



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 11:07 pm BST

PDB ID : 2WJ7  
Title : human alphaB crystallin  
Authors : Naylor, C.E.; Bagneris, C.; Bateman, O.A.; Cronin, N.; Keep, N.H.; Slingsby, C.  
Deposited on : 2009-05-22  
Resolution : 2.63 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

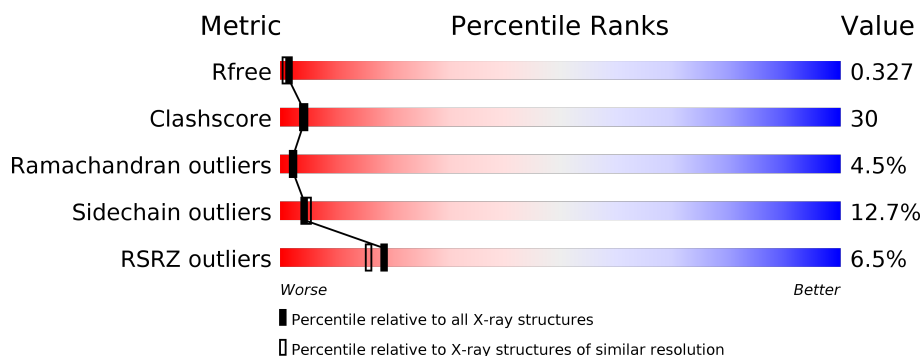
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	94	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>27%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	94	<div> <div>2%</div> <div> <div></div> <div>41%</div> <div>21%</div> <div>14%</div> <div>23%</div> </div> </div>
1	C	94	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>9%</div> <div>10%</div> </div> </div>
1	D	94	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>22%</div> <div>12%</div> <div>24%</div> </div> </div>
1	E	94	<div> <div>17%</div> <div> <div></div> <div>43%</div> <div>30%</div> <div>6%</div> <div>21%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3038 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.

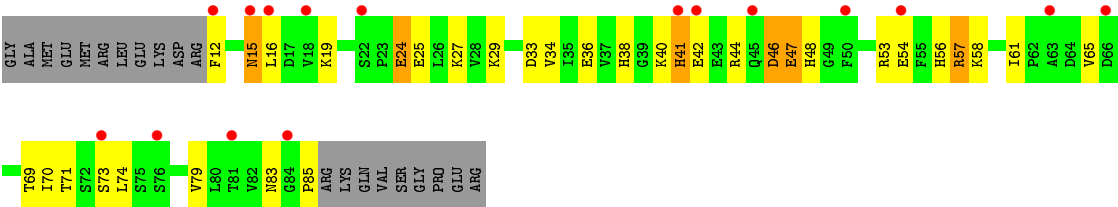
- Molecule 1 is a protein called ALPHA-CRYSTALLIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			650	409	113	127	1			
1	B	72	Total	C	N	O		0	0	0
			560	353	101	106				
1	C	85	Total	C	N	O	S	0	0	0
			640	401	113	125	1			
1	D	71	Total	C	N	O		0	0	0
			528	331	95	102				
1	E	74	Total	C	N	O		0	0	0
			575	363	100	112				

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total	O	0	0
			24	24		
2	B	26	Total	O	0	0
			26	26		
2	C	24	Total	O	0	0
			24	24		
2	D	5	Total	O	0	0
			5	5		
2	E	6	Total	O	0	0
			6	6		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.46 Å 66.07 Å 190.97 Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	39.03 – 2.63 63.59 – 2.63	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.03-2.63) 96.8 (63.59-2.63)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.252 , 0.320 0.256 , 0.327	Depositor DCC
$R_{free}$ test set	916 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.20	2/663 (0.3%)	1.17	4/899 (0.4%)
1	B	1.06	0/571	1.07	1/773 (0.1%)
1	C	0.98	0/653	1.03	0/885
1	D	0.92	0/538	1.03	1/732 (0.1%)
1	E	0.87	0/588	0.91	0/797
All	All	1.02	2/3013 (0.1%)	1.05	6/4086 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLU	CG-CD	7.56	1.63	1.51
1	A	4	GLU	CB-CG	7.37	1.66	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	D	51	ILE	CB-CA-C	-6.84	97.91	111.60
1	B	16	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	A	53	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	26	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	A	4	GLU	OE1-CD-OE2	-5.04	117.26	123.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	650	0	603	30	0
1	B	560	0	543	51	0
1	C	640	0	578	24	1
1	D	528	0	490	40	0
1	E	575	0	546	30	0
2	A	24	0	0	5	0
2	B	26	0	0	4	0
2	C	24	0	0	2	0
2	D	5	0	0	1	0
2	E	6	0	0	0	0
All	All	3038	0	2760	172	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (172) 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:D:41:HIS:HE1	1:D:53:ARG:HH11	1.05	0.98
1:B:41:HIS:CE1	1:B:53:ARG:HH11	1.84	0.95
1:E:41:HIS:CE1	1:E:53:ARG:HH11	1.84	0.95
1:E:41:HIS:HE1	1:E:53:ARG:HH11	0.96	0.95
1:D:41:HIS:CE1	1:D:53:ARG:HH11	1.85	0.94
1:A:9:LYS:NZ	2:A:2003:HOH:O	1.96	0.94
1:B:33:ASP:O	1:B:61:ILE:HG13	1.69	0.93
1:C:41:HIS:HE1	1:C:53:ARG:HH11	1.07	0.93
1:A:41:HIS:HE1	1:A:53:ARG:HH11	0.97	0.93
1:E:12:PHE:HE2	1:E:65:VAL:HG11	1.32	0.92
1:A:41:HIS:CE1	1:A:53:ARG:HH11	1.87	0.90
1:B:41:HIS:HE1	1:B:53:ARG:HH11	0.97	0.90
1:B:41:HIS:HE1	1:B:53:ARG:NH1	1.72	0.87
1:D:65:VAL:CA	1:D:66:ASP:HB2	2.04	0.87
1:E:33:ASP:OD1	1:E:34:VAL:HG23	1.75	0.87
1:E:41:HIS:HE1	1:E:53:ARG:NH1	1.73	0.86
1:D:65:VAL:HA	1:D:66:ASP:HB2	1.57	0.86
1:B:65:VAL:HA	1:B:66:ASP:HB2	1.57	0.85
1:D:65:VAL:HA	1:D:66:ASP:CB	2.06	0.85
1:B:71:THR:HG22	2:C:2023:HOH:O	1.78	0.84
1:A:9:LYS:CE	2:A:2003:HOH:O	2.24	0.84
1:B:65:VAL:CA	1:B:66:ASP:HB2	2.07	0.84
1:D:41:HIS:HE1	1:D:53:ARG:NH1	1.74	0.84
1:B:65:VAL:HA	1:B:66:ASP:CB	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2004:HOH:O	1:E:71:THR:HA	1.81	0.79
1:A:41:HIS:HE1	1:A:53:ARG:NH1	1.80	0.79
1:B:68:LEU:O	1:B:70:ILE:N	2.16	0.79
1:E:12:PHE:CE2	1:E:65:VAL:HG11	2.16	0.79
1:A:9:LYS:HZ2	1:A:9:LYS:HB3	1.48	0.78
1:C:41:HIS:CE1	1:C:53:ARG:HH11	1.97	0.77
1:D:64:ASP:O	1:D:65:VAL:HG23	1.86	0.76
1:A:9:LYS:CB	1:A:9:LYS:HZ2	2.00	0.75
1:D:65:VAL:HG13	1:D:66:ASP:HB2	1.67	0.74
1:E:69:THR:OG1	1:E:85:PRO:HD2	1.87	0.73
1:D:31:LEU:HD12	1:D:36:GLU:OE2	1.89	0.72
1:B:65:VAL:HG13	1:B:66:ASP:HB2	1.71	0.72
1:D:65:VAL:CB	1:D:66:ASP:HB2	2.21	0.70
1:C:41:HIS:HE1	1:C:53:ARG:NH1	1.86	0.70
1:C:86:ARG:O	1:C:87:LYS:CB	2.39	0.70
1:A:45:GLN:NE2	2:A:2015:HOH:O	2.25	0.69
1:A:9:LYS:HE3	2:A:2003:HOH:O	1.86	0.69
1:B:61:ILE:HB	1:B:65:VAL:HG12	1.75	0.69
1:E:74:LEU:HD12	1:E:79:VAL:O	1.93	0.68
1:D:68:LEU:O	1:D:70:ILE:N	2.28	0.67
1:D:57:ARG:HG3	1:D:58:LYS:N	2.10	0.66
1:B:33:ASP:O	1:B:61:ILE:CG1	2.42	0.66
1:B:70:ILE:HA	1:B:83:ASN:O	1.97	0.65
1:D:65:VAL:CG1	1:D:66:ASP:HB2	2.25	0.65
1:D:41:HIS:CE1	1:D:53:ARG:NH1	2.58	0.65
1:A:69:THR:OG1	1:A:85:PRO:HD2	1.98	0.64
1:B:61:ILE:O	1:B:63:ALA:N	2.31	0.64
1:B:64:ASP:O	1:B:65:VAL:HG23	1.98	0.63
1:A:31:LEU:HD12	1:A:36:GLU:OE2	1.98	0.63
1:D:25:GLU:HB3	1:D:40:LYS:O	1.97	0.63
1:E:24:GLU:H	1:E:24:GLU:CD	2.02	0.63
1:A:9:LYS:CB	1:A:9:LYS:NZ	2.62	0.63
1:D:66:ASP:OD1	1:D:69:THR:HG21	1.98	0.62
1:B:38:HIS:HE1	1:B:54:GLU:OE2	1.83	0.62
1:D:66:ASP:HB3	1:D:69:THR:OG1	2.00	0.62
1:B:31:LEU:HD23	2:B:2017:HOH:O	1.99	0.62
1:B:31:LEU:HD12	1:B:36:GLU:OE2	1.99	0.61
1:B:65:VAL:CB	1:B:66:ASP:HB2	2.31	0.61
1:C:24:GLU:H	1:C:24:GLU:CD	2.03	0.61
1:C:3:MET:HB2	1:C:15:ASN:O	2.00	0.61
1:C:9:LYS:NZ	1:C:9:LYS:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:CG1	1:B:66:ASP:HB2	2.31	0.60
1:C:41:HIS:HD2	1:C:42:GLU:O	1.83	0.60
1:B:29:LYS:HE2	2:B:2017:HOH:O	2.02	0.60
1:D:66:ASP:O	1:D:67:PRO:O	2.20	0.60
1:C:9:LYS:NZ	1:C:9:LYS:CB	2.64	0.60
1:B:15:ASN:N	1:B:15:ASN:HD22	2.01	0.59
1:E:25:GLU:HB3	1:E:40:LYS:O	2.03	0.59
1:A:15:ASN:N	1:A:15:ASN:HD22	2.01	0.58
1:E:57:ARG:HG3	1:E:58:LYS:N	2.17	0.58
1:B:66:ASP:HB3	1:B:69:THR:OG1	2.03	0.58
1:E:33:ASP:O	1:E:61:ILE:HD12	2.03	0.58
1:B:66:ASP:O	1:B:67:PRO:O	2.21	0.58
1:B:41:HIS:CE1	1:B:53:ARG:NH1	2.58	0.57
1:D:64:ASP:O	1:D:64:ASP:OD2	2.22	0.57
1:D:63:ALA:C	1:D:65:VAL:H	2.07	0.57
1:B:33:ASP:CB	1:B:61:ILE:HD11	2.35	0.56
1:A:24:GLU:H	1:A:24:GLU:CD	2.08	0.56
1:C:12:PHE:HE2	1:C:65:VAL:HG11	1.71	0.56
1:C:9:LYS:HZ2	1:C:9:LYS:HB2	1.69	0.56
1:B:64:ASP:O	1:B:64:ASP:OD2	2.24	0.56
1:B:67:PRO:O	1:B:68:LEU:C	2.43	0.56
1:B:41:HIS:HD2	1:B:42:GLU:O	1.88	0.55
1:B:63:ALA:C	1:B:65:VAL:H	2.07	0.55
1:C:15:ASN:N	1:C:15:ASN:HD22	2.02	0.55
1:A:14:VAL:C	1:A:15:ASN:HD22	2.10	0.55
1:E:41:HIS:HD2	1:E:42:GLU:O	1.90	0.55
1:E:71:THR:N	1:E:83:ASN:O	2.40	0.54
1:A:57:ARG:HG3	1:A:58:LYS:N	2.21	0.54
1:E:36:GLU:HB3	1:E:56:HIS:HE1	1.72	0.54
1:B:57:ARG:HG3	1:B:58:LYS:N	2.22	0.54
1:E:46:ASP:O	1:E:47:GLU:CB	2.55	0.54
1:A:9:LYS:NZ	1:A:9:LYS:HB2	2.22	0.53
1:A:49:GLY:HA2	1:B:60:ARG:NH1	2.24	0.53
1:E:46:ASP:OD2	1:E:48:HIS:HB2	2.07	0.53
1:E:15:ASN:C	1:E:16:LEU:HD12	2.29	0.53
1:A:43:GLU:OE2	1:B:58:LYS:HE2	2.10	0.52
1:E:29:LYS:HB2	1:E:29:LYS:NZ	2.25	0.52
1:A:12:PHE:HE2	1:A:65:VAL:HG11	1.75	0.52
1:D:15:ASN:HD22	1:D:15:ASN:N	2.07	0.52
1:A:73:SER:O	1:A:80:LEU:HD12	2.10	0.51
1:E:41:HIS:CE1	1:E:53:ARG:NH1	2.60	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:C	2:B:2013:HOH:O	2.48	0.51
1:D:15:ASN:C	1:D:16:LEU:HD12	2.31	0.51
1:D:41:HIS:HD2	1:D:42:GLU:O	1.94	0.51
1:D:63:ALA:C	1:D:65:VAL:N	2.64	0.51
1:E:41:HIS:C	1:E:41:HIS:CD2	2.85	0.50
1:C:30:VAL:HG11	1:C:67:PRO:HB3	1.92	0.50
1:D:51:ILE:HD13	1:D:53:ARG:HH12	1.77	0.50
1:D:38:HIS:HE1	1:D:54:GLU:OE2	1.94	0.50
1:C:14:VAL:C	1:C:15:ASN:HD22	2.14	0.50
1:B:63:ALA:C	1:B:65:VAL:N	2.65	0.50
1:E:33:ASP:N	1:E:33:ASP:OD1	2.44	0.50
1:E:38:HIS:HE1	1:E:54:GLU:OE2	1.93	0.50
1:C:44:ARG:NH1	2:C:2014:HOH:O	2.26	0.50
1:C:38:HIS:HE1	1:C:54:GLU:OE2	1.94	0.50
1:E:70:ILE:HA	1:E:83:ASN:O	2.11	0.50
1:C:36:GLU:HB3	1:C:56:HIS:HE1	1.77	0.49
1:B:33:ASP:CG	1:B:61:ILE:HD11	2.32	0.49
1:D:70:ILE:HA	1:D:83:ASN:O	2.12	0.49
1:B:29:LYS:HE3	1:B:29:LYS:CA	2.41	0.49
1:D:67:PRO:O	1:D:68:LEU:C	2.51	0.49
1:D:40:LYS:HG2	1:D:41:HIS:H	1.79	0.48
1:C:57:ARG:HG3	1:C:58:LYS:N	2.26	0.48
1:D:40:LYS:HG2	1:D:41:HIS:N	2.28	0.48
1:E:12:PHE:CD2	1:E:65:VAL:HG21	2.48	0.48
1:D:65:VAL:HG13	1:D:66:ASP:CB	2.39	0.48
1:A:41:HIS:HD2	1:A:42:GLU:O	1.96	0.48
1:D:65:VAL:HG22	1:D:66:ASP:OD2	2.14	0.47
1:A:78:GLY:HA2	2:A:2010:HOH:O	2.15	0.47
1:B:35:ILE:O	1:B:58:LYS:HA	2.15	0.47
1:B:62:PRO:O	1:B:64:ASP:N	2.48	0.46
1:C:12:PHE:CE2	1:C:65:VAL:HG11	2.50	0.46
1:A:12:PHE:CE2	1:A:65:VAL:HG11	2.50	0.46
1:B:33:ASP:O	1:B:61:ILE:CD1	2.64	0.46
1:A:38:HIS:HE1	1:A:54:GLU:OE2	1.98	0.46
1:B:66:ASP:OD1	1:B:69:THR:HG21	2.16	0.46
1:B:33:ASP:OD1	1:B:61:ILE:HD11	2.16	0.45
1:A:15:ASN:C	1:A:16:LEU:HD12	2.36	0.45
1:E:15:ASN:HD22	1:E:15:ASN:N	2.13	0.45
1:D:61:ILE:HA	1:D:62:PRO:HD3	1.78	0.45
1:C:9:LYS:HZ3	1:C:9:LYS:CB	2.29	0.45
1:A:4:GLU:HG2	1:A:5:MET:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:C	1:B:15:ASN:HD22	2.20	0.44
1:C:9:LYS:HZ3	1:C:9:LYS:HB3	1.82	0.44
1:D:45:GLN:HG2	1:D:46:ASP:H	1.83	0.44
1:B:65:VAL:HG13	1:B:66:ASP:CB	2.45	0.44
1:D:62:PRO:O	1:D:64:ASP:N	2.49	0.44
1:D:65:VAL:HA	1:D:66:ASP:CG	2.38	0.44
1:B:15:ASN:C	1:B:16:LEU:HD12	2.38	0.44
1:B:19:LYS:HB3	2:B:2009:HOH:O	2.18	0.43
1:B:38:HIS:CE1	1:B:54:GLU:OE2	2.68	0.43
1:B:61:ILE:HD12	1:B:61:ILE:N	2.33	0.43
1:A:41:HIS:C	1:A:41:HIS:CD2	2.91	0.43
1:A:41:HIS:CE1	1:A:53:ARG:NH1	2.67	0.43
1:B:65:VAL:HA	1:B:66:ASP:CG	2.40	0.43
1:E:41:HIS:CD2	1:E:41:HIS:O	2.71	0.42
1:E:70:ILE:HG23	1:E:83:ASN:O	2.19	0.42
1:D:38:HIS:CE1	1:D:54:GLU:OE2	2.72	0.42
1:A:46:ASP:OD2	1:A:51:ILE:HG21	2.19	0.42
1:D:81:THR:HG22	1:D:82:VAL:N	2.35	0.42
1:E:40:LYS:O	1:E:41:HIS:HB3	2.20	0.41
1:B:40:LYS:HG2	1:B:41:HIS:N	2.35	0.41
1:C:55:PHE:CD1	1:C:55:PHE:C	2.94	0.41
1:B:61:ILE:HA	1:B:62:PRO:HD3	1.74	0.41
1:C:15:ASN:C	1:C:16:LEU:HD12	2.41	0.41
1:C:57:ARG:NH2	1:D:46:ASP:OD1	2.52	0.40
1:D:74:LEU:HD12	1:D:79:VAL:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LEU:N	1:C:45:GLN:NE2[3_445]	1.90	0.30

## 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	83/94 (88%)	79 (95%)	3 (4%)	1 (1%)	13	18
1	B	70/94 (74%)	59 (84%)	5 (7%)	6 (9%)	1	0
1	C	83/94 (88%)	79 (95%)	4 (5%)	0	100	100
1	D	69/94 (73%)	58 (84%)	4 (6%)	7 (10%)	0	0
1	E	72/94 (77%)	64 (89%)	5 (7%)	3 (4%)	3	2
All	All	377/470 (80%)	339 (90%)	21 (6%)	17 (4%)	2	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	PRO
1	B	69	THR
1	D	67	PRO
1	D	69	THR
1	E	47	GLU
1	A	4	GLU
1	B	64	ASP
1	D	64	ASP
1	D	66	ASP
1	D	68	LEU
1	E	46	ASP
1	B	62	PRO
1	B	66	ASP
1	D	62	PRO
1	E	19	LYS
1	D	65	VAL
1	B	65	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	69/85 (81%)	62 (90%)	7 (10%)	7	10
1	B	62/85 (73%)	54 (87%)	8 (13%)	4	5
1	C	65/85 (76%)	54 (83%)	11 (17%)	2	2
1	D	55/85 (65%)	48 (87%)	7 (13%)	4	5
1	E	64/85 (75%)	57 (89%)	7 (11%)	6	8
All	All	315/425 (74%)	275 (87%)	40 (13%)	4	5

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	LYS
1	A	41	HIS
1	A	44	ARG
1	A	47	GLU
1	A	57	ARG
1	A	73	SER
1	B	15	ASN
1	B	29	LYS
1	B	41	HIS
1	B	51	ILE
1	B	55	PHE
1	B	57	ARG
1	B	60	ARG
1	B	61	ILE
1	C	8	GLU
1	C	9	LYS
1	C	15	ASN
1	C	24	GLU
1	C	41	HIS
1	C	44	ARG
1	C	45	GLN
1	C	55	PHE
1	C	57	ARG
1	C	73	SER
1	C	83	ASN
1	D	15	ASN
1	D	41	HIS
1	D	44	ARG
1	D	51	ILE
1	D	56	HIS

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Mol	Chain	Res	Type
1	D	57	ARG
1	D	83	ASN
1	E	15	ASN
1	E	24	GLU
1	E	27	LYS
1	E	41	HIS
1	E	44	ARG
1	E	57	ARG
1	E	73	SER

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

Mol	Chain	Res	Type
1	A	15	ASN
1	A	38	HIS
1	A	41	HIS
1	B	15	ASN
1	B	20	HIS
1	B	38	HIS
1	B	41	HIS
1	C	15	ASN
1	C	20	HIS
1	C	38	HIS
1	C	41	HIS
1	C	56	HIS
1	D	15	ASN
1	D	38	HIS
1	D	41	HIS
1	E	15	ASN
1	E	20	HIS
1	E	38	HIS
1	E	41	HIS
1	E	56	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	85/94 (90%)	0.56	2 (2%) 59 55	28, 48, 78, 88	0
1	B	72/94 (76%)	0.58	2 (2%) 53 49	33, 56, 94, 104	0
1	C	85/94 (90%)	0.55	3 (3%) 44 40	36, 55, 81, 107	0
1	D	71/94 (75%)	0.42	2 (2%) 53 49	43, 64, 103, 112	0
1	E	74/94 (78%)	1.26	16 (21%) 0 0	54, 74, 106, 119	0
All	All	387/470 (82%)	0.67	25 (6%) 18 16	28, 59, 96, 119	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	63	ALA	11.1
1	B	61	ILE	5.4
1	E	45	GLN	4.7
1	B	34	VAL	4.6
1	E	50	PHE	3.8
1	E	66	ASP	3.7
1	E	22	SER	3.7
1	E	76	SER	3.3
1	E	16	LEU	2.8
1	C	32	GLY	2.8
1	E	81	THR	2.7
1	A	39	GLY	2.7
1	D	34	VAL	2.5
1	E	42	GLU	2.4
1	E	84	GLY	2.4
1	E	54	GLU	2.4
1	E	12	PHE	2.4
1	E	18	VAL	2.3
1	E	73	SER	2.3
1	C	12	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	85	PRO	2.2
1	A	12	PHE	2.2
1	D	83	ASN	2.2
1	E	41	HIS	2.2
1	E	15	ASN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.