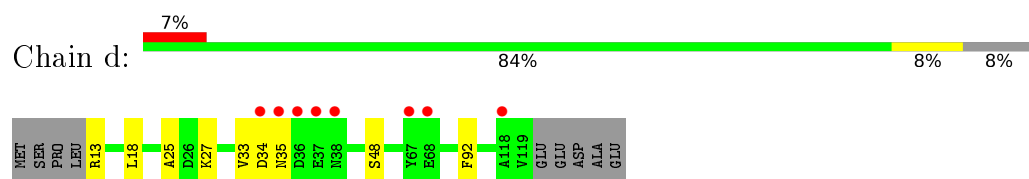
## • Molecule 1: Nucleophosmin



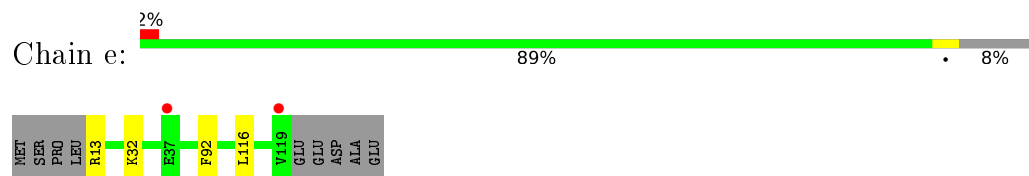
## • Molecule 1: Nucleophosmin



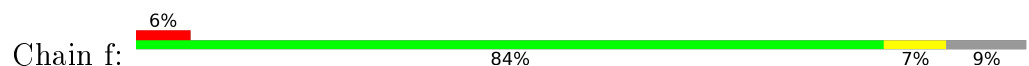
## • Molecule 1: Nucleophosmin

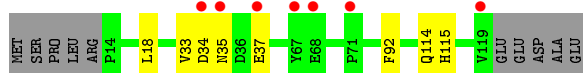


## • Molecule 1: Nucleophosmin

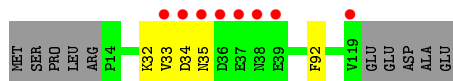
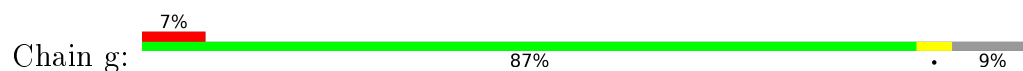


## • Molecule 1: Nucleophosmin

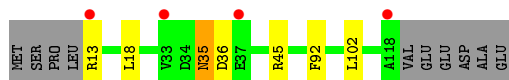
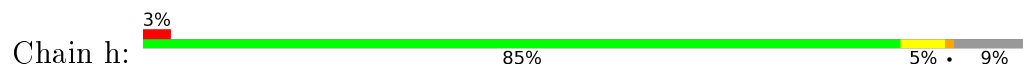




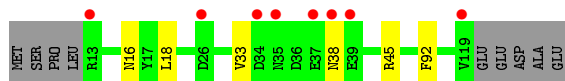
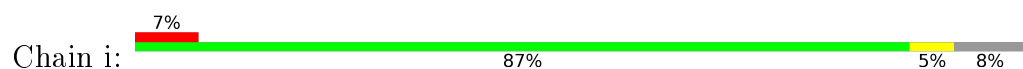
• Molecule 1: Nucleophosmin



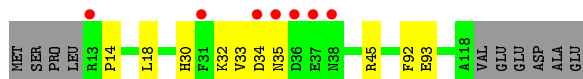
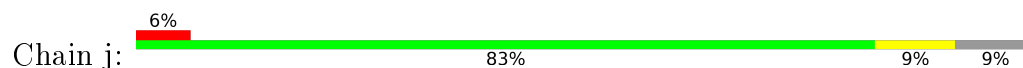
• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin



• Molecule 1: Nucleophosmin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.80Å 179.72Å 104.30Å 90.00° 94.32° 90.00°	Depositor
Resolution (Å)	45.53 – 2.55 45.53 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.53-2.55) 99.6 (45.53-2.55)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.164 , 0.229 0.160 , 0.159	Depositor DCC
$R_{free}$ test set	3426 reflections (4.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
CL

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	0.45	0/823	0.66	0/1115
1	B	0.44	0/816	0.77	1/1105 (0.1%)
1	C	0.42	0/834	0.65	0/1130
1	D	0.41	0/816	0.66	0/1105
1	E	0.52	1/823 (0.1%)	0.76	1/1115 (0.1%)
1	F	0.47	0/834	0.70	0/1130
1	G	0.44	0/823	0.67	0/1115
1	H	0.46	0/834	0.71	0/1130
1	I	0.51	1/834 (0.1%)	0.71	0/1130
1	J	0.53	0/832	0.74	1/1127 (0.1%)
1	a	0.42	0/823	0.65	0/1115
1	b	0.44	0/816	0.72	1/1105 (0.1%)
1	c	0.46	0/823	0.71	0/1115
1	d	0.44	0/834	0.68	0/1130
1	e	0.46	0/834	0.72	1/1130 (0.1%)
1	f	0.44	0/823	0.70	0/1115
1	g	0.44	0/823	0.76	1/1115 (0.1%)
1	h	0.48	0/827	0.71	0/1120
1	i	0.48	0/834	0.76	1/1130 (0.1%)
1	j	0.51	0/827	0.80	2/1120 (0.2%)
All	All	0.46	2/16533 (0.0%)	0.71	9/22397 (0.0%)

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	J	0	1
1	b	0	1
1	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	69	GLY	C-N	-7.22	1.17	1.34
1	E	32	LYS	CD-CE	-6.57	1.34	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	93	GLU	CA-CB-CG	-7.47	96.97	113.40
1	g	32	LYS	C-N-CA	6.43	137.76	121.70
1	b	32	LYS	C-N-CA	5.95	136.57	121.70
1	e	116	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	31	PHE	C-N-CA	5.64	135.80	121.70
1	E	93	GLU	CA-CB-CG	-5.62	101.03	113.40
1	i	45	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	J	103	LYS	CD-CE-NZ	5.21	123.67	111.70
1	j	45	ARG	NE-CZ-NH2	-5.11	117.74	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	35	ASN	Peptide
1	b	32	LYS	Peptide
1	f	35	ASN	Peptide
1	f	37	GLU	Peptide

## 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	807	0	807	26	0
1	B	800	0	798	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	818	0	819	28	0
1	D	800	0	798	33	0
1	E	807	0	807	32	0
1	F	818	0	819	38	0
1	G	807	0	807	35	0
1	H	818	0	819	51	0
1	I	818	0	818	27	0
1	J	816	0	813	28	0
1	a	807	0	807	0	0
1	b	800	0	798	0	0
1	c	807	0	807	0	0
1	d	818	0	819	0	0
1	e	818	0	819	0	0
1	f	807	0	807	0	0
1	g	807	0	807	0	0
1	h	811	0	810	0	0
1	i	818	0	819	0	0
1	j	811	0	810	0	0
2	A	1	0	0	0	0
2	G	1	0	0	0	0
2	b	1	0	0	0	0
2	f	1	0	0	0	0
3	A	6	0	0	1	0
3	B	7	0	0	0	0
3	C	1	0	0	1	0
3	D	6	0	0	2	0
3	E	9	0	0	3	0
3	F	20	0	0	1	0
3	G	14	0	0	0	0
3	H	15	0	0	5	0
3	I	17	0	0	1	0
3	J	12	0	0	2	0
3	a	8	0	0	0	0
3	b	5	0	0	0	0
3	c	8	0	0	0	0
3	d	16	0	0	0	0
3	e	14	0	0	0	0
3	f	12	0	0	0	0
3	g	18	0	0	0	0
3	h	12	0	0	0	0
3	i	16	0	0	0	0
3	j	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16452	0	16208	302	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 10.

All (302) 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:G:32:LYS:HD3	1:G:33:VAL:CG1	9.75	1.22
1:G:32:LYS:HD3	1:G:33:VAL:HG12	9.69	1.06
1:G:54:LYS:HD2	1:G:55:ASP:H	1.21	1.06
1:C:35:ASN:HA	1:C:36:ASP:HB2	5.98	1.01
1:G:32:LYS:HD3	1:G:33:VAL:HG11	10.28	1.00
1:G:32:LYS:CD	1:G:33:VAL:HG12	8.94	0.97
1:B:32:LYS:HB3	1:B:33:VAL:HG22	5.98	0.90
1:F:33:VAL:HG23	1:F:34:ASP:H	5.01	0.89
1:C:24:LYS:HB2	1:C:27:LYS:HG2	4.68	0.88
1:I:106:SER:O	3:I:201:HOH:O	1.92	0.87
1:B:31:PHE:HA	1:B:32:LYS:HB3	1.58	0.84
1:G:58:HIS:HE1	1:G:107:GLY:H	3.89	0.83
1:D:33:VAL:O	1:D:35:ASN:N	3.37	0.82
1:F:58:HIS:HE1	1:F:107:GLY:H	1.28	0.81
1:E:117:VAL:HG12	1:E:118:ALA:H	1.47	0.79
1:G:54:LYS:HD2	1:G:55:ASP:N	1.98	0.78
1:B:32:LYS:HA	1:B:33:VAL:HG13	4.92	0.78
1:F:32:LYS:NZ	3:F:201:HOH:O	2.16	0.77
1:G:32:LYS:CD	1:G:33:VAL:CG1	9.03	0.77
1:J:15:GLN:NE2	1:J:17:TYR:OH	2.19	0.76
1:I:33:VAL:HG13	1:I:34:ASP:HB3	5.68	0.75
1:E:36:ASP:OD1	3:E:201:HOH:O	35.70	0.74
1:C:63:GLU:OE2	1:C:101:ARG:NH1	2.20	0.74
1:G:34:ASP:O	1:G:36:ASP:N	2.82	0.74
1:G:58:HIS:CE1	1:G:107:GLY:H	3.43	0.74
1:C:32:LYS:HB2	1:C:33:VAL:HA	5.84	0.74
1:B:63:GLU:HB3	1:B:99:VAL:HG12	1.70	0.74
1:F:40:HIS:HD2	1:F:115:HIS:NE2	1.87	0.73
1:H:32:LYS:N	3:H:202:HOH:O	2.21	0.72
1:E:64:ALA:HB2	1:E:98:VAL:HG12	1.71	0.72
1:H:58:HIS:HE1	1:H:107:GLY:H	3.93	0.71
1:C:58:HIS:HE1	1:C:107:GLY:H	3.95	0.71
1:B:33:VAL:HG12	1:B:96:PRO:HB2	4.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:O	3:A:301:HOH:O	2.07	0.71
1:I:13:ARG:HH11	1:I:14:PRO:HD3	1.57	0.70
1:G:40:HIS:ND1	1:G:115:HIS:HE1	1.89	0.70
1:E:38:ASN:OD1	3:E:201:HOH:O	39.45	0.70
1:H:39:GLU:CD	1:H:39:GLU:H	4.78	0.69
1:J:56:GLU:OE2	3:J:201:HOH:O	28.30	0.69
1:F:36:ASP:CG	1:F:37:GLU:H	1.94	0.69
1:F:58:HIS:CE1	1:F:107:GLY:H	2.09	0.68
1:D:33:VAL:HG21	1:D:40:HIS:CD2	2.28	0.68
1:H:58:HIS:CE1	1:H:107:GLY:H	3.46	0.68
1:H:68:GLU:OE2	3:H:201:HOH:O	31.52	0.68
1:C:14:PRO:HB3	1:C:118:ALA:HB2	1.74	0.68
1:D:35:ASN:ND2	1:F:26:ASP:OD2	87.72	0.67
1:I:55:ASP:OD2	1:J:80:LYS:NZ	14.90	0.67
1:E:28:ASP:OD2	3:E:202:HOH:O	7.07	0.66
1:H:65:MET:HE2	1:H:70:SER:C	5.52	0.66
1:H:56:GLU:O	3:H:201:HOH:O	2.13	0.66
1:C:58:HIS:CE1	1:C:107:GLY:H	3.48	0.66
1:A:18:LEU:HD12	1:E:64:ALA:HB3	1.79	0.65
1:G:57:LEU:HD11	1:H:81:MET:HE2	1.79	0.65
1:C:38:ASN:HB3	1:C:119:VAL:HA	5.40	0.64
1:H:33:VAL:HG12	1:H:34:ASP:OD2	1.97	0.64
1:A:55:ASP:OD2	1:B:80:LYS:NZ	15.09	0.64
1:D:40:HIS:HD2	1:D:115:HIS:NE2	5.64	0.64
1:G:68:GLU:OE2	1:G:68:GLU:N	4.17	0.64
1:J:40:HIS:HD2	1:J:115:HIS:NE2	5.75	0.64
1:B:63:GLU:OE1	1:B:73:LYS:NZ	2.26	0.63
1:H:65:MET:HE1	1:H:69:GLY:O	2.75	0.63
1:F:41:GLN:HE22	1:G:16:ASN:HD22	1.46	0.62
1:H:114:GLN:HE21	1:H:116:LEU:HD21	1.63	0.62
1:A:74:VAL:HG22	1:B:20:GLY:HA3	1.80	0.62
1:H:65:MET:CE	1:H:69:GLY:O	3.06	0.62
1:D:32:LYS:O	1:D:34:ASP:N	3.78	0.62
1:I:13:ARG:NH1	1:I:14:PRO:HD3	2.15	0.62
1:D:14:PRO:HB3	1:D:118:ALA:HB2	5.84	0.61
1:B:31:PHE:CD1	1:B:32:LYS:HG2	2.36	0.61
1:G:32:LYS:HA	1:G:33:VAL:HB	4.72	0.61
1:H:66:ASN:ND2	1:H:68:GLU:OE1	2.33	0.61
1:H:97:PRO:HA	3:H:202:HOH:O	1.98	0.61
1:B:32:LYS:CB	1:B:33:VAL:HG22	5.29	0.61
1:C:40:HIS:ND1	1:C:115:HIS:HE1	3.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LYS:NZ	3:D:202:HOH:O	33.85	0.61
1:H:45:ARG:HD2	1:H:114:GLN:HE21	7.03	0.61
1:E:15:GLN:NE2	1:E:15:GLN:O	2.35	0.60
1:F:74:VAL:HG22	1:G:20:GLY:HA3	1.83	0.60
1:G:32:LYS:HE2	1:G:97:PRO:HB3	7.74	0.59
1:C:32:LYS:CB	1:C:33:VAL:HA	4.96	0.59
1:F:40:HIS:ND1	1:F:115:HIS:HE1	5.41	0.59
1:J:54:LYS:HB2	1:J:56:GLU:OE1	3.71	0.59
1:D:79:LEU:HD21	1:D:87:VAL:HG23	1.83	0.59
1:E:38:ASN:OD1	1:E:119:VAL:HA	2.03	0.59
1:J:42:LEU:O	1:J:93:GLU:HA	2.35	0.59
1:J:36:ASP:OD2	1:J:38:ASN:N	5.79	0.58
1:D:38:ASN:OD1	1:D:39:GLU:N	2.36	0.58
1:D:61:GLU:OE1	1:D:73:LYS:HB3	3.24	0.58
1:F:49:LEU:HD23	1:F:109:VAL:HG22	2.00	0.58
1:H:34:ASP:CG	1:H:35:ASN:H	2.07	0.57
1:F:20:GLY:HA3	1:J:74:VAL:HG22	1.87	0.57
1:B:32:LYS:O	1:B:33:VAL:HG13	2.05	0.57
1:B:74:VAL:HG22	1:C:20:GLY:HA3	1.86	0.57
1:E:47:VAL:HG12	1:E:79:LEU:HD11	1.87	0.56
1:G:49:LEU:HD23	1:G:109:VAL:HG22	1.87	0.56
1:D:58:HIS:HE1	1:D:107:GLY:H	3.78	0.56
1:C:42:LEU:HD12	1:C:98:VAL:HG11	6.00	0.56
1:I:74:VAL:HG22	1:J:20:GLY:HA3	1.87	0.56
1:F:36:ASP:OD2	1:F:40:HIS:HE1	1.89	0.56
1:J:28:ASP:OD1	1:J:101:ARG:NH1	2.40	0.55
1:H:33:VAL:HG22	1:H:96:PRO:HB2	3.90	0.55
1:E:67:TYR:HD1	1:E:68:GLU:H	1.55	0.55
1:A:115:HIS:ND1	1:E:67:TYR:CD2	2.72	0.55
1:A:57:LEU:HD11	1:B:81:MET:HE2	1.88	0.55
1:I:43:SER:HB2	1:I:116:LEU:HD21	4.25	0.55
1:D:58:HIS:CE1	1:D:107:GLY:H	3.34	0.55
1:F:114:GLN:HE21	1:F:116:LEU:HD21	3.41	0.55
1:E:117:VAL:HG12	1:E:118:ALA:N	2.19	0.54
1:J:58:HIS:HE1	1:J:107:GLY:H	3.90	0.54
1:A:20:GLY:HA3	1:B:74:VAL:HG22	35.94	0.54
1:C:42:LEU:O	1:C:93:GLU:HA	2.26	0.54
1:F:33:VAL:HG23	1:F:34:ASP:N	5.02	0.54
1:A:47:VAL:HG12	1:A:79:LEU:HD11	1.90	0.54
1:B:31:PHE:CE2	1:B:42:LEU:HG	2.42	0.54
1:E:37:GLU:N	1:E:37:GLU:OE1	5.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:PRO:HA	1:F:98:VAL:HG23	1.89	0.54
1:J:58:HIS:CE1	1:J:107:GLY:H	3.45	0.54
1:F:13:ARG:NH1	1:F:15:GLN:HA	2.23	0.53
1:F:36:ASP:CG	1:F:40:HIS:HE1	2.11	0.53
1:B:55:ASP:OD2	1:C:80:LYS:NZ	14.49	0.53
1:B:35:ASN:OD1	1:B:36:ASP:N	5.14	0.53
1:B:49:LEU:HD23	1:B:109:VAL:HG22	2.11	0.53
1:H:34:ASP:O	1:H:35:ASN:HB2	2.08	0.53
1:A:33:VAL:HG21	1:A:40:HIS:CE1	4.11	0.53
1:G:41:GLN:HE22	1:H:16:ASN:HD22	1.56	0.53
1:B:34:ASP:O	1:B:36:ASP:N	2.42	0.53
1:B:37:GLU:N	1:B:37:GLU:OE1	2.41	0.53
1:F:25:ALA:HB2	1:F:106:SER:HA	2.19	0.53
1:G:74:VAL:HG22	1:H:20:GLY:HA3	1.89	0.53
1:H:31:PHE:HB3	3:H:202:HOH:O	2.09	0.52
1:G:32:LYS:HD2	1:G:33:VAL:HG12	8.45	0.52
1:H:41:GLN:HE22	1:I:16:ASN:HD22	1.56	0.52
1:I:49:LEU:HD23	1:I:109:VAL:HG22	1.95	0.52
1:B:81:MET:HE3	1:B:85:PRO:HB3	1.92	0.52
1:H:81:MET:HE3	1:H:85:PRO:HB3	1.91	0.52
1:A:22:GLU:OE2	1:A:27:LYS:NZ	2.44	0.51
1:F:16:ASN:ND2	3:J:201:HOH:O	2.43	0.51
1:H:47:VAL:HG12	1:H:79:LEU:HD11	1.92	0.51
1:I:30:HIS:NE2	1:I:32:LYS:HE3	2.26	0.51
1:F:40:HIS:ND1	1:F:115:HIS:CE1	5.55	0.51
1:I:30:HIS:CE1	1:I:32:LYS:HE3	2.46	0.51
1:C:33:VAL:HG21	1:C:40:HIS:ND1	5.77	0.50
1:E:15:GLN:HE22	1:E:117:VAL:C	2.14	0.50
1:E:15:GLN:CD	1:E:15:GLN:N	2.65	0.50
1:E:102:LEU:HD21	1:E:109:VAL:HG21	1.93	0.50
1:H:32:LYS:HG3	1:H:33:VAL:HG23	1.94	0.50
1:H:81:MET:CE	1:H:85:PRO:HB3	2.42	0.50
1:I:73:LYS:HE3	1:I:101:ARG:NH1	6.41	0.50
1:G:61:GLU:OE1	1:G:73:LYS:HD2	4.42	0.50
1:J:25:ALA:HB2	1:J:106:SER:HA	2.01	0.50
1:B:42:LEU:O	1:B:93:GLU:HA	2.12	0.50
1:I:79:LEU:HD21	1:I:87:VAL:HG23	3.39	0.49
1:J:19:PHE:CD1	1:J:42:LEU:HD11	2.47	0.49
1:B:68:GLU:H	1:B:68:GLU:CD	3.52	0.49
1:B:66:ASN:ND2	1:B:68:GLU:OE2	4.64	0.49
1:I:54:LYS:HB2	1:I:56:GLU:OE1	4.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:LEU:O	1:I:93:GLU:HA	2.12	0.49
1:G:37:GLU:N	1:G:37:GLU:OE1	4.76	0.49
1:G:92:PHE:CG	1:H:45:ARG:HD3	4.55	0.49
1:F:36:ASP:CG	1:F:37:GLU:N	2.66	0.49
1:A:64:ALA:HB3	1:B:18:LEU:HD12	1.95	0.48
1:J:34:ASP:C	1:J:36:ASP:H	2.44	0.48
1:D:38:ASN:HD21	1:D:118:ALA:C	2.17	0.48
1:D:38:ASN:OD1	1:D:118:ALA:HB3	2.13	0.48
1:G:58:HIS:HE1	1:G:107:GLY:N	4.66	0.48
1:F:36:ASP:OD2	1:F:40:HIS:CE1	2.66	0.48
1:G:32:LYS:CD	1:G:33:VAL:HG11	9.62	0.48
1:A:36:ASP:OD2	1:A:38:ASN:N	2.41	0.48
1:F:40:HIS:CD2	1:F:115:HIS:NE2	2.76	0.47
1:H:39:GLU:N	1:H:39:GLU:CD	4.91	0.47
1:B:35:ASN:CG	1:B:36:ASP:H	5.10	0.47
1:C:49:LEU:HD23	1:C:109:VAL:HG22	2.01	0.47
1:F:41:GLN:HE22	1:G:16:ASN:ND2	2.09	0.47
1:I:13:ARG:HD3	1:I:14:PRO:HD3	1.96	0.47
1:I:25:ALA:HB2	1:I:106:SER:HA	2.14	0.47
1:J:61:GLU:OE1	1:J:73:LYS:HB3	4.78	0.47
1:E:38:ASN:ND2	1:E:119:VAL:HG12	2.58	0.47
1:I:15:GLN:HG3	1:I:17:TYR:CZ	4.67	0.47
1:A:34:ASP:N	1:A:34:ASP:OD1	4.66	0.47
1:H:31:PHE:HB3	1:H:98:VAL:HG13	1.97	0.47
1:G:40:HIS:ND1	1:G:115:HIS:CE1	2.78	0.47
1:A:34:ASP:CG	1:A:35:ASN:H	2.18	0.47
1:J:34:ASP:O	1:J:36:ASP:N	2.93	0.47
1:A:33:VAL:HG21	1:A:40:HIS:ND1	3.22	0.47
1:D:33:VAL:HG21	1:D:40:HIS:NE2	2.30	0.47
1:F:33:VAL:O	1:F:34:ASP:HB2	4.83	0.47
1:G:74:VAL:HG12	1:H:20:GLY:HA3	5.00	0.47
1:D:19:PHE:CD2	1:D:42:LEU:HD11	2.50	0.46
1:E:42:LEU:HD12	1:E:98:VAL:HG11	5.27	0.46
1:H:31:PHE:HD1	1:H:96:PRO:HB3	1.81	0.46
1:I:26:ASP:OD1	1:I:26:ASP:N	2.47	0.46
1:A:26:ASP:N	1:A:26:ASP:OD2	4.71	0.46
1:A:57:LEU:HA	1:A:57:LEU:HD12	1.76	0.46
1:H:15:GLN:HG2	1:H:117:VAL:HG22	1.97	0.46
1:H:74:VAL:HG13	1:I:20:GLY:HA3	2.79	0.46
1:H:42:LEU:O	1:H:93:GLU:HA	2.16	0.46
1:J:31:PHE:CD1	1:J:32:LYS:HB2	6.01	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASN:HB2	1:C:116:LEU:HD23	1.97	0.46
1:J:49:LEU:HD23	1:J:109:VAL:HG22	1.98	0.46
1:C:25:ALA:HB2	1:C:106:SER:HA	1.97	0.46
1:D:33:VAL:HG21	1:D:115:HIS:CE1	5.10	0.46
1:C:35:ASN:HA	1:C:36:ASP:CB	5.15	0.46
1:D:25:ALA:HB2	1:D:106:SER:HA	1.98	0.46
1:D:40:HIS:CD2	1:D:117:VAL:HG12	5.05	0.46
1:E:30:HIS:HB3	1:E:32:LYS:HZ1	1.80	0.46
1:H:32:LYS:HA	1:H:33:VAL:HG22	1.97	0.46
1:D:99:VAL:HG11	1:D:101:ARG:NH2	2.30	0.45
1:G:34:ASP:OD2	1:G:40:HIS:NE2	2.49	0.45
1:D:74:VAL:HG22	1:E:18:LEU:HD21	1.99	0.45
1:E:15:GLN:CD	1:E:15:GLN:H	2.19	0.45
1:H:102:LEU:HD11	1:H:109:VAL:HG21	3.33	0.45
1:C:34:ASP:O	1:C:36:ASP:N	2.47	0.45
1:A:49:LEU:HD23	1:A:109:VAL:HG22	2.03	0.45
1:B:81:MET:CE	1:B:85:PRO:HB3	2.45	0.45
1:E:39:GLU:O	1:E:117:VAL:HA	2.17	0.45
1:E:38:ASN:HB3	1:E:118:ALA:O	2.57	0.45
1:H:33:VAL:HG13	1:H:96:PRO:HB2	1.97	0.45
1:C:61:GLU:HG2	1:C:101:ARG:HG3	1.98	0.45
1:E:25:ALA:HB2	1:E:106:SER:HA	2.46	0.45
1:F:79:LEU:HD21	1:F:87:VAL:HG23	2.23	0.45
1:D:30:HIS:CE1	1:D:32:LYS:NZ	2.85	0.45
1:I:79:LEU:CD2	1:I:87:VAL:HG23	3.63	0.44
1:E:49:LEU:HD23	1:E:109:VAL:HG22	2.07	0.44
1:I:96:PRO:HA	1:I:98:VAL:HG23	5.43	0.44
1:D:100:LEU:HD13	1:D:111:ILE:HD12	2.00	0.44
1:C:34:ASP:OD1	1:C:34:ASP:N	3.42	0.44
1:C:63:GLU:HA	1:C:72:ILE:O	2.56	0.44
1:B:31:PHE:CD2	1:B:42:LEU:HG	2.52	0.44
1:H:46:THR:HG1	1:H:112:SER:HG	2.02	0.44
1:J:14:PRO:O	1:J:15:GLN:HB2	4.79	0.44
1:A:57:LEU:CD1	1:B:81:MET:HE2	2.48	0.43
1:H:13:ARG:HB2	1:H:14:PRO:HD3	1.99	0.43
1:H:13:ARG:O	1:H:13:ARG:HD3	6.10	0.43
1:E:19:PHE:CG	1:E:42:LEU:HD21	2.53	0.43
1:B:33:VAL:CG1	1:B:96:PRO:HB2	3.68	0.43
1:C:18:LEU:HD12	1:D:64:ALA:HB3	34.30	0.43
1:E:30:HIS:CD2	1:E:99:VAL:HG22	2.54	0.43
1:D:66:ASN:HB3	1:D:72:ILE:HD13	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ASN:HD21	1:J:41:GLN:HE22	3.54	0.43
1:D:16:ASN:ND2	1:D:114:GLN:HB3	2.46	0.43
1:D:96:PRO:HA	1:D:98:VAL:HG23	2.01	0.42
1:G:64:ALA:HB3	1:H:18:LEU:HD12	5.08	0.42
1:G:57:LEU:CD1	1:H:81:MET:HE2	2.46	0.42
1:J:35:ASN:OD1	1:J:35:ASN:N	2.78	0.42
1:B:67:TYR:CE1	1:C:117:VAL:HG11	2.55	0.42
1:F:33:VAL:CG2	1:F:34:ASP:H	4.77	0.42
1:F:79:LEU:CD2	1:F:87:VAL:HG23	2.61	0.42
1:H:31:PHE:CD1	1:H:96:PRO:HB3	2.54	0.42
1:J:36:ASP:CG	1:J:40:HIS:HE1	3.88	0.42
1:B:43:SER:HB2	1:B:93:GLU:HG2	3.23	0.42
1:C:54:LYS:HD2	3:C:201:HOH:O	19.41	0.42
1:G:102:LEU:HD21	1:G:109:VAL:HG21	2.46	0.42
1:A:96:PRO:HA	1:A:98:VAL:HG23	2.11	0.42
1:E:41:GLN:NE2	1:E:95:THR:OG1	4.21	0.42
1:J:31:PHE:HB3	1:J:98:VAL:CG1	2.50	0.42
1:B:61:GLU:OE1	1:B:103:LYS:HE3	2.20	0.42
1:D:39:GLU:OE1	1:D:39:GLU:HA	2.18	0.42
1:F:102:LEU:HA	1:F:102:LEU:HD23	1.87	0.42
1:H:35:ASN:HB2	1:H:36:ASP:H	4.53	0.42
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.75	0.42
1:A:19:PHE:CD1	1:A:42:LEU:HD11	2.55	0.42
1:B:47:VAL:HG13	1:B:111:ILE:HD13	2.02	0.42
1:G:57:LEU:HA	1:G:57:LEU:HD12	1.85	0.42
1:E:66:ASN:ND2	1:E:68:GLU:OE1	6.00	0.41
1:H:14:PRO:HA	1:H:118:ALA:HA	2.72	0.41
1:H:34:ASP:CG	1:H:35:ASN:N	2.72	0.41
1:F:80:LYS:NZ	1:H:55:ASP:OD2	18.60	0.41
1:I:35:ASN:O	1:I:36:ASP:O	2.38	0.41
1:J:27:LYS:HA	1:J:27:LYS:HD2	1.78	0.41
1:A:59:ILE:HG23	1:A:75:THR:HG23	2.03	0.41
1:E:38:ASN:CG	1:E:119:VAL:HG12	2.82	0.41
1:E:94:ILE:CG2	1:E:98:VAL:HG11	2.51	0.41
1:F:36:ASP:OD1	1:F:37:GLU:N	2.54	0.41
1:I:13:ARG:N	1:I:14:PRO:CD	2.90	0.41
1:J:33:VAL:HG12	1:J:34:ASP:H	1.85	0.41
1:D:57:LEU:HA	1:D:57:LEU:HD12	1.88	0.41
1:I:18:LEU:HA	1:I:18:LEU:HD23	1.86	0.41
1:F:43:SER:HB3	1:F:114:GLN:HG3	4.06	0.41
1:A:114:GLN:HB2	1:A:114:GLN:HE21	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:PHE:HB3	1:F:98:VAL:HG12	4.66	0.41
1:J:31:PHE:HA	1:J:32:LYS:HG3	5.55	0.41
1:B:100:LEU:HD13	1:B:111:ILE:HD12	3.95	0.41
1:B:31:PHE:CE1	1:B:32:LYS:HG2	2.55	0.41
1:D:49:LEU:HD23	1:D:109:VAL:HG22	2.02	0.41
1:A:62:ALA:HB2	1:A:76:LEU:HD11	2.28	0.41
1:D:25:ALA:O	3:D:201:HOH:O	10.26	0.41
1:F:36:ASP:HB2	1:F:37:GLU:OE2	2.20	0.41
1:F:57:LEU:HA	1:F:57:LEU:HD12	1.88	0.41
1:C:32:LYS:CB	1:C:33:VAL:CA	4.73	0.40
1:G:38:ASN:OD1	1:G:119:VAL:HA	4.71	0.40
1:H:54:LYS:HA	1:H:54:LYS:HD2	3.74	0.40
1:H:63:GLU:O	1:H:98:VAL:HA	2.21	0.40
1:A:38:ASN:HD22	1:A:119:VAL:HB	1.86	0.40
1:C:32:LYS:HB3	1:C:34:ASP:N	5.89	0.40
1:F:32:LYS:HD3	1:F:97:PRO:HB3	2.03	0.40
1:J:39:GLU:O	1:J:117:VAL:HA	2.22	0.40
1:D:61:GLU:OE2	1:D:101:ARG:HD2	4.33	0.40
1:D:65:MET:HE2	1:D:65:MET:HA	4.86	0.40
1:E:15:GLN:NE2	1:E:117:VAL:C	2.73	0.40
1:H:41:GLN:HE22	1:I:16:ASN:ND2	2.20	0.40
1:H:65:MET:CE	1:H:70:SER:C	4.61	0.40
1:I:65:MET:HE1	1:I:71:PRO:HB3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	104/116 (90%)	95 (91%)	7 (7%)	2 (2%)	10 15
1	B	103/116 (89%)	96 (93%)	4 (4%)	3 (3%)	6 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	105/116 (90%)	100 (95%)	4 (4%)	1 (1%)	19	33
1	D	103/116 (89%)	98 (95%)	4 (4%)	1 (1%)	19	33
1	E	104/116 (90%)	97 (93%)	7 (7%)	0	100	100
1	F	105/116 (90%)	97 (92%)	6 (6%)	2 (2%)	10	15
1	G	104/116 (90%)	97 (93%)	5 (5%)	2 (2%)	10	15
1	H	105/116 (90%)	96 (91%)	5 (5%)	4 (4%)	4	4
1	I	105/116 (90%)	99 (94%)	4 (4%)	2 (2%)	10	15
1	J	105/116 (90%)	98 (93%)	6 (6%)	1 (1%)	19	33
1	a	104/116 (90%)	100 (96%)	4 (4%)	0	100	100
1	b	103/116 (89%)	95 (92%)	5 (5%)	3 (3%)	6	7
1	c	104/116 (90%)	95 (91%)	5 (5%)	4 (4%)	4	4
1	d	105/116 (90%)	96 (91%)	5 (5%)	4 (4%)	4	4
1	e	105/116 (90%)	100 (95%)	5 (5%)	0	100	100
1	f	104/116 (90%)	95 (91%)	7 (7%)	2 (2%)	10	15
1	g	104/116 (90%)	99 (95%)	3 (3%)	2 (2%)	10	15
1	h	104/116 (90%)	98 (94%)	4 (4%)	2 (2%)	10	15
1	i	105/116 (90%)	94 (90%)	10 (10%)	1 (1%)	19	33
1	j	104/116 (90%)	96 (92%)	4 (4%)	4 (4%)	4	4
All	All	2085/2320 (90%)	1941 (93%)	104 (5%)	40 (2%)	10	15

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	32	LYS
1	B	33	VAL
1	B	35	ASN
1	F	36	ASP
1	H	35	ASN
1	I	36	ASP
1	I	37	GLU
1	b	35	ASN
1	c	32	LYS
1	c	35	ASN
1	d	25	ALA
1	d	33	VAL
1	d	34	ASP

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Mol	Chain	Res	Type
1	f	33	VAL
1	g	33	VAL
1	g	35	ASN
1	h	35	ASN
1	h	36	ASP
1	j	14	PRO
1	j	32	LYS
1	A	118	ALA
1	C	35	ASN
1	D	35	ASN
1	H	34	ASP
1	b	33	VAL
1	c	34	ASP
1	d	35	ASN
1	j	35	ASN
1	A	33	VAL
1	H	32	LYS
1	J	36	ASP
1	c	28	ASP
1	i	33	VAL
1	b	36	ASP
1	F	33	VAL
1	G	36	ASP
1	G	118	ALA
1	f	34	ASP
1	j	33	VAL
1	H	33	VAL

### 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	90/99 (91%)	86 (96%)	4 (4%)	35	58
1	B	89/99 (90%)	88 (99%)	1 (1%)	80	93
1	C	91/99 (92%)	88 (97%)	3 (3%)	45	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	89/99 (90%)	88 (99%)	1 (1%)	80	93
1	E	90/99 (91%)	88 (98%)	2 (2%)	60	83
1	F	91/99 (92%)	89 (98%)	2 (2%)	60	83
1	G	90/99 (91%)	88 (98%)	2 (2%)	60	83
1	H	91/99 (92%)	87 (96%)	4 (4%)	35	58
1	I	91/99 (92%)	86 (94%)	5 (6%)	27	46
1	J	91/99 (92%)	89 (98%)	2 (2%)	60	83
1	a	90/99 (91%)	88 (98%)	2 (2%)	60	83
1	b	89/99 (90%)	86 (97%)	3 (3%)	44	70
1	c	90/99 (91%)	85 (94%)	5 (6%)	26	45
1	d	91/99 (92%)	86 (94%)	5 (6%)	27	46
1	e	91/99 (92%)	88 (97%)	3 (3%)	45	71
1	f	90/99 (91%)	86 (96%)	4 (4%)	35	58
1	g	90/99 (91%)	88 (98%)	2 (2%)	60	83
1	h	90/99 (91%)	84 (93%)	6 (7%)	20	35
1	i	91/99 (92%)	87 (96%)	4 (4%)	35	58
1	j	90/99 (91%)	86 (96%)	4 (4%)	35	58
All	All	1805/1980 (91%)	1741 (96%)	64 (4%)	43	68

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	26	ASP
1	A	35	ASN
1	A	92	PHE
1	B	92	PHE
1	C	16	ASN
1	C	32	LYS
1	C	92	PHE
1	D	92	PHE
1	E	67	TYR
1	E	92	PHE
1	F	65	MET
1	F	92	PHE
1	G	92	PHE

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Mol	Chain	Res	Type
1	G	115	HIS
1	H	15	GLN
1	H	36	ASP
1	H	92	PHE
1	H	98	VAL
1	I	13	ARG
1	I	18	LEU
1	I	48	SER
1	I	65	MET
1	I	92	PHE
1	J	18	LEU
1	J	92	PHE
1	a	37	GLU
1	a	92	PHE
1	b	36	ASP
1	b	54	LYS
1	b	92	PHE
1	c	18	LEU
1	c	36	ASP
1	c	38	ASN
1	c	92	PHE
1	c	115	HIS
1	d	13	ARG
1	d	18	LEU
1	d	27	LYS
1	d	48	SER
1	d	92	PHE
1	e	13	ARG
1	e	32	LYS
1	e	92	PHE
1	f	18	LEU
1	f	92	PHE
1	f	114	GLN
1	f	115	HIS
1	g	34	ASP
1	g	92	PHE
1	h	13	ARG
1	h	18	LEU
1	h	35	ASN
1	h	45	ARG
1	h	92	PHE
1	h	102	LEU

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Mol	Chain	Res	Type
1	i	16	ASN
1	i	18	LEU
1	i	38	ASN
1	i	92	PHE
1	j	18	LEU
1	j	30	HIS
1	j	34	ASP
1	j	92	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	16	ASN
1	A	38	ASN
1	A	84	GLN
1	A	110	HIS
1	A	114	GLN
1	C	30	HIS
1	C	38	ASN
1	C	84	GLN
1	D	15	GLN
1	D	16	ASN
1	D	84	GLN
1	E	30	HIS
1	E	84	GLN
1	F	40	HIS
1	F	58	HIS
1	F	114	GLN
1	G	16	ASN
1	G	41	GLN
1	G	84	GLN
1	G	114	GLN
1	G	115	HIS
1	H	114	GLN
1	I	16	ASN
1	I	114	GLN
1	J	15	GLN
1	J	38	ASN
1	J	114	GLN
1	a	16	ASN
1	a	114	GLN

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Mol	Chain	Res	Type
1	b	30	HIS
1	b	84	GLN
1	c	16	ASN
1	c	38	ASN
1	c	58	HIS
1	c	115	HIS
1	d	16	ASN
1	d	30	HIS
1	d	40	HIS
1	d	41	GLN
1	d	58	HIS
1	e	38	ASN
1	e	41	GLN
1	e	84	GLN
1	e	114	GLN
1	f	16	ASN
1	f	41	GLN
1	f	114	GLN
1	f	115	HIS
1	g	16	ASN
1	g	58	HIS
1	g	84	GLN
1	g	114	GLN
1	h	41	GLN
1	h	58	HIS
1	h	84	GLN
1	h	114	GLN
1	i	16	ASN
1	i	38	ASN
1	i	114	GLN
1	j	15	GLN
1	j	40	HIS
1	j	58	HIS
1	j	114	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	69:GLY	C	70:SER	N	1.17

## 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	106/116 (91%)	0.24	9 (8%) 13 15	39, 53, 109, 142	0
1	B	105/116 (90%)	0.55	14 (13%) 4 5	36, 54, 99, 130	0
1	C	107/116 (92%)	0.64	12 (11%) 7 8	39, 60, 123, 165	0
1	D	105/116 (90%)	0.40	8 (7%) 17 19	39, 59, 100, 137	0
1	E	106/116 (91%)	0.32	10 (9%) 11 12	40, 57, 99, 117	0
1	F	107/116 (92%)	0.18	6 (5%) 28 33	31, 44, 89, 119	0
1	G	106/116 (91%)	0.10	6 (5%) 27 32	33, 43, 86, 121	0
1	H	107/116 (92%)	0.07	4 (3%) 45 51	31, 46, 94, 134	0
1	I	107/116 (92%)	0.14	5 (4%) 35 41	32, 47, 84, 102	0
1	J	107/116 (92%)	0.31	6 (5%) 28 33	32, 46, 91, 129	0
1	a	106/116 (91%)	0.32	7 (6%) 22 25	36, 52, 96, 129	0
1	b	105/116 (90%)	0.32	9 (8%) 13 14	35, 53, 93, 122	0
1	c	106/116 (91%)	0.29	7 (6%) 22 25	35, 52, 123, 141	0
1	d	107/116 (92%)	0.26	8 (7%) 17 19	34, 50, 104, 132	0
1	e	107/116 (92%)	0.04	2 (1%) 70 74	34, 46, 77, 98	0
1	f	106/116 (91%)	0.30	7 (6%) 22 25	29, 46, 92, 122	0
1	g	106/116 (91%)	0.26	8 (7%) 17 19	32, 45, 88, 140	0
1	h	106/116 (91%)	0.11	4 (3%) 44 50	28, 43, 87, 100	0
1	i	107/116 (92%)	0.17	8 (7%) 17 19	30, 44, 89, 117	0
1	j	106/116 (91%)	0.25	7 (6%) 22 25	30, 43, 84, 125	0
All	All	2125/2320 (91%)	0.26	147 (6%) 20 23	28, 50, 99, 165	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	34	ASP	9.1
1	j	35	ASN	9.0
1	C	119	VAL	7.7
1	B	35	ASN	7.1
1	C	35	ASN	6.9
1	g	35	ASN	6.8
1	d	36	ASP	5.6
1	f	35	ASN	5.4
1	a	119	VAL	5.1
1	b	36	ASP	4.9
1	D	37	GLU	4.8
1	d	34	ASP	4.8
1	j	37	GLU	4.6
1	f	67	TYR	4.5
1	I	119	VAL	4.5
1	c	36	ASP	4.4
1	B	33	VAL	4.4
1	J	120	GLU	4.3
1	c	119	VAL	4.3
1	F	37	GLU	4.2
1	C	33	VAL	4.2
1	E	119	VAL	4.2
1	g	36	ASP	4.1
1	i	119	VAL	4.1
1	G	37	GLU	4.1
1	B	37	GLU	4.1
1	A	35	ASN	4.1
1	c	37	GLU	4.1
1	j	13	ARG	4.1
1	H	37	GLU	4.0
1	J	33	VAL	4.0
1	a	37	GLU	4.0
1	F	34	ASP	3.8
1	g	119	VAL	3.7
1	j	36	ASP	3.7
1	A	38	ASN	3.6
1	J	34	ASP	3.6
1	G	36	ASP	3.6
1	B	67	TYR	3.6
1	A	119	VAL	3.5
1	d	38	ASN	3.5
1	C	37	GLU	3.5
1	E	117	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	c	34	ASP	3.4
1	E	67	TYR	3.4
1	B	34	ASP	3.4
1	E	33	VAL	3.4
1	b	34	ASP	3.4
1	B	118	ALA	3.3
1	f	34	ASP	3.3
1	C	34	ASP	3.3
1	D	36	ASP	3.3
1	J	35	ASN	3.3
1	c	68	GLU	3.3
1	B	32	LYS	3.3
1	D	35	ASN	3.3
1	a	36	ASP	3.2
1	h	37	GLU	3.2
1	f	119	VAL	3.2
1	C	38	ASN	3.2
1	F	36	ASP	3.2
1	e	119	VAL	3.2
1	G	35	ASN	3.2
1	D	118	ALA	3.1
1	c	38	ASN	3.1
1	e	37	GLU	3.1
1	C	68	GLU	3.1
1	g	38	ASN	3.1
1	C	67	TYR	3.1
1	B	38	ASN	3.0
1	B	26	ASP	3.0
1	g	34	ASP	3.0
1	g	39	GLU	3.0
1	a	35	ASN	3.0
1	g	37	GLU	2.9
1	J	36	ASP	2.9
1	f	68	GLU	2.9
1	I	67	TYR	2.9
1	b	38	ASN	2.8
1	i	13	ARG	2.8
1	b	39	GLU	2.8
1	h	118	ALA	2.8
1	b	35	ASN	2.8
1	C	13	ARG	2.7
1	C	14	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	36	ASP	2.7
1	B	39	GLU	2.7
1	A	39	GLU	2.6
1	i	37	GLU	2.6
1	F	13	ARG	2.6
1	H	34	ASP	2.6
1	f	37	GLU	2.6
1	d	67	TYR	2.6
1	A	33	VAL	2.6
1	d	37	GLU	2.6
1	h	13	ARG	2.6
1	H	39	GLU	2.6
1	j	34	ASP	2.5
1	G	34	ASP	2.5
1	E	39	GLU	2.5
1	F	70	SER	2.5
1	d	68	GLU	2.5
1	D	117	VAL	2.5
1	b	31	PHE	2.5
1	I	36	ASP	2.5
1	I	13	ARG	2.4
1	d	118	ALA	2.4
1	i	35	ASN	2.4
1	f	71	PRO	2.4
1	G	38	ASN	2.4
1	d	35	ASN	2.4
1	b	26	ASP	2.4
1	c	26	ASP	2.3
1	A	36	ASP	2.3
1	A	37	GLU	2.3
1	B	14	PRO	2.3
1	A	34	ASP	2.3
1	B	36	ASP	2.3
1	i	38	ASN	2.3
1	a	34	ASP	2.2
1	G	33	VAL	2.2
1	b	33	VAL	2.2
1	E	95	THR	2.2
1	a	31	PHE	2.2
1	F	67	TYR	2.2
1	i	39	GLU	2.2
1	a	38	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	b	67	TYR	2.2
1	E	38	ASN	2.2
1	h	33	VAL	2.1
1	E	35	ASN	2.1
1	E	68	GLU	2.1
1	C	70	SER	2.1
1	D	38	ASN	2.1
1	J	38	ASN	2.1
1	A	118	ALA	2.1
1	i	26	ASP	2.1
1	i	34	ASP	2.1
1	B	31	PHE	2.1
1	j	38	ASN	2.1
1	g	33	VAL	2.0
1	E	37	GLU	2.0
1	H	13	ARG	2.0
1	I	33	VAL	2.0
1	j	31	PHE	2.0
1	B	65	MET	2.0
1	D	33	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CL	f	201	1/1	0.93	0.44	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	201	1/1	0.90	0.53	-	86,86,86,86	0
2	CL	b	201	1/1	0.94	0.54	-	88,88,88,88	0
2	CL	G	201	1/1	0.93	0.47	-	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.