



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:23 PM UTC

PDB ID : 4PH0 / pdb\_00004ph0  
Title : capsid protein from bovine leukemia virus  
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Deposited on : 2014-05-03  
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

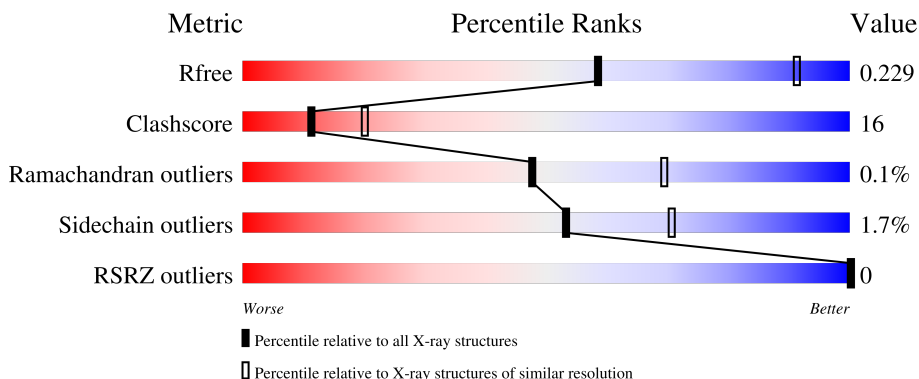
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	215	 55% 36% 7%
1	B	215	 56% 31% 13%
1	C	215	 67% 24% 7%
1	D	215	 66% 26% 8%
1	E	215	 63% 26% 10%

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Mol	Chain	Length	Quality of chain
1	F	215	 53% 35% 5% 7%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9078 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 BLV capsid.

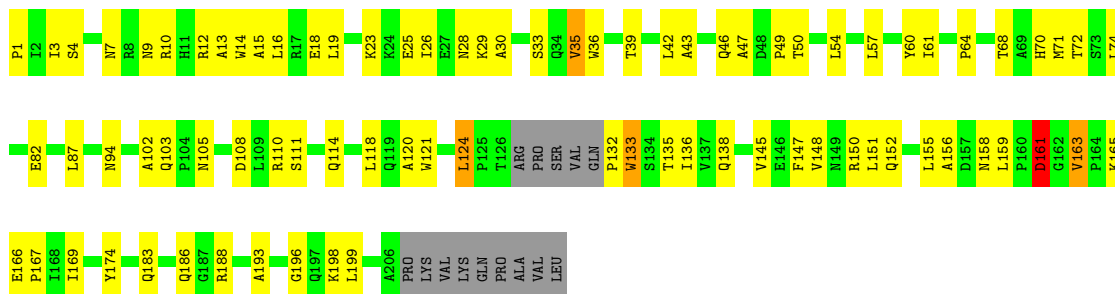
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1549	972	278	295	4	0	0	0
1	B	188	1450	907	259	280	4	0	0	0
1	C	199	1532	960	273	295	4	0	0	0
1	D	198	1535	962	276	293	4	0	0	0
1	E	193	1493	937	267	285	4	0	0	0
1	F	199	1519	957	267	291	4	0	0	0

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

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

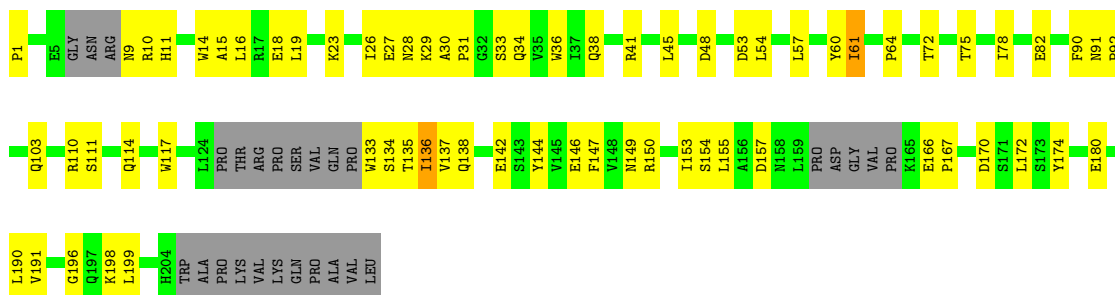
- Molecule 1: BLV capsid

Chain A: 



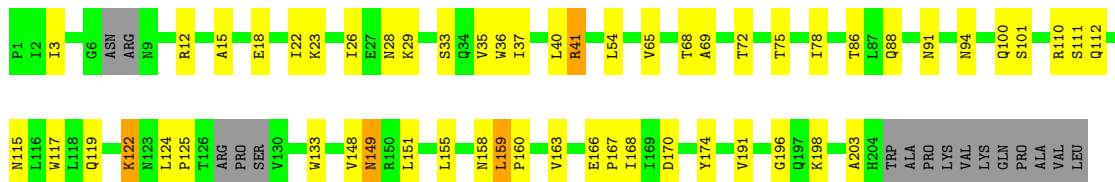
- Molecule 1: BLV capsid

Chain B: 



- Molecule 1: BLV capsid

Chain C: 



- Molecule 1: BLV capsid



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.28Å 94.28Å 257.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.14 – 2.75 47.14 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.14-2.75) 99.9 (47.14-2.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.180 , 0.221 0.182 , 0.229	Depositor DCC
$R_{free}$ test set	1676 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.2	Xtrriage
Anisotropy	0.498	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 135.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.398 for h,-h-k,-l	Xtrriage
Reported twinning fraction	0.420 for k,h,-l	Depositor
Outliers	0 of 33497 reflections	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9078	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.59	0/1582	1.08	8/2159 (0.4%)
1	B	0.62	1/1474 (0.1%)	1.12	7/2005 (0.3%)
1	C	0.62	0/1562	1.07	7/2131 (0.3%)
1	D	0.64	0/1567	1.09	9/2138 (0.4%)
1	E	0.57	0/1523	1.07	5/2077 (0.2%)
1	F	0.63	0/1552	1.23	15/2123 (0.7%)
All	All	0.61	1/9260 (0.0%)	1.11	51/12633 (0.4%)

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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	ILE	CA-CB	5.76	1.61	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LEU	CA-C-N	9.03	128.68	119.56
1	A	124	LEU	C-N-CA	9.03	128.68	119.56
1	D	86	THR	N-CA-C	-8.26	103.19	113.18
1	F	14	TRP	N-CA-C	7.48	121.05	110.50
1	B	48	ASP	CA-C-N	7.45	128.78	120.66
1	B	48	ASP	C-N-CA	7.45	128.78	120.66
1	E	33	SER	N-CA-C	-7.29	100.22	110.50
1	F	131	GLN	N-CA-C	7.04	125.36	109.81
1	D	158	ASN	N-CA-C	6.72	122.31	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	THR	N-CA-C	-6.69	104.86	113.16
1	F	159	LEU	CA-C-N	-6.53	113.25	119.85
1	F	159	LEU	C-N-CA	-6.53	113.25	119.85
1	B	190	LEU	N-CA-C	-6.35	104.84	112.59
1	A	163	VAL	N-CA-C	6.31	114.84	107.77
1	F	103	GLN	CA-C-N	6.29	126.49	119.32
1	F	103	GLN	C-N-CA	6.29	126.49	119.32
1	A	133	TRP	N-CA-C	6.24	118.89	111.71
1	C	91	ASN	CA-C-N	6.14	125.82	119.56
1	C	91	ASN	C-N-CA	6.14	125.82	119.56
1	F	44	ILE	N-CA-C	6.07	116.24	110.42
1	F	48	ASP	CA-C-N	6.00	126.50	120.14
1	F	48	ASP	C-N-CA	6.00	126.50	120.14
1	D	88	GLN	N-CA-C	5.99	117.95	108.67
1	E	86	THR	N-CA-C	-5.96	105.78	113.16
1	D	103	GLN	CA-C-N	5.80	125.93	119.32
1	D	103	GLN	C-N-CA	5.80	125.93	119.32
1	F	86	THR	N-CA-C	-5.79	106.22	113.28
1	A	7	ASN	N-CA-C	-5.77	106.20	113.18
1	F	124	LEU	CA-C-N	-5.77	112.63	119.84
1	F	124	LEU	C-N-CA	-5.77	112.63	119.84
1	E	163	VAL	CA-C-N	5.71	125.90	119.90
1	E	163	VAL	C-N-CA	5.71	125.90	119.90
1	E	42	LEU	N-CA-C	5.69	117.28	111.14
1	A	161	ASP	N-CA-C	5.47	116.92	111.07
1	B	135	THR	CA-C-N	5.44	129.17	121.66
1	B	135	THR	C-N-CA	5.44	129.17	121.66
1	F	127	ARG	CA-C-N	5.35	125.56	120.31
1	F	127	ARG	C-N-CA	5.35	125.56	120.31
1	C	124	LEU	CA-C-N	5.33	126.04	120.12
1	C	124	LEU	C-N-CA	5.33	126.04	120.12
1	D	91	ASN	CA-C-N	5.28	124.94	119.56
1	D	91	ASN	C-N-CA	5.28	124.94	119.56
1	B	61	ILE	N-CA-C	5.25	118.21	112.96
1	C	122	LYS	N-CA-C	-5.24	105.24	111.69
1	D	48	ASP	CA-C-N	5.17	125.62	120.14
1	D	48	ASP	C-N-CA	5.17	125.62	120.14
1	C	203	ALA	N-CA-C	-5.14	106.84	113.01
1	F	158	ASN	N-CA-C	5.13	117.73	107.62
1	A	3	ILE	N-CA-C	5.12	115.34	108.17
1	A	94	ASN	N-CA-C	-5.10	106.65	112.92
1	B	180	GLU	N-CA-C	5.02	116.44	110.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	124	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1549	0	1527	61	0
1	B	1450	0	1431	63	0
1	C	1532	0	1517	44	1
1	D	1535	0	1516	37	1
1	E	1493	0	1474	45	0
1	F	1519	0	1494	63	0
All	All	9078	0	8959	293	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 16.

All (293) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TRP:HB3	1:A:158:ASN:HD22	1.29	0.94
1:C:133:TRP:HD1	1:C:158:ASN:HB2	1.32	0.94
1:F:124:LEU:O	1:F:126:THR:N	2.06	0.86
1:F:136:ILE:O	1:F:176:ASN:ND2	2.10	0.84
1:A:25:GLU:O	1:A:29:LYS:NZ	2.13	0.82
1:D:159:LEU:HD22	1:D:160:PRO:HD2	1.62	0.82
1:A:145:VAL:HG13	1:F:65:VAL:HG11	1.62	0.80
1:F:23:LYS:HB2	1:F:60:TYR:HE2	1.48	0.78
1:C:133:TRP:CD1	1:C:158:ASN:HB2	2.18	0.78
1:E:193:ALA:O	1:E:198:LYS:NZ	2.15	0.78
1:B:138:GLN:NE2	1:B:142:GLU:O	2.17	0.77
1:A:161:ASP:OD1	1:A:161:ASP:N	2.16	0.77
1:A:72:THR:HG23	1:B:196:GLY:HA2	1.67	0.77
1:C:170:ASP:O	1:C:198:LYS:NZ	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLU:OE1	1:B:150:ARG:NH1	2.18	0.75
1:F:163:VAL:HG12	1:F:168:ILE:HD11	1.67	0.75
1:A:12:ARG:NH1	1:A:13:ALA:O	2.20	0.74
1:F:142:GLU:OE1	1:F:150:ARG:NH1	2.22	0.73
1:F:16:LEU:HA	1:F:19:LEU:HD12	1.71	0.72
1:F:119:GLN:O	1:F:122:LYS:HG2	1.88	0.72
1:F:193:ALA:O	1:F:198:LYS:NZ	2.23	0.72
1:F:95:GLY:O	1:F:100:GLN:NE2	2.24	0.71
1:C:75:THR:HA	1:C:78:ILE:HD12	1.73	0.71
1:F:161:ASP:OD1	1:F:161:ASP:N	2.24	0.70
1:A:16:LEU:HA	1:A:19:LEU:HD12	1.73	0.70
1:A:42:LEU:HD11	1:F:14:TRP:HB2	1.74	0.69
1:E:75:THR:HA	1:E:78:ILE:HD12	1.74	0.69
1:B:82:GLU:HG3	1:B:90:PHE:CE2	2.27	0.69
1:B:150:ARG:HA	1:B:153:ILE:HD12	1.74	0.69
1:D:15:ALA:HB3	1:D:18:GLU:HG3	1.75	0.69
1:C:101:SER:HB2	1:C:110:ARG:HA	1.76	0.67
1:B:166:GLU:CD	1:B:166:GLU:H	2.03	0.66
1:B:57:LEU:O	1:B:61:ILE:HG12	1.96	0.66
1:C:166:GLU:H	1:C:166:GLU:CD	2.04	0.65
1:B:170:ASP:O	1:B:198:LYS:NZ	2.29	0.65
1:C:159:LEU:HD22	1:C:160:PRO:HD2	1.79	0.65
1:F:133:TRP:HB3	1:F:158:ASN:HD22	1.62	0.65
1:F:131:GLN:O	1:F:133:TRP:N	2.30	0.64
1:A:70:HIS:NE2	1:A:120:ALA:HB3	2.11	0.64
1:E:166:GLU:HB2	1:E:167:PRO:HD3	1.79	0.64
1:F:159:LEU:HD22	1:F:165:LYS:HG2	1.80	0.64
1:B:75:THR:HA	1:B:78:ILE:HD12	1.78	0.64
1:C:3:ILE:HD11	1:C:12:ARG:HE	1.63	0.64
1:A:166:GLU:H	1:A:166:GLU:CD	2.06	0.64
1:F:34:GLN:HE21	1:F:156:ALA:HB1	1.63	0.63
1:E:160:PRO:HB2	1:E:163:VAL:HG21	1.81	0.63
1:C:88:GLN:O	1:C:112:GLN:NE2	2.30	0.62
1:F:75:THR:HA	1:F:78:ILE:HD12	1.81	0.62
1:F:26:ILE:HD12	1:F:39:THR:HB	1.80	0.62
1:C:41:ARG:HH21	1:C:41:ARG:HB2	1.64	0.62
1:B:9:ASN:C	1:B:10:ARG:HD3	2.25	0.61
1:B:138:GLN:HB2	1:B:147:PHE:CD1	2.36	0.61
1:B:133:TRP:HB3	1:B:154:SER:HB3	1.81	0.61
1:A:26:ILE:HA	1:A:29:LYS:HD3	1.82	0.61
1:D:65:VAL:HG11	1:E:145:VAL:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:LYS:HA	1:F:168:ILE:HD12	1.83	0.61
1:A:71:MET:SD	1:A:74:LEU:HD23	2.41	0.60
1:E:65:VAL:HG11	1:F:145:VAL:HG13	1.81	0.60
1:B:34:GLN:O	1:B:38:GLN:HG2	2.01	0.60
1:F:166:GLU:H	1:F:166:GLU:CD	2.10	0.60
1:D:136:ILE:HD12	1:D:151:LEU:HA	1.84	0.60
1:E:136:ILE:HD12	1:E:151:LEU:HA	1.84	0.60
1:B:54:LEU:HD23	1:B:57:LEU:HD12	1.84	0.60
1:E:166:GLU:CD	1:E:166:GLU:H	2.10	0.59
1:C:65:VAL:HG11	1:D:145:VAL:HG13	1.83	0.59
1:C:69:ALA:HB1	1:C:125:PRO:HD2	1.83	0.59
1:E:163:VAL:HG12	1:E:168:ILE:HD11	1.85	0.59
1:C:29:LYS:HE2	1:C:35:VAL:HG11	1.84	0.58
1:B:23:LYS:HD2	1:B:60:TYR:CE2	2.39	0.58
1:D:57:LEU:O	1:D:61:ILE:HG12	2.03	0.58
1:C:68:THR:HG21	1:D:195:VAL:HG13	1.85	0.58
1:E:160:PRO:HB2	1:E:163:VAL:CG2	2.34	0.57
1:A:25:GLU:OE1	1:F:60:TYR:OH	2.18	0.57
1:F:53:ASP:O	1:F:56:GLN:HB2	2.03	0.57
1:D:32:GLY:H	1:D:36:TRP:CD1	2.21	0.57
1:E:23:LYS:HD2	1:E:60:TYR:CE1	2.40	0.57
1:B:33:SER:O	1:B:36:TRP:HB3	2.05	0.56
1:F:70:HIS:NE2	1:F:117:TRP:O	2.35	0.56
1:E:57:LEU:O	1:E:61:ILE:HG12	2.04	0.56
1:F:26:ILE:HB	1:F:39:THR:HG21	1.87	0.56
1:B:23:LYS:O	1:B:27:GLU:N	2.39	0.56
1:A:103:GLN:HG2	1:A:105:ASN:H	1.72	0.55
1:E:4:SER:O	1:E:9:ASN:N	2.40	0.55
1:F:57:LEU:O	1:F:61:ILE:HG12	2.07	0.55
1:F:33:SER:O	1:F:36:TRP:HB3	2.07	0.54
1:B:166:GLU:HB2	1:B:167:PRO:HD3	1.89	0.54
1:C:111:SER:O	1:C:115:ASN:ND2	2.40	0.54
1:E:115:ASN:O	1:E:119:GLN:HG2	2.07	0.54
1:F:96:THR:O	1:F:100:GLN:HG3	2.07	0.54
1:A:14:TRP:CG	1:A:19:LEU:HD21	2.43	0.54
1:A:68:THR:OG1	1:B:149:ASN:OD1	2.22	0.54
1:F:124:LEU:HB3	1:F:125:PRO:HD3	1.88	0.54
1:E:138:GLN:HB2	1:E:147:PHE:CG	2.43	0.54
1:C:101:SER:HB2	1:C:110:ARG:CA	2.37	0.53
1:F:70:HIS:NE2	1:F:120:ALA:HB3	2.24	0.53
1:A:82:GLU:HG2	1:A:87:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:TYR:O	1:E:148:VAL:HG23	2.09	0.52
1:A:174:TYR:HB2	1:A:198:LYS:HE2	1.91	0.52
1:B:15:ALA:O	1:B:18:GLU:HB2	2.10	0.52
1:B:16:LEU:HA	1:B:19:LEU:HD12	1.91	0.52
1:B:154:SER:O	1:B:157:ASP:HB2	2.09	0.52
1:A:166:GLU:HB2	1:A:167:PRO:HD3	1.91	0.52
1:D:75:THR:HA	1:D:78:ILE:HD12	1.91	0.52
1:E:136:ILE:CD1	1:E:151:LEU:HA	2.40	0.51
1:D:136:ILE:HD12	1:D:151:LEU:HD12	1.92	0.51
1:E:65:VAL:HG21	1:F:145:VAL:O	2.10	0.51
1:E:29:LYS:HE3	1:E:35:VAL:HG11	1.92	0.51
1:A:156:ALA:HA	1:A:165:LYS:NZ	2.26	0.50
1:F:54:LEU:HD23	1:F:57:LEU:HD12	1.91	0.50
1:A:155:LEU:HD22	1:A:159:LEU:HB2	1.92	0.50
1:C:72:THR:OG1	1:D:196:GLY:HA3	2.11	0.50
1:F:185:LEU:O	1:F:190:LEU:N	2.41	0.50
1:C:33:SER:O	1:C:36:TRP:HB3	2.12	0.50
1:E:35:VAL:O	1:E:39:THR:OG1	2.17	0.50
1:A:29:LYS:HG2	1:A:35:VAL:HG22	1.94	0.50
1:B:28:ASN:OD1	1:B:28:ASN:N	2.42	0.50
1:B:111:SER:HA	1:B:114:GLN:OE1	2.12	0.50
1:A:148:VAL:HG12	1:F:65:VAL:HG22	1.93	0.50
1:C:148:VAL:O	1:C:151:LEU:HB3	2.12	0.50
1:D:23:LYS:O	1:D:27:GLU:N	2.45	0.50
1:E:133:TRP:CE3	1:E:134:SER:HB3	2.47	0.50
1:F:161:ASP:C	1:F:163:VAL:H	2.20	0.50
1:C:15:ALA:HB3	1:C:18:GLU:HG3	1.94	0.49
1:E:19:LEU:HB3	1:E:60:TYR:CE2	2.47	0.49
1:A:49:PRO:O	1:A:110:ARG:HD2	2.12	0.49
1:D:136:ILE:HD11	1:D:154:SER:CB	2.43	0.49
1:B:38:GLN:HA	1:B:41:ARG:NH1	2.28	0.49
1:C:3:ILE:HD11	1:C:12:ARG:NE	2.26	0.49
1:C:163:VAL:HG12	1:C:168:ILE:HD11	1.95	0.49
1:A:136:ILE:CD1	1:A:151:LEU:HA	2.43	0.49
1:D:136:ILE:CD1	1:D:151:LEU:HA	2.43	0.49
1:A:152:GLN:NE2	1:F:68:THR:OG1	2.24	0.48
1:F:77:ALA:HB1	1:F:116:LEU:HD22	1.94	0.48
1:D:32:GLY:HA2	1:D:121:TRP:HB3	1.95	0.48
1:A:30:ALA:HB3	1:A:33:SER:HB3	1.95	0.48
1:A:136:ILE:HG22	1:A:150:ARG:HH21	1.78	0.48
1:A:28:ASN:OD1	1:A:28:ASN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LYS:HA	1:C:26:ILE:HG22	1.96	0.48
1:A:64:PRO:HB2	1:B:149:ASN:HD21	1.78	0.48
1:D:8:ARG:HB3	1:D:10:ARG:HG2	1.96	0.48
1:A:183:GLN:HA	1:A:186:GLN:OE1	2.12	0.48
1:E:180:GLU:HG3	1:E:205:TRP:CZ2	2.49	0.48
1:F:163:VAL:CG1	1:F:168:ILE:HD11	2.40	0.47
1:B:142:GLU:CD	1:B:150:ARG:HH11	2.22	0.47
1:C:166:GLU:HB2	1:C:167:PRO:HD3	1.96	0.47
1:E:15:ALA:HB3	1:E:18:GLU:HG3	1.96	0.47
1:A:33:SER:O	1:A:36:TRP:HB3	2.14	0.47
1:C:159:LEU:HD22	1:C:160:PRO:CD	2.43	0.47
1:C:54:LEU:HB3	1:C:117:TRP:CE2	2.49	0.47
1:E:2:ILE:HD13	1:E:11:HIS:HA	1.97	0.47
1:E:174:TYR:HD1	1:E:185:LEU:HD12	1.79	0.47
1:E:180:GLU:HG3	1:E:205:TRP:HZ2	1.79	0.47
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.73	0.47
1:A:72:THR:HG23	1:B:196:GLY:CA	2.42	0.47
1:D:23:LYS:HD2	1:D:60:TYR:CE1	2.50	0.47
1:A:121:TRP:CE3	1:A:124:LEU:HD11	2.50	0.46
1:C:155:LEU:HD22	1:C:159:LEU:HD23	1.97	0.46
1:F:166:GLU:HB2	1:F:167:PRO:HD3	1.97	0.46
1:B:150:ARG:O	1:B:153:ILE:HB	2.14	0.46
1:C:29:LYS:HD2	1:C:29:LYS:N	2.30	0.46
1:E:78:ILE:HG23	1:E:97:LEU:HD23	1.96	0.46
1:F:132:PRO:HB2	1:F:135:THR:HG21	1.97	0.46
1:A:161:ASP:C	1:A:163:VAL:H	2.22	0.46
1:C:36:TRP:O	1:C:40:LEU:HG	2.15	0.46
1:E:33:SER:O	1:E:36:TRP:HB3	2.15	0.46
1:D:69:ALA:HB1	1:D:124:LEU:HD22	1.97	0.46
1:A:4:SER:HA	1:A:9:ASN:OD1	2.16	0.46
1:B:34:GLN:HE21	1:B:38:GLN:NE2	2.14	0.46
1:F:91:ASN:HA	1:F:92:PRO:HD2	1.81	0.46
1:D:88:GLN:HB3	1:D:112:GLN:HE22	1.81	0.46
1:A:50:THR:HB	1:A:102:ALA:HA	1.98	0.46
1:A:121:TRP:HE3	1:A:124:LEU:HD11	1.81	0.46
1:E:19:LEU:HB3	1:E:60:TYR:CD2	2.51	0.45
1:A:193:ALA:O	1:A:198:LYS:NZ	2.37	0.45
1:B:34:GLN:HG2	1:B:38:GLN:HE21	1.80	0.45
1:B:133:TRP:HB3	1:B:154:SER:CB	2.46	0.45
1:F:130:VAL:C	1:F:132:PRO:HD2	2.40	0.45
1:A:57:LEU:O	1:A:61:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASP:C	1:D:163:VAL:H	2.24	0.45
1:E:180:GLU:H	1:E:180:GLU:HG2	1.60	0.45
1:F:23:LYS:HB2	1:F:60:TYR:CE2	2.39	0.45
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.78	0.45
1:E:174:TYR:CD2	1:E:191:VAL:HG13	2.51	0.45
1:A:110:ARG:HG2	1:A:114:GLN:NE2	2.32	0.45
1:B:138:GLN:HB2	1:B:147:PHE:CG	2.51	0.45
1:D:14:TRP:HE1	1:D:53:ASP:HB3	1.80	0.45
1:F:174:TYR:CG	1:F:191:VAL:HG13	2.52	0.45
1:E:60:TYR:O	1:E:60:TYR:HD1	2.00	0.45
1:F:34:GLN:NE2	1:F:156:ALA:HB1	2.29	0.45
1:A:183:GLN:HA	1:A:186:GLN:CD	2.42	0.44
1:E:103:GLN:O	1:E:110:ARG:NH1	2.44	0.44
1:B:144:TYR:CD2	1:B:199:LEU:HD23	2.52	0.44
1:D:14:TRP:HB3	1:D:19:LEU:HD11	2.00	0.44
1:D:196:GLY:HA2	1:D:199:LEU:HD12	1.99	0.44
1:C:37:ILE:HG22	1:C:41:ARG:HH22	1.81	0.44
1:F:20:GLN:NE2	1:F:60:TYR:OH	2.50	0.44
1:A:54:LEU:O	1:A:57:LEU:HB2	2.18	0.44
1:C:155:LEU:O	1:C:159:LEU:N	2.50	0.44
1:D:12:ARG:NH1	1:D:13:ALA:O	2.51	0.44
1:E:23:LYS:HD2	1:E:60:TYR:HE1	1.81	0.44
1:C:119:GLN:O	1:C:122:LYS:HB2	2.17	0.44
1:F:15:ALA:HB3	1:F:18:GLU:HG3	1.98	0.44
1:F:142:GLU:OE2	1:F:150:ARG:HD3	2.18	0.44
1:A:196:GLY:HA2	1:A:199:LEU:HD12	2.00	0.44
1:B:26:ILE:HD11	1:B:36:TRP:CD2	2.52	0.44
1:B:54:LEU:HB3	1:B:117:TRP:NE1	2.32	0.44
1:B:103:GLN:O	1:B:110:ARG:NH1	2.51	0.44
1:E:3:ILE:HD13	1:E:12:ARG:NE	2.33	0.44
1:A:23:LYS:HD2	1:A:60:TYR:CE2	2.52	0.44
1:A:136:ILE:HG22	1:A:150:ARG:NH2	2.32	0.44
1:D:150:ARG:HA	1:D:153:ILE:HD12	1.99	0.44
1:E:65:VAL:HG23	1:F:149:ASN:OD1	2.18	0.44
1:B:38:GLN:CD	1:B:41:ARG:HH12	2.26	0.44
1:B:166:GLU:CD	1:B:166:GLU:N	2.74	0.44
1:F:15:ALA:HB3	1:F:18:GLU:CG	2.48	0.44
1:D:118:LEU:HA	1:D:118:LEU:HD23	1.85	0.43
1:A:138:GLN:HB2	1:A:147:PHE:CG	2.53	0.43
1:C:41:ARG:HB2	1:C:41:ARG:NH2	2.31	0.43
1:D:194:PRO:HD2	1:D:197:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:GLN:HA	1:F:104:PRO:HD3	1.84	0.43
1:D:54:LEU:HD23	1:D:57:LEU:HD12	1.99	0.43
1:D:144:TYR:O	1:D:148:VAL:HG23	2.18	0.43
1:A:118:LEU:O	1:A:121:TRP:HD1	2.02	0.43
1:D:49:PRO:HB2	1:D:53:ASP:HB2	2.00	0.43
1:E:54:LEU:O	1:E:57:LEU:HB2	2.18	0.43
1:B:57:LEU:HA	1:B:57:LEU:HD23	1.78	0.43
1:C:155:LEU:O	1:C:159:LEU:HB2	2.18	0.43
1:E:164:PRO:HB2	1:E:167:PRO:HD2	2.01	0.43
1:F:161:ASP:C	1:F:163:VAL:N	2.75	0.43
1:A:108:ASP:O	1:A:111:SER:HB2	2.19	0.43
1:A:15:ALA:HB3	1:A:18:GLU:HG3	2.01	0.43
1:B:41:ARG:O	1:B:45:LEU:HG	2.19	0.43
1:B:54:LEU:O	1:B:57:LEU:HB2	2.19	0.43
1:B:72:THR:HG23	1:C:196:GLY:O	2.18	0.43
1:B:142:GLU:CD	1:B:150:ARG:NH1	2.76	0.43
1:F:63:SER:O	1:F:67:GLN:HG3	2.18	0.43
1:C:15:ALA:HA	1:D:46:GLN:CD	2.44	0.43
1:A:133:TRP:HB3	1:A:158:ASN:ND2	2.12	0.43
1:D:34:GLN:HG2	1:D:156:ALA:HB1	2.00	0.43
1:E:122:LYS:HG3	1:E:123:ASN:N	2.34	0.43
1:E:154:SER:O	1:E:158:ASN:ND2	2.42	0.43
1:F:16:LEU:O	1:F:20:GLN:N	2.49	0.43
1:F:23:LYS:O	1:F:27:GLU:N	2.43	0.43
1:B:174:TYR:CG	1:B:191:VAL:HG13	2.54	0.42
1:A:64:PRO:CB	1:B:149:ASN:HD21	2.31	0.42
1:B:137:VAL:HG12	1:B:138:GLN:N	2.33	0.42
1:D:136:ILE:HD11	1:D:154:SER:HB2	2.00	0.42
1:C:23:LYS:O	1:C:26:ILE:HG22	2.19	0.42
1:E:164:PRO:HB2	1:E:167:PRO:CD	2.49	0.42
1:F:170:ASP:CG	1:F:194:PRO:HA	2.45	0.42
1:B:26:ILE:HA	1:B:29:LYS:HD3	2.02	0.42
1:C:94:ASN:HB2	1:C:100:GLN:NE2	2.33	0.42
1:C:174:TYR:CG	1:C:191:VAL:HG13	2.55	0.42
1:B:9:ASN:O	1:B:10:ARG:HD3	2.20	0.42
1:E:29:LYS:HD3	1:E:29:LYS:HA	1.91	0.42
1:F:44:ILE:HG23	1:F:49:PRO:HD2	2.01	0.42
1:B:133:TRP:CZ3	1:B:172:LEU:HD11	2.55	0.42
1:F:30:ALA:HA	1:F:31:PRO:HD3	1.90	0.42
1:A:155:LEU:HD12	1:A:169:ILE:HD11	2.03	0.41
1:B:34:GLN:CG	1:B:38:GLN:HE21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLU:O	1:C:22:ILE:HG13	2.19	0.41
1:D:2:ILE:HD13	1:D:11:HIS:HA	2.02	0.41
1:F:96:THR:HG23	1:F:99:GLN:OE1	2.20	0.41
1:A:35:VAL:O	1:A:39:THR:OG1	2.23	0.41
1:A:156:ALA:HA	1:A:165:LYS:HZ3	1.85	0.41
1:D:161:ASP:O	1:D:163:VAL:HG23	2.21	0.41
1:F:29:LYS:HE2	1:F:35:VAL:HG21	2.02	0.41
1:B:30:ALA:HA	1:B:31:PRO:HD3	1.90	0.41
1:B:136:ILE:HD12	1:B:136:ILE:HG23	1.93	0.41
1:B:144:TYR:HD2	1:B:199:LEU:HD23	1.84	0.41
1:B:146:GLU:HA	1:B:149:ASN:HB2	2.03	0.41
1:A:43:ALA:O	1:A:46:GLN:HB2	2.20	0.41
1:F:205:TRP:CG	1:F:206:ALA:N	2.89	0.41
1:A:138:GLN:HB2	1:A:147:PHE:CD1	2.55	0.41
1:A:1:PRO:HG3	1:A:47:ALA:HB1	2.02	0.41
1:A:136:ILE:HD12	1:A:151:LEU:HA	2.03	0.41
1:B:64:PRO:HB2	1:C:149:ASN:OD1	2.21	0.41
1:B:133:TRP:CZ3	1:B:134:SER:HB3	2.56	0.41
1:D:15:ALA:HB3	1:D:18:GLU:CG	2.48	0.41
1:D:58:CYS:HB3	1:D:67:GLN:HG2	2.02	0.41
1:E:133:TRP:CZ3	1:E:155:LEU:HD21	2.56	0.41
1:E:174:TYR:CG	1:E:191:VAL:HG13	2.56	0.41
1:F:82:GLU:CD	1:F:90:PHE:HE2	2.29	0.41
1:B:14:TRP:HE1	1:B:53:ASP:HB3	1.87	0.40
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.83	0.40
1:B:144:TYR:CE2	1:B:199:LEU:HA	2.56	0.40
1:B:1:PRO:O	1:B:11:HIS:HA	2.22	0.40
1:F:174:TYR:CD1	1:F:191:VAL:HG13	2.57	0.40
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.89	0.40
1:C:15:ALA:O	1:C:18:GLU:HB2	2.22	0.40
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.77	0.40
1:A:132:PRO:HB2	1:A:135:THR:HG23	2.02	0.40
1:C:54:LEU:HB3	1:C:117:TRP:NE1	2.36	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:28:ASN:O	1:D:10:ARG:NH2[6_654]	2.11	0.09

## 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	197/215 (92%)	195 (99%)	2 (1%)	0	100	100
1	B	180/215 (84%)	176 (98%)	4 (2%)	0	100	100
1	C	193/215 (90%)	192 (100%)	1 (0%)	0	100	100
1	D	194/215 (90%)	192 (99%)	2 (1%)	0	100	100
1	E	187/215 (87%)	184 (98%)	3 (2%)	0	100	100
1	F	195/215 (91%)	190 (97%)	4 (2%)	1 (0%)	24	40
All	All	1146/1290 (89%)	1129 (98%)	16 (1%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	132	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/177 (92%)	158 (98%)	4 (2%)	42	63
1	B	152/177 (86%)	152 (100%)	0	100	100
1	C	163/177 (92%)	160 (98%)	3 (2%)	51	69
1	D	162/177 (92%)	160 (99%)	2 (1%)	63	77
1	E	157/177 (89%)	155 (99%)	2 (1%)	61	75
1	F	159/177 (90%)	154 (97%)	5 (3%)	35	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	955/1062 (90%)	939 (98%)	16 (2%)	53 71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	35	VAL
1	A	161	ASP
1	A	188	ARG
1	C	41	ARG
1	C	149	ASN
1	C	159	LEU
1	D	159	LEU
1	D	188	ARG
1	E	28	ASN
1	E	188	ARG
1	F	24	LYS
1	F	35	VAL
1	F	91	ASN
1	F	161	ASP
1	F	173	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	158	ASN
1	B	34	GLN
1	B	200	GLN
1	C	59	GLN
1	C	197	GLN
1	D	34	GLN
1	D	38	GLN
1	D	100	GLN
1	D	152	GLN
1	E	103	GLN
1	E	105	ASN
1	E	197	GLN
1	F	20	GLN
1	F	152	GLN
1	F	158	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	201/215 (93%)	-0.79	0 100 100	66, 99, 131, 157	0
1	B	188/215 (87%)	-0.60	0 100 100	79, 118, 167, 212	0
1	C	199/215 (92%)	-0.94	0 100 100	52, 85, 117, 150	0
1	D	198/215 (92%)	-1.02	0 100 100	55, 82, 121, 150	0
1	E	193/215 (89%)	-0.83	0 100 100	75, 102, 146, 188	0
1	F	199/215 (92%)	-0.69	0 100 100	64, 110, 158, 183	0
All	All	1178/1290 (91%)	-0.81	0 100 100	52, 99, 151, 212	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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.