



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:42 AM GMT

PDB ID : 3BIM  
Title : Crystal structure of the BCL6 BTB domain dimer in complex with the BCOR  
BBD corepressor peptide  
Authors : Prive, G.G.; Ghetu, A.F.  
Deposited on : 2007-11-30  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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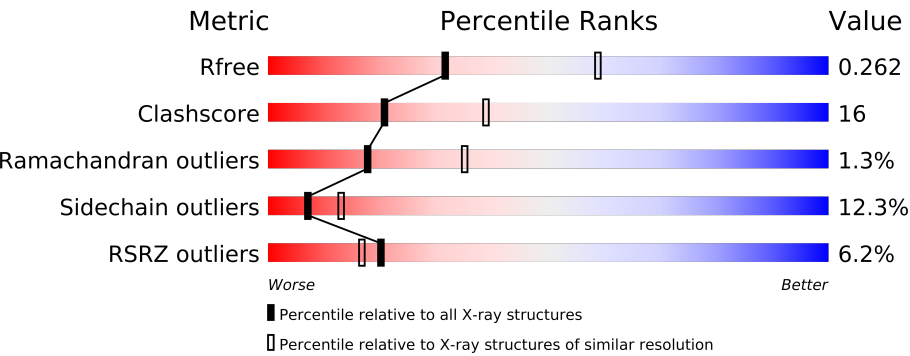
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance i

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	127	
1	B	127	
1	C	127	
1	D	127	
1	E	127	
1	F	127	
1	G	127	
1	H	127	
2	I	19	
2	J	19	
2	K	19	
2	L	19	
2	M	19	
2	N	19	

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Mol	Chain	Length	Quality of chain
2	O	19	
2	P	19	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9091 atoms, of which 0 are hydrogen and 0 are deuterium.

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 B-cell lymphoma 6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			1008	636	178	186	8			
1	B	124	Total	C	N	O	S	0	0	0
			998	631	177	182	8			
1	C	125	Total	C	N	O	S	0	0	0
			1008	636	178	186	8			
1	D	124	Total	C	N	O	S	0	0	0
			998	631	177	182	8			
1	E	123	Total	C	N	O	S	0	0	0
			993	628	176	181	8			
1	F	122	Total	C	N	O	S	0	0	0
			987	625	175	179	8			
1	G	122	Total	C	N	O	S	0	0	0
			985	624	175	178	8			
1	H	122	Total	C	N	O	S	0	0	0
			987	625	175	179	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	EXPRESSION TAG	UNP P41182
A	4	SER	-	EXPRESSION TAG	UNP P41182
A	8	GLN	CYS	ENGINEERED	UNP P41182
A	67	ARG	CYS	ENGINEERED	UNP P41182
A	84	ASN	CYS	ENGINEERED	UNP P41182
B	3	GLY	-	EXPRESSION TAG	UNP P41182
B	4	SER	-	EXPRESSION TAG	UNP P41182
B	8	GLN	CYS	ENGINEERED	UNP P41182
B	67	ARG	CYS	ENGINEERED	UNP P41182
B	84	ASN	CYS	ENGINEERED	UNP P41182
C	3	GLY	-	EXPRESSION TAG	UNP P41182
C	4	SER	-	EXPRESSION TAG	UNP P41182
C	8	GLN	CYS	ENGINEERED	UNP P41182

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Chain	Residue	Modelled	Actual	Comment	Reference
C	67	ARG	CYS	ENGINEERED	UNP P41182
C	84	ASN	CYS	ENGINEERED	UNP P41182
D	3	GLY	-	EXPRESSION TAG	UNP P41182
D	4	SER	-	EXPRESSION TAG	UNP P41182
D	8	GLN	CYS	ENGINEERED	UNP P41182
D	67	ARG	CYS	ENGINEERED	UNP P41182
D	84	ASN	CYS	ENGINEERED	UNP P41182
E	3	GLY	-	EXPRESSION TAG	UNP P41182
E	4	SER	-	EXPRESSION TAG	UNP P41182
E	8	GLN	CYS	ENGINEERED	UNP P41182
E	67	ARG	CYS	ENGINEERED	UNP P41182
E	84	ASN	CYS	ENGINEERED	UNP P41182
F	3	GLY	-	EXPRESSION TAG	UNP P41182
F	4	SER	-	EXPRESSION TAG	UNP P41182
F	8	GLN	CYS	ENGINEERED	UNP P41182
F	67	ARG	CYS	ENGINEERED	UNP P41182
F	84	ASN	CYS	ENGINEERED	UNP P41182
G	3	GLY	-	EXPRESSION TAG	UNP P41182
G	4	SER	-	EXPRESSION TAG	UNP P41182
G	8	GLN	CYS	ENGINEERED	UNP P41182
G	67	ARG	CYS	ENGINEERED	UNP P41182
G	84	ASN	CYS	ENGINEERED	UNP P41182
H	3	GLY	-	EXPRESSION TAG	UNP P41182
H	4	SER	-	EXPRESSION TAG	UNP P41182
H	8	GLN	CYS	ENGINEERED	UNP P41182
H	67	ARG	CYS	ENGINEERED	UNP P41182
H	84	ASN	CYS	ENGINEERED	UNP P41182

- Molecule 2 is a protein called BCL-6 corepressor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	0	0	0
			126	80	21	25			
2	J	17	Total	C	N	O	0	0	0
			126	80	21	25			
2	K	17	Total	C	N	O	0	0	0
			126	80	21	25			
2	L	16	Total	C	N	O	0	0	0
			115	74	17	24			
2	M	17	Total	C	N	O	0	0	0
			126	80	21	25			
2	N	16	Total	C	N	O	0	0	0
			115	74	17	24			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	17	Total	C	N	O	0	0	0
			126	80	21	25			
2	P	17	Total	C	N	O	0	0	0
			126	80	21	25			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
I	497	SER	-	EXPRESSION TAG	UNP Q6W2J9
J	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
J	497	SER	-	EXPRESSION TAG	UNP Q6W2J9
K	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
K	497	SER	-	EXPRESSION TAG	UNP Q6W2J9
L	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
L	497	SER	-	EXPRESSION TAG	UNP Q6W2J9
M	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
M	497	SER	-	EXPRESSION TAG	UNP Q6W2J9
N	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
N	497	SER	-	EXPRESSION TAG	UNP Q6W2J9
O	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
O	497	SER	-	EXPRESSION TAG	UNP Q6W2J9
P	496	GLY	-	EXPRESSION TAG	UNP Q6W2J9
P	497	SER	-	EXPRESSION TAG	UNP Q6W2J9

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	23	Total	O	0	0
			23	23		
3	C	11	Total	O	0	0
			11	11		
3	D	23	Total	O	0	0
			23	23		
3	E	12	Total	O	0	0
			12	12		
3	F	15	Total	O	0	0
			15	15		
3	G	15	Total	O	0	0
			15	15		

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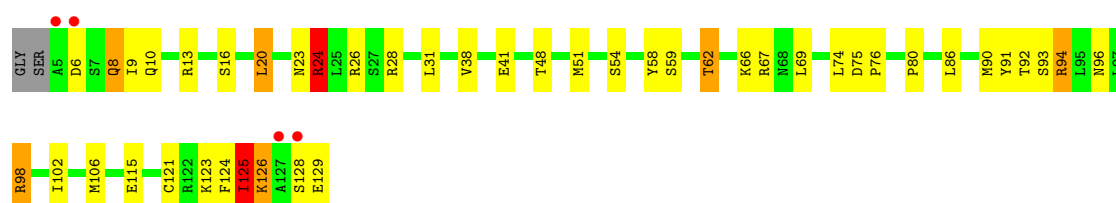
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	7	Total	O	0	0
			7	7		
3	I	1	Total	O	0	0
			1	1		
3	J	3	Total	O	0	0
			3	3		
3	K	1	Total	O	0	0
			1	1		
3	L	1	Total	O	0	0
			1	1		
3	M	1	Total	O	0	0
			1	1		
3	N	1	Total	O	0	0
			1	1		
3	O	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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.

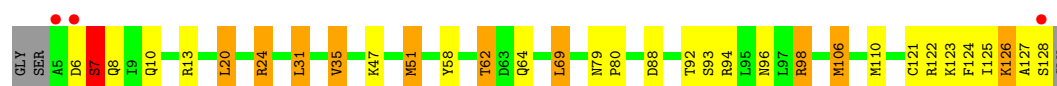
- Molecule 1: B-cell lymphoma 6 protein

Chain A: 



- Molecule 1: B-cell lymphoma 6 protein

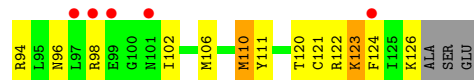
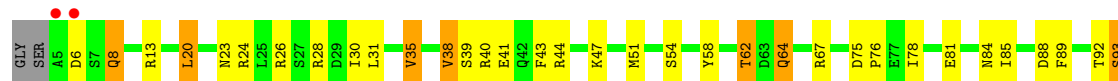
Chain B: 





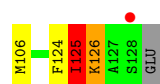
- Molecule 1: B-cell lymphoma 6 protein

Chain F:



- Molecule 1: B-cell lymphoma 6 protein

Chain G:



- Molecule 1: B-cell lymphoma 6 protein

Chain H:



- Molecule 2: BCL-6 corepressor

Chain I:



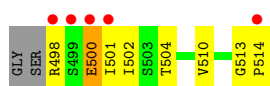
- Molecule 2: BCL-6 corepressor

Chain J:



- Molecule 2: BCL-6 corepressor

Chain K:



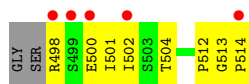
- Molecule 2: BCL-6 corepressor

Chain L:



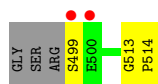
- Molecule 2: BCL-6 corepressor

Chain M:



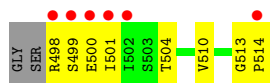
- Molecule 2: BCL-6 corepressor

Chain N:



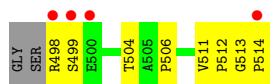
- Molecule 2: BCL-6 corepressor

Chain O:



- Molecule 2: BCL-6 corepressor

Chain P:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.55Å 150.55Å 312.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.70 – 2.60 48.68 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.70-2.60) 98.3 (48.68-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.219 , 0.260 0.223 , 0.262	Depositor DCC
$R_{free}$ test set	3969 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 80574 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.88	1/1022 (0.1%)	0.93	2/1377 (0.1%)
1	B	0.93	0/1012	0.95	2/1365 (0.1%)
1	C	0.85	1/1022 (0.1%)	0.95	3/1377 (0.2%)
1	D	0.91	0/1012	1.00	2/1365 (0.1%)
1	E	0.80	0/1007	0.86	0/1358
1	F	0.87	0/1001	0.97	3/1350 (0.2%)
1	G	0.79	0/999	0.85	1/1347 (0.1%)
1	H	0.76	0/1001	0.83	0/1350
2	I	0.86	0/130	0.74	0/178
2	J	0.99	0/130	0.82	0/178
2	K	0.83	0/130	0.67	0/178
2	L	0.79	0/119	0.80	0/164
2	M	0.78	0/130	0.72	0/178
2	N	0.79	0/119	0.78	0/164
2	O	0.76	0/130	0.75	0/178
2	P	0.79	0/130	0.73	0/178
All	All	0.85	2/9094 (0.0%)	0.90	13/12285 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	E	0	1
2	I	0	1
2	J	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	CYS	CB-SG	-5.30	1.73	1.81
1	A	16	SER	CB-OG	-5.06	1.35	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	PHE	CB-CG-CD2	10.34	128.03	120.80
1	C	33	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	91	TYR	CB-CG-CD1	6.86	125.11	121.00
1	F	88	ASP	CB-CG-OD2	6.62	124.26	118.30
1	D	124	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	C	91	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	24	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	F	88	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	B	35	VAL	CB-CA-C	-5.39	101.16	111.40
1	F	31	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	B	51	MET	CG-SD-CE	5.14	108.42	100.20
1	G	63	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	28	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	31	LEU	Mainchain
1	D	124	PHE	Sidechain
1	E	31	LEU	Mainchain
2	I	513	GLY	Peptide
2	J	513	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1008	0	1023	36	0
1	B	998	0	1017	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1008	0	1023	40	0
1	D	998	0	1017	40	0
1	E	993	0	1012	35	0
1	F	987	0	1007	52	0
1	G	985	0	1008	24	0
1	H	987	0	1007	44	0
2	I	126	0	124	3	0
2	J	126	0	124	5	0
2	K	126	0	124	13	0
2	L	115	0	111	6	0
2	M	126	0	124	7	0
2	N	115	0	111	6	0
2	O	126	0	124	7	0
2	P	126	0	124	4	0
3	A	26	0	0	4	0
3	B	23	0	0	2	0
3	C	11	0	0	1	0
3	D	23	0	0	0	0
3	E	12	0	0	2	0
3	F	15	0	0	2	0
3	G	15	0	0	1	0
3	H	7	0	0	3	0
3	I	1	0	0	0	0
3	J	3	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	1	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
All	All	9091	0	9080	282	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (282) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:8:GLN:HG3	1:B:96:ASN:ND2	1.49	1.25
1:E:8:GLN:HG3	1:F:96:ASN:ND2	1.56	1.19
1:A:24:ARG:HG3	1:A:24:ARG:NH1	1.40	1.15
1:A:24:ARG:HH11	1:A:24:ARG:CG	1.57	1.13
1:H:43:PHE:HE2	1:H:84:ASN:HD22	0.98	0.94
1:B:110:MET:HG2	1:H:110:MET:CE	1.99	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:110:MET:HG2	1:H:110:MET:HE2	1.51	0.92
1:B:69:LEU:HD13	1:D:69:LEU:HD13	1.51	0.91
1:C:62:THR:CG2	1:E:28:ARG:HE	1.85	0.88
1:E:96:ASN:ND2	1:F:8:GLN:HG2	1.90	0.87
1:E:8:GLN:HG3	1:F:96:ASN:HD22	1.36	0.86
2:O:510:VAL:CG1	1:H:24:ARG:HH22	1.87	0.86
1:E:8:GLN:HG3	1:F:96:ASN:HD21	1.41	0.85
1:D:58:TYR:O	1:D:62:THR:HB	1.77	0.84
1:D:23:ASN:HD21	1:D:26:ARG:HH21	1.25	0.84
1:A:8:GLN:HG3	1:B:96:ASN:HD21	1.41	0.83
1:H:106:MET:HE2	1:H:121:CYS:HB3	1.60	0.83
1:B:69:LEU:CD1	1:D:69:LEU:HD13	2.09	0.82
1:A:58:TYR:O	1:A:62:THR:HB	1.79	0.82
1:G:96:ASN:ND2	1:H:8:GLN:HG3	1.96	0.81
1:D:126:LYS:HE3	1:D:126:LYS:HA	1.64	0.79
1:F:92:THR:O	1:F:93:SER:HB2	1.80	0.79
1:F:58:TYR:O	1:F:62:THR:HB	1.83	0.79
2:I:498:ARG:HB2	1:B:6:ASP:HB2	1.65	0.77
1:H:43:PHE:HE2	1:H:84:ASN:ND2	1.78	0.76
1:D:35:VAL:HG23	1:D:44:ARG:NH1	2.01	0.76
1:C:23:ASN:HD21	1:C:26:ARG:HH21	1.32	0.75
1:A:23:ASN:HD21	1:A:26:ARG:HH21	1.34	0.75
2:J:513:GLY:O	2:J:514:PRO:O	2.05	0.75
1:F:81:GLU:O	1:F:85:ILE:HG13	1.86	0.74
1:G:66:LYS:HA	1:G:69:LEU:HD22	1.68	0.74
2:P:512:PRO:C	2:P:514:PRO:HD3	2.07	0.74
1:G:31:LEU:HD12	1:H:51:MET:SD	2.28	0.73
3:G:130:HOH:O	1:H:95:LEU:HB2	1.87	0.73
1:B:122:ARG:NH1	3:B:151:HOH:O	2.22	0.72
1:C:13:ARG:HG2	3:L:74:HOH:O	1.89	0.72
1:A:24:ARG:HH11	1:A:24:ARG:HG3	0.66	0.71
2:K:498:ARG:HB2	1:D:6:ASP:HB3	1.72	0.71
1:C:58:TYR:O	1:C:62:THR:HB	1.91	0.71
2:O:510:VAL:CG1	1:H:24:ARG:NH2	2.56	0.69
1:D:23:ASN:ND2	1:D:26:ARG:HH21	1.90	0.69
1:D:106:MET:HE2	1:D:121:CYS:HB3	1.75	0.69
1:B:92:THR:O	1:B:93:SER:HB2	1.92	0.69
1:D:24:ARG:HH11	1:D:24:ARG:HG3	1.58	0.69
1:E:8:GLN:OE1	1:F:94:ARG:NH1	2.26	0.68
1:A:24:ARG:CG	1:A:24:ARG:NH1	2.28	0.68
1:C:97:LEU:HD21	1:C:105:VAL:HG11	1.76	0.68
1:H:43:PHE:CE2	1:H:84:ASN:ND2	2.58	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:98:ARG:HH11	1:H:98:ARG:HB3	1.59	0.67
1:F:106:MET:HE3	1:F:121:CYS:HB3	1.77	0.67
1:E:94:ARG:HB3	1:F:8:GLN:HE22	1.59	0.67
1:D:35:VAL:CG2	1:D:44:ARG:HH11	2.07	0.67
1:H:61:PHE:O	1:H:67:ARG:HG3	1.95	0.67
1:D:24:ARG:HG3	1:D:24:ARG:NH1	2.09	0.67
2:O:510:VAL:HG13	1:H:24:ARG:HH22	1.60	0.67
1:A:106:MET:HE2	1:A:121:CYS:HB3	1.77	0.66
1:A:24:ARG:HD3	3:A:140:HOH:O	1.96	0.66
1:G:24:ARG:HG3	2:P:511:VAL:HB	1.76	0.66
2:O:504:THR:O	2:O:504:THR:HG22	1.95	0.66
1:B:20:LEU:O	1:B:24:ARG:HG2	1.95	0.66
1:B:110:MET:HG2	1:H:110:MET:HE1	1.77	0.66
1:F:106:MET:CE	1:F:121:CYS:HB3	2.26	0.66
1:C:64:GLN:H	1:C:64:GLN:CD	1.99	0.65
1:C:62:THR:HG23	1:E:28:ARG:NE	2.10	0.65
1:F:75:ASP:O	1:F:78:ILE:HG12	1.97	0.65
1:B:122:ARG:C	1:B:124:PHE:H	1.99	0.65
1:B:122:ARG:O	1:B:124:PHE:N	2.29	0.65
1:C:62:THR:CG2	1:E:28:ARG:NE	2.59	0.64
1:F:28:ARG:HB2	1:F:30:ILE:HD12	1.80	0.64
1:B:58:TYR:O	1:B:62:THR:HB	1.97	0.64
1:G:31:LEU:CD1	1:H:51:MET:SD	2.86	0.64
1:C:62:THR:HG23	1:E:28:ARG:HE	1.64	0.63
1:D:35:VAL:CG2	1:D:44:ARG:NH1	2.62	0.63
1:E:44:ARG:NH1	3:E:130:HOH:O	2.32	0.63
1:D:97:LEU:HD13	1:D:102:ILE:CD1	2.28	0.62
2:I:512:PRO:HB2	2:I:514:PRO:HD3	1.80	0.62
1:D:23:ASN:HD21	1:D:26:ARG:NH2	1.95	0.62
2:M:498:ARG:HA	1:F:6:ASP:O	1.98	0.62
1:D:75:ASP:OD1	1:D:77:GLU:HB2	1.98	0.62
1:E:96:ASN:HD22	1:F:8:GLN:HG2	1.62	0.62
1:D:92:THR:O	1:D:93:SER:HB2	2.00	0.61
1:G:47:LYS:O	1:G:51:MET:HG3	2.00	0.61
1:G:21:ASN:HA	1:G:24:ARG:HG2	1.83	0.61
1:D:66:LYS:HA	1:D:69:LEU:HD22	1.81	0.61
1:H:98:ARG:HB3	1:H:98:ARG:NH1	2.15	0.61
1:F:28:ARG:HB2	1:F:30:ILE:CD1	2.29	0.61
1:G:64:GLN:OE1	1:G:64:GLN:N	2.32	0.61
1:H:35:VAL:HB	3:H:137:HOH:O	2.01	0.61
2:K:504:THR:O	2:K:504:THR:HG22	2.01	0.60
2:O:513:GLY:N	2:O:514:PRO:HD3	2.15	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:512:PRO:C	2:L:514:PRO:HD2	2.21	0.60
1:D:126:LYS:HA	1:D:126:LYS:CE	2.30	0.60
1:D:97:LEU:HD13	1:D:102:ILE:HD12	1.84	0.60
1:F:40:ARG:NH2	3:F:142:HOH:O	2.22	0.59
1:H:92:THR:O	1:H:93:SER:HB2	2.03	0.59
1:A:98:ARG:HG3	1:B:6:ASP:OD1	2.03	0.59
1:C:64:GLN:HE22	2:N:514:PRO:HD2	1.68	0.59
1:B:110:MET:CG	1:H:110:MET:HE2	2.28	0.59
1:G:53:CYS:SG	1:G:90:MET:HG2	2.43	0.58
1:G:51:MET:SD	1:H:31:LEU:HD12	2.44	0.58
1:G:47:LYS:NZ	1:G:67:ARG:O	2.37	0.58
1:C:92:THR:O	1:C:93:SER:HB2	2.04	0.58
1:E:96:ASN:ND2	1:F:8:GLN:HE21	2.02	0.57
1:E:92:THR:O	1:E:93:SER:HB2	2.04	0.57
1:A:41:GLU:HG3	1:A:80:PRO:HB3	1.87	0.57
2:N:513:GLY:O	2:N:514:PRO:C	2.41	0.57
1:A:62:THR:HG21	3:A:146:HOH:O	2.05	0.57
1:B:6:ASP:O	1:B:7:SER:HB2	2.05	0.56
1:B:69:LEU:HD13	1:D:69:LEU:CD1	2.29	0.56
1:C:64:GLN:NE2	2:N:514:PRO:HG2	2.21	0.56
1:A:51:MET:SD	1:B:31:LEU:HD12	2.46	0.56
1:D:127:ALA:O	1:D:128:SER:HB2	2.06	0.56
1:G:106:MET:HE3	1:G:125:ILE:HD11	1.88	0.56
2:L:513:GLY:N	2:L:514:PRO:HD2	2.21	0.56
1:G:58:TYR:O	1:G:62:THR:HB	2.06	0.56
1:B:126:LYS:HA	1:B:126:LYS:HE3	1.88	0.55
2:O:510:VAL:HG13	1:H:24:ARG:NH2	2.22	0.55
1:H:35:VAL:HG22	1:H:44:ARG:HD2	1.88	0.55
1:A:92:THR:O	1:A:93:SER:HB2	2.07	0.55
1:H:122:ARG:O	1:H:124:PHE:N	2.40	0.55
1:C:8:GLN:HB2	1:D:96:ASN:ND2	2.21	0.55
1:G:35:VAL:HG22	1:G:44:ARG:HH11	1.70	0.55
1:E:44:ARG:HD2	3:E:130:HOH:O	2.05	0.55
1:C:111:TYR:O	1:F:67:ARG:NH2	2.41	0.54
1:E:94:ARG:HB3	1:F:8:GLN:NE2	2.21	0.54
1:B:124:PHE:C	1:B:126:LYS:H	2.11	0.54
2:K:498:ARG:CB	1:D:6:ASP:HB3	2.37	0.54
2:P:512:PRO:HB2	2:P:514:PRO:HD3	1.88	0.54
2:K:513:GLY:N	2:K:514:PRO:CD	2.71	0.54
1:A:8:GLN:OE1	1:B:94:ARG:NH1	2.41	0.54
1:E:14:HIS:O	1:E:18:VAL:HG23	2.08	0.54
1:G:32:THR:HA	1:G:46:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:64:GLN:HE21	2:N:514:PRO:HG2	1.73	0.53
1:A:86:LEU:O	1:A:90:MET:HG3	2.09	0.53
1:G:93:SER:HA	1:H:14:HIS:CD2	2.44	0.53
2:M:513:GLY:N	2:M:514:PRO:CD	2.72	0.53
1:F:122:ARG:C	1:F:124:PHE:H	2.12	0.53
1:E:43:PHE:HE2	1:E:84:ASN:HD22	1.57	0.53
1:F:64:GLN:H	1:F:64:GLN:CD	2.12	0.52
1:C:96:ASN:ND2	1:D:8:GLN:HG3	2.24	0.52
2:J:512:PRO:HB2	2:J:514:PRO:HD3	1.90	0.52
1:F:123:LYS:O	1:F:123:LYS:HG3	2.08	0.52
1:A:66:LYS:HA	1:A:69:LEU:HD23	1.90	0.52
1:C:97:LEU:CD2	1:C:105:VAL:HG11	2.38	0.52
1:A:51:MET:SD	1:B:31:LEU:CD1	2.98	0.52
1:E:8:GLN:CG	1:F:96:ASN:ND2	2.50	0.52
1:A:62:THR:CG2	3:A:146:HOH:O	2.57	0.52
1:B:122:ARG:C	1:B:124:PHE:N	2.63	0.52
1:F:110:MET:HG2	1:F:111:TYR:N	2.24	0.52
1:G:28:ARG:HD2	2:P:513:GLY:HA2	1.92	0.51
1:H:62:THR:O	1:H:62:THR:HG22	2.09	0.51
1:C:46:HIS:CD2	1:D:48:THR:HG21	2.46	0.51
1:A:125:ILE:HG22	1:A:128:SER:OG	2.11	0.51
1:H:33:ASP:N	1:H:33:ASP:OD2	2.44	0.50
1:B:47:LYS:O	1:B:51:MET:HG3	2.11	0.50
1:E:98:ARG:HG2	1:F:6:ASP:OD1	2.12	0.50
1:B:6:ASP:O	1:B:7:SER:CB	2.59	0.50
2:M:504:THR:O	2:M:504:THR:HG22	2.12	0.50
1:F:35:VAL:HG13	1:F:44:ARG:HG2	1.93	0.49
1:D:127:ALA:O	1:D:128:SER:CB	2.60	0.49
1:G:126:LYS:HE3	1:G:126:LYS:HA	1.93	0.49
1:A:20:LEU:O	1:A:24:ARG:HG2	2.13	0.49
1:F:106:MET:HE2	1:F:121:CYS:C	2.33	0.49
2:K:513:GLY:N	2:K:514:PRO:HD3	2.27	0.49
1:C:103:MET:HA	1:C:103:MET:CE	2.42	0.49
1:C:122:ARG:C	1:C:124:PHE:H	2.16	0.49
1:E:106:MET:HE2	1:E:121:CYS:HB3	1.95	0.49
1:E:96:ASN:HD21	1:F:8:GLN:HG2	1.72	0.48
1:D:92:THR:O	1:D:93:SER:CB	2.61	0.48
2:O:504:THR:O	2:O:504:THR:CG2	2.61	0.48
1:B:126:LYS:C	1:B:128:SER:H	2.17	0.48
1:A:96:ASN:ND2	1:B:8:GLN:HG2	2.28	0.48
1:E:125:ILE:HG22	1:E:125:ILE:O	2.13	0.48
2:K:501:ILE:HG13	2:K:502:ILE:N	2.27	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:512:PRO:HB2	1:F:28:ARG:HH12	1.78	0.48
1:A:94:ARG:HB3	1:B:8:GLN:NE2	2.28	0.48
1:E:8:GLN:CG	1:F:96:ASN:HD22	2.17	0.47
1:C:13:ARG:HD3	2:L:504:THR:O	2.13	0.47
1:C:64:GLN:HE22	2:N:514:PRO:CD	2.27	0.47
1:C:75:ASP:HB3	1:C:78:ILE:HG12	1.96	0.47
1:E:6:ASP:HA	1:F:98:ARG:HB3	1.95	0.47
1:F:120:THR:O	1:F:124:PHE:HB2	2.15	0.47
1:E:6:ASP:OD1	1:F:98:ARG:HD3	2.14	0.47
1:F:43:PHE:HE2	1:F:84:ASN:HD22	1.63	0.46
1:H:44:ARG:O	3:H:133:HOH:O	2.20	0.46
1:E:21:ASN:O	1:E:25:LEU:HG	2.16	0.46
1:F:106:MET:CE	1:F:121:CYS:CB	2.93	0.46
1:C:21:ASN:HA	1:C:24:ARG:HG2	1.96	0.46
1:A:38:VAL:HG22	1:A:74:LEU:HD12	1.96	0.46
1:C:124:PHE:C	1:C:126:LYS:H	2.18	0.46
1:E:124:PHE:C	1:E:126:LYS:H	2.19	0.46
1:C:35:VAL:HG22	1:C:44:ARG:HD2	1.97	0.46
1:F:20:LEU:O	1:F:24:ARG:HG2	2.16	0.46
1:F:123:LYS:O	1:F:123:LYS:CG	2.64	0.46
1:C:118:VAL:O	1:C:121:CYS:HB2	2.16	0.45
1:D:20:LEU:O	1:D:24:ARG:HG2	2.16	0.45
1:F:106:MET:HE2	1:F:121:CYS:CB	2.47	0.45
1:E:106:MET:HB2	1:E:106:MET:HE2	1.60	0.45
1:F:106:MET:HE2	1:F:121:CYS:HB3	1.99	0.45
1:C:86:LEU:HD12	1:C:108:THR:HB	1.99	0.45
1:A:23:ASN:ND2	1:A:26:ARG:HE	2.15	0.45
2:I:504:THR:HG22	2:I:504:THR:O	2.16	0.45
2:M:501:ILE:HG13	2:M:502:ILE:N	2.31	0.45
1:H:79:ASN:OD1	1:H:104:ALA:HB1	2.17	0.45
1:B:110:MET:HE1	1:H:122:ARG:NE	2.32	0.45
1:H:11:PHE:HB2	1:H:14:HIS:HB2	1.99	0.45
1:B:88:ASP:OD2	3:B:141:HOH:O	2.21	0.44
2:K:498:ARG:CA	1:D:6:ASP:HB3	2.47	0.44
1:A:123:LYS:O	1:A:123:LYS:CG	2.64	0.44
2:K:510:VAL:CG1	1:D:24:ARG:HH12	2.30	0.44
1:B:106:MET:HE2	1:B:121:CYS:HB3	1.99	0.44
1:F:67:ARG:NH1	3:F:134:HOH:O	2.49	0.44
1:F:122:ARG:O	1:F:124:PHE:N	2.51	0.44
1:C:106:MET:CE	1:C:121:CYS:HB3	2.48	0.44
1:H:47:LYS:O	1:H:51:MET:HG3	2.18	0.44
1:A:6:ASP:OD1	1:B:98:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:137:HOH:O	1:F:62:THR:CG2	2.65	0.44
1:H:62:THR:CG2	1:H:62:THR:O	2.65	0.44
1:F:85:ILE:HD13	1:F:96:ASN:O	2.17	0.43
1:A:125:ILE:CG2	1:A:128:SER:OG	2.66	0.43
1:D:24:ARG:HH11	1:D:24:ARG:CG	2.24	0.43
1:D:63:ASP:OD1	1:D:63:ASP:C	2.57	0.43
1:F:23:ASN:HD21	1:F:26:ARG:HH21	1.66	0.43
1:F:28:ARG:CB	1:F:30:ILE:HD12	2.48	0.43
1:G:92:THR:O	1:G:93:SER:CB	2.67	0.43
1:C:96:ASN:HD21	1:D:8:GLN:HG3	1.83	0.43
2:L:513:GLY:N	2:L:514:PRO:CD	2.82	0.43
1:C:8:GLN:CD	1:D:94:ARG:HG2	2.39	0.43
1:H:122:ARG:C	1:H:124:PHE:N	2.72	0.43
2:M:512:PRO:CB	2:M:514:PRO:HD2	2.49	0.42
1:E:121:CYS:O	1:E:124:PHE:HB3	2.20	0.42
2:J:512:PRO:HB2	2:J:514:PRO:CD	2.49	0.42
1:F:75:ASP:HA	1:F:76:PRO:HD3	1.80	0.42
1:E:53:CYS:SG	1:E:90:MET:HG2	2.59	0.42
1:G:96:ASN:CG	1:H:8:GLN:HG3	2.39	0.42
1:B:6:ASP:HB3	1:B:7:SER:H	1.68	0.42
1:A:126:LYS:HA	1:A:126:LYS:HE3	2.00	0.42
1:H:23:ASN:HD21	1:H:26:ARG:HH21	1.68	0.42
1:H:106:MET:HE2	1:H:106:MET:HB2	1.89	0.42
2:K:513:GLY:HA2	1:D:28:ARG:HD2	2.02	0.42
2:K:500:GLU:H	2:K:500:GLU:HG3	1.67	0.42
1:H:35:VAL:CG2	3:H:137:HOH:O	2.68	0.42
1:C:106:MET:HB2	1:C:106:MET:HE2	1.88	0.42
1:G:35:VAL:HG22	1:G:44:ARG:NH1	2.34	0.42
1:B:110:MET:HE2	1:H:122:ARG:HE	1.85	0.42
1:E:87:LEU:HD12	1:E:87:LEU:HA	1.85	0.42
1:E:66:LYS:HA	1:E:69:LEU:HD22	2.02	0.42
2:M:512:PRO:C	2:M:514:PRO:HD2	2.40	0.41
1:G:75:ASP:HA	1:G:76:PRO:HD3	1.79	0.41
2:K:504:THR:O	2:K:504:THR:CG2	2.68	0.41
1:H:122:ARG:O	1:H:123:LYS:C	2.59	0.41
2:K:498:ARG:HA	1:D:6:ASP:C	2.41	0.41
1:A:9:ILE:HG12	2:J:501:ILE:HG12	2.03	0.41
1:B:110:MET:CE	1:H:122:ARG:NE	2.84	0.41
1:A:23:ASN:HD22	1:A:26:ARG:HE	1.67	0.41
1:C:86:LEU:HD13	1:C:112:LEU:HD12	2.03	0.41
1:A:75:ASP:HA	1:A:76:PRO:HD3	1.84	0.41
1:A:26:ARG:HD3	1:A:91:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:13:ARG:CD	2:L:504:THR:O	2.69	0.41
1:H:110:MET:HE3	1:H:110:MET:HB2	1.96	0.41
1:F:28:ARG:CB	1:F:30:ILE:CD1	2.98	0.41
1:A:124:PHE:O	1:A:126:LYS:N	2.54	0.41
1:C:106:MET:HE2	1:C:121:CYS:HB3	2.03	0.41
1:E:11:PHE:CD1	1:F:89:PHE:HE1	2.38	0.41
1:H:20:LEU:HG	1:H:20:LEU:O	2.17	0.41
1:B:79:ASN:HA	1:B:80:PRO:HD3	1.98	0.41
1:H:38:VAL:HG22	1:H:74:LEU:HD12	2.02	0.41
2:J:513:GLY:N	2:J:514:PRO:CD	2.84	0.40
1:C:6:ASP:OD2	1:D:98:ARG:HG3	2.21	0.40
1:F:38:VAL:HG13	1:F:78:ILE:HB	2.02	0.40
1:G:124:PHE:C	1:G:126:LYS:H	2.25	0.40
1:G:99:GLU:O	1:G:102:ILE:HG22	2.21	0.40
1:D:66:LYS:O	1:D:67:ARG:C	2.60	0.40
2:K:498:ARG:HA	1:D:6:ASP:O	2.21	0.40
1:C:28:ARG:NH1	2:L:512:PRO:O	2.52	0.40
1:C:55:GLY:HA3	1:E:29:ASP:OD1	2.21	0.40
1:F:47:LYS:O	1:F:51:MET:HG3	2.22	0.40
1:A:48:THR:HG23	3:A:153:HOH:O	2.21	0.40
2:N:513:GLY:N	2:N:514:PRO:HD3	2.37	0.40
1:C:103:MET:HE2	1:C:103:MET:HA	2.03	0.40
1:C:98:ARG:O	1:C:102:ILE:HB	2.22	0.40
1:F:38:VAL:CG1	1:F:78:ILE:HB	2.51	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	123/127 (97%)	111 (90%)	11 (9%)	1 (1%)	27	53
1	B	122/127 (96%)	112 (92%)	6 (5%)	4 (3%)	6	9
1	C	123/127 (97%)	112 (91%)	8 (6%)	3 (2%)	9	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	122/127 (96%)	109 (89%)	12 (10%)	1 (1%)	27	53
1	E	121/127 (95%)	113 (93%)	7 (6%)	1 (1%)	27	53
1	F	120/127 (94%)	111 (92%)	7 (6%)	2 (2%)	14	26
1	G	120/127 (94%)	110 (92%)	9 (8%)	1 (1%)	27	53
1	H	120/127 (94%)	108 (90%)	11 (9%)	1 (1%)	27	53
2	I	15/19 (79%)	15 (100%)	0	0	100	100
2	J	15/19 (79%)	15 (100%)	0	0	100	100
2	K	15/19 (79%)	14 (93%)	1 (7%)	0	100	100
2	L	14/19 (74%)	14 (100%)	0	0	100	100
2	M	15/19 (79%)	14 (93%)	1 (7%)	0	100	100
2	N	14/19 (74%)	14 (100%)	0	0	100	100
2	O	15/19 (79%)	13 (87%)	2 (13%)	0	100	100
2	P	15/19 (79%)	14 (93%)	1 (7%)	0	100	100
All	All	1089/1168 (93%)	999 (92%)	76 (7%)	14 (1%)	18	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	SER
1	B	123	LYS
1	A	125	ILE
1	C	123	LYS
1	C	125	ILE
1	F	123	LYS
1	G	125	ILE
1	D	126	LYS
1	E	125	ILE
1	H	123	LYS
1	B	125	ILE
1	B	127	ALA
1	F	39	SER
1	C	102	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/115 (99%)	97 (85%)	17 (15%)	4	7
1	B	113/115 (98%)	101 (89%)	12 (11%)	10	18
1	C	114/115 (99%)	97 (85%)	17 (15%)	4	7
1	D	113/115 (98%)	104 (92%)	9 (8%)	17	33
1	E	113/115 (98%)	97 (86%)	16 (14%)	5	8
1	F	112/115 (97%)	99 (88%)	13 (12%)	8	14
1	G	112/115 (97%)	101 (90%)	11 (10%)	12	21
1	H	112/115 (97%)	102 (91%)	10 (9%)	14	26
2	I	15/16 (94%)	14 (93%)	1 (7%)	23	44
2	J	15/16 (94%)	9 (60%)	6 (40%)	0	0
2	K	15/16 (94%)	14 (93%)	1 (7%)	23	44
2	L	14/16 (88%)	11 (79%)	3 (21%)	1	2
2	M	15/16 (94%)	14 (93%)	1 (7%)	23	44
2	N	14/16 (88%)	13 (93%)	1 (7%)	21	40
2	O	15/16 (94%)	11 (73%)	4 (27%)	1	1
2	P	15/16 (94%)	11 (73%)	4 (27%)	1	1
All	All	1021/1048 (97%)	895 (88%)	126 (12%)	7	13

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	10	GLN
1	A	13	ARG
1	A	20	LEU
1	A	24	ARG
1	A	31	LEU
1	A	54	SER
1	A	59	SER
1	A	62	THR
1	A	67	ARG
1	A	94	ARG
1	A	98	ARG
1	A	102	ILE
1	A	115	GLU

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Mol	Chain	Res	Type
1	A	125	ILE
1	A	126	LYS
1	A	129	GLU
2	I	500	GLU
1	B	7	SER
1	B	10	GLN
1	B	13	ARG
1	B	20	LEU
1	B	24	ARG
1	B	35	VAL
1	B	62	THR
1	B	64	GLN
1	B	69	LEU
1	B	98	ARG
1	B	106	MET
1	B	126	LYS
2	J	498	ARG
2	J	499	SER
2	J	500	GLU
2	J	501	ILE
2	J	502	ILE
2	J	504	THR
1	C	23	ASN
1	C	24	ARG
1	C	31	LEU
1	C	54	SER
1	C	62	THR
1	C	64	GLN
1	C	65	LEU
1	C	69	LEU
1	C	94	ARG
1	C	98	ARG
1	C	102	ILE
1	C	106	MET
1	C	110	MET
1	C	115	GLU
1	C	119	ASP
1	C	123	LYS
1	C	129	GLU
2	K	500	GLU
1	D	8	GLN
1	D	31	LEU

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Mol	Chain	Res	Type
1	D	62	THR
1	D	64	GLN
1	D	69	LEU
1	D	77	GLU
1	D	94	ARG
1	D	102	ILE
1	D	126	LYS
2	L	499	SER
2	L	500	GLU
2	L	504	THR
1	E	6	ASP
1	E	8	GLN
1	E	24	ARG
1	E	31	LEU
1	E	35	VAL
1	E	42	GLN
1	E	54	SER
1	E	64	GLN
1	E	67	ARG
1	E	69	LEU
1	E	70	SER
1	E	86	LEU
1	E	106	MET
1	E	115	GLU
1	E	126	LYS
1	E	128	SER
2	M	500	GLU
1	F	8	GLN
1	F	13	ARG
1	F	20	LEU
1	F	35	VAL
1	F	38	VAL
1	F	41	GLU
1	F	54	SER
1	F	62	THR
1	F	64	GLN
1	F	93	SER
1	F	102	ILE
1	F	110	MET
1	F	126	LYS
2	N	499	SER
1	G	13	ARG

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Mol	Chain	Res	Type
1	G	24	ARG
1	G	27	SER
1	G	40	ARG
1	G	54	SER
1	G	62	THR
1	G	64	GLN
1	G	69	LEU
1	G	86	LEU
1	G	125	ILE
1	G	126	LYS
2	O	498	ARG
2	O	499	SER
2	O	500	GLU
2	O	501	ILE
1	H	6	ASP
1	H	8	GLN
1	H	13	ARG
1	H	24	ARG
1	H	54	SER
1	H	64	GLN
1	H	65	LEU
1	H	103	MET
1	H	125	ILE
1	H	126	LYS
2	P	498	ARG
2	P	499	SER
2	P	504	THR
2	P	506	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	96	ASN
1	B	8	GLN
1	B	10	GLN
1	B	23	ASN
1	B	96	ASN
1	C	10	GLN
1	C	23	ASN
1	C	64	GLN
1	C	96	ASN

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Mol	Chain	Res	Type
1	C	113	GLN
1	D	23	ASN
1	D	96	ASN
1	E	23	ASN
1	E	84	ASN
1	E	96	ASN
1	F	8	GLN
1	F	23	ASN
1	F	84	ASN
1	F	96	ASN
1	F	101	ASN
1	G	8	GLN
1	G	23	ASN
1	G	84	ASN
1	G	96	ASN
1	H	23	ASN
1	H	96	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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(Å²)	Q<0.9	
1	A	125/127 (98%)	-0.03	4 (3%)	45	42	40, 58, 98, 124	0
1	B	124/127 (97%)	-0.00	3 (2%)	56	53	41, 56, 95, 116	0
1	C	125/127 (98%)	0.33	11 (8%)	10	7	46, 70, 112, 134	0
1	D	124/127 (97%)	-0.16	4 (3%)	45	42	43, 55, 98, 114	0
1	E	123/127 (96%)	0.04	1 (0%)	83	85	48, 67, 97, 125	0
1	F	122/127 (96%)	0.04	7 (5%)	23	19	50, 67, 100, 115	0
1	G	122/127 (96%)	-0.02	4 (3%)	44	41	50, 72, 103, 125	0
1	H	122/127 (96%)	0.08	5 (4%)	35	32	55, 75, 107, 117	0
2	I	17/19 (89%)	1.18	3 (17%)	2	1	59, 70, 109, 116	0
2	J	17/19 (89%)	0.21	2 (11%)	5	4	49, 58, 105, 113	0
2	K	17/19 (89%)	1.22	5 (29%)	1	1	61, 81, 119, 122	0
2	L	16/19 (84%)	0.44	4 (25%)	1	1	64, 77, 104, 104	0
2	M	17/19 (89%)	0.88	5 (29%)	1	1	68, 82, 115, 122	0
2	N	16/19 (84%)	1.07	2 (12%)	5	3	61, 78, 107, 107	0
2	O	17/19 (89%)	1.36	6 (35%)	1	1	68, 93, 123, 126	0
2	P	17/19 (89%)	1.20	4 (23%)	1	1	79, 97, 122, 127	0
All	All	1121/1168 (95%)	0.14	70 (6%)	20	17	40, 68, 109, 134	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	499	SER	7.8
2	P	514	PRO	7.3
2	K	499	SER	6.6
2	M	499	SER	5.7
1	D	5	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	127	ALA	5.5
2	J	498	ARG	5.3
2	O	502	ILE	5.2
2	O	499	SER	5.0
2	O	498	ARG	5.0
2	N	499	SER	5.0
1	A	5	ALA	4.8
2	M	498	ARG	4.8
1	C	129	GLU	4.6
2	N	500	GLU	4.6
1	F	5	ALA	4.4
2	O	500	GLU	4.3
2	P	498	ARG	4.1
2	K	514	PRO	4.1
2	P	499	SER	4.0
1	C	40	ARG	3.8
1	E	6	ASP	3.7
1	C	128	SER	3.7
2	O	501	ILE	3.6
2	L	514	PRO	3.5
1	C	97	LEU	3.5
1	C	98	ARG	3.5
1	D	6	ASP	3.4
1	F	98	ARG	3.3
2	K	500	GLU	3.2
2	K	498	ARG	3.2
2	L	499	SER	3.2
1	H	98	ARG	3.1
2	M	514	PRO	3.1
1	A	128	SER	3.1
2	O	514	PRO	3.0
1	D	7	SER	2.9
2	I	500	GLU	2.9
1	F	124	PHE	2.9
2	J	499	SER	2.9
2	K	501	ILE	2.8
2	I	498	ARG	2.8
2	P	500	GLU	2.8
1	C	126	LYS	2.8
1	D	127	ALA	2.7
1	C	99	GLU	2.5
1	G	128	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	7	SER	2.5
1	C	127	ALA	2.5
2	M	500	GLU	2.4
1	G	99	GLU	2.4
1	A	6	ASP	2.4
1	B	5	ALA	2.4
1	B	128	SER	2.3
1	F	101	ASN	2.3
1	F	97	LEU	2.3
1	C	38	VAL	2.2
1	F	6	ASP	2.2
1	C	124	PHE	2.2
1	H	40	ARG	2.2
1	H	97	LEU	2.2
2	L	513	GLY	2.2
2	M	502	ILE	2.2
1	C	5	ALA	2.1
1	B	6	ASP	2.1
1	H	64	GLN	2.1
1	G	98	ARG	2.1
2	L	500	GLU	2.1
1	G	40	ARG	2.0
1	F	99	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.