

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8TOO
Title	:	Crystal structure of Epstein-Barr virus gp42 in complex with antibody 4C12
Authors	:	Bu, W.; Kumar, A.; Board, N.; Kim, J.; Dowdell, K.; Zhang, S.; Lei, Y.;
		Hostal, A.; Krogmann, T.; Wang, Y.; Pittaluga, S.; Marcotrigiano, J.; Cohen,
		J.I.
Deposited on	:	2023-08-03
Resolution	:	2.60 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	А	214	2% 8 4%	14%	•
1	С	214	% 	20%	••
1	Е	214	79%	17%	•••
1	F	214	2% 8 2%	16%	·
2	В	234	^{2%} 70% 22%	•	6%



Mol	Chain	Length	Quality of chain		
	D	22.4	3%		
2	D	234	76%	18%	6%
0	C	994	3%		
	G	234	73%	21%	• 6%
2	Н	234	68%	26%	6%
_	-		4%		
3	I	139	76%	19%	••
3	J	139	% 8 3%	13%	•••
			8%		
3	K	139	73%	22%	••
	Ŧ	100	7%		
3	L	139	81%	15%	••



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2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17213 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	011	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	211	1589	987	266	331	5	0	0	0
1	С	911	Total	С	Ν	0	S	0	0	0
	U	211	1582	985	266	326	5	0	0	0
1	Б	011	Total	С	Ν	0	S	0	0	0
	E	211	1597	999	272	321	5	0	0	0
1	Б	911	Total	С	Ν	0	S	0	0	0
		211	1579	984	268	322	5	U	U	U

• Molecule 1 is a protein called 4C12 light chain.

• Molecule 2 is a protein called 4C12 heavy chain.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
0	D	220	Total	С	Ν	0	\mathbf{S}	0	0	0
	D	220	1605	1015	259	324	$\overline{7}$	0	0	0
0	Л	220	Total	С	Ν	0	\mathbf{S}	0	0	0
	D	220	1603	1014	261	321	$\overline{7}$	0	0	0
0	C	220	Total	С	Ν	0	S	0	0	0
	G	220	1622	1025	265	325	$\overline{7}$	0	0	0
0	и	220	Total	С	Ν	0	S	0	0	0
	п	220	1633	1032	266	328	$\overline{7}$	0	0	0

• Molecule 3 is a protein called Glycoprotein 42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	т	196	Total	С	Ν	0	\mathbf{S}	0	0	0
3	1	130	1044	684	168	181	11	0	0	0
2	т	126	Total	al C I	Ν	0	S	0	0	0
3	J	130	1045	681	167	186	11			0
9	V	196	Total	С	Ν	0	S	0	0	0
3	n	130	1057	688	170	188	11	0	0	0
2	т	126	Total	С	Ν	0	S	0	0	0
	130	1066	692	174	189	11	U	U	0	



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	15	Total O 15 15	0	0
4	В	20	TotalO2020	0	0
4	С	14	Total O 14 14	0	0
4	D	23	TotalO2323	0	0
4	Ε	22	TotalO2222	0	0
4	F	21	Total O 21 21	0	0
4	G	19	Total O 19 19	0	0
4	Н	20	Total O 20 20	0	0
4	Ι	11	Total O 11 11	0	0
4	J	8	Total O 8 8	0	0
4	К	9	Total O 9 9	0	0
4	L	9	Total O 9 9	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: 4C12 light chain











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	53.30Å 63.57Å 199.28Å	Deneiten
a, b, c, α , β , γ	89.81° 89.75° 88.86°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	53.51 - 2.60	Depositor
Resolution (A)	63.56 - 2.60	EDS
% Data completeness	91.5 (53.51-2.60)	Depositor
(in resolution range)	90.5(63.56-2.60)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) > 1$	$2.24 (at 2.61 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
B B.	0.226 , 0.275	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.225 , 0.274	DCC
R_{free} test set	3755 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	42.5	Xtriage
Anisotropy	0.800	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 23.1	EDS
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.31$	Xtriage
	0.095 for h,-k,-l	
Estimated twinning fraction	0.094 for -h,k,-l	Xtriage
	0.400 for -h,-k,l	
F_o, F_c correlation	0.92	EDS
Total number of atoms	17213	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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).

Mal	Mol Chain		lengths	Bond angles		
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.26	0/1620	0.51	0/2210	
1	С	0.26	0/1613	0.54	0/2201	
1	Ε	0.27	0/1628	0.53	0/2214	
1	F	0.27	0/1610	0.51	0/2194	
2	В	0.28	0/1649	0.54	0/2261	
2	D	0.30	0/1647	0.50	0/2257	
2	G	0.34	0/1666	0.55	0/2281	
2	Н	0.30	0/1677	0.53	0/2292	
3	Ι	0.26	0/1082	0.46	0/1482	
3	J	0.32	0/1083	0.49	0/1485	
3	Κ	0.42	0/1095	0.60	0/1500	
3	L	0.27	0/1104	0.50	0/1511	
All	All	0.30	0/17474	0.53	0/23888	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1589	0	1482	15	0
1	С	1582	0	1478	24	0
1	Е	1597	0	1539	33	0
1	F	1579	0	1486	17	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	1605	0	1473	33	0
2	D	1603	0	1469	24	0
2	G	1622	0	1508	24	0
2	Н	1633	0	1530	32	0
3	Ι	1044	0	947	15	0
3	J	1045	0	934	12	0
3	Κ	1057	0	956	17	0
3	L	1066	0	971	12	0
4	А	15	0	0	0	0
4	В	20	0	0	0	0
4	С	14	0	0	1	0
4	D	23	0	0	1	0
4	Ε	22	0	0	2	0
4	F	21	0	0	0	0
4	G	19	0	0	0	0
4	Н	20	0	0	3	0
4	Ι	11	0	0	0	0
4	J	8	0	0	0	0
4	Κ	9	0	0	0	0
4	L	9	0	0	1	0
All	All	17213	0	15773	243	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 7.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:G:131:LEU:HD21	2:G:148:LEU:HB2	1.59	0.85
2:B:48:ILE:HG21	2:B:81:MET:HE3	1.59	0.83
1:F:142:ARG:HD2	1:F:163:VAL:HG11	1.65	0.78
1:E:136:LEU:HD21	1:E:196:VAL:HG21	1.68	0.75
2:G:99:ASP:HA	2:G:107:MET:HA	1.68	0.74
2:H:213:LYS:NZ	4:H:301:HOH:O	2.22	0.72
2:B:99:ASP:HA	2:B:107:MET:HA	1.71	0.70
2:B:30:THR:HB	2:B:54:TYR:HD1	1.56	0.69
1:E:3:GLN:NE2	4:E:302:HOH:O	2.24	0.69
3:K:184:VAL:HG22	3:K:202:PRO:HB2	1.77	0.67
1:F:164:THR:HG22	1:F:174:SER:H	1.59	0.66
2:H:166:LEU:HD21	2:H:189:VAL:HG21	1.77	0.66
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.76	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:91:SER:HA	2:D:116:VAL:O	1.95	0.66
2:H:99:ASP:HA	2:H:107:MET:HA	1.76	0.66
1:F:37:GLN:HB2	1:F:47:LEU:HD11	1.78	0.66
2:B:148:LEU:HD21	2:B:150:LYS:HD2	1.77	0.65
1:E:149:LYS:HG2	1:E:152:ASN:HA	1.78	0.65
2:H:51:ILE:HG13	2:H:58:THR:HG22	1.79	0.65
3:K:189:GLY:HA3	3:K:204:SER:HB3	1.77	0.65
1:F:135:LEU:HD22	2:G:188:VAL:HG11	1.78	0.65
2:B:67:LYS:NZ	2:B:90:ASP:OD1	2.30	0.64
2:D:34:MET:HE3	2:D:96:CYS:HB2	1.78	0.63
2:H:102:GLY:HA3	3:L:196:SER:HB2	1.79	0.63
1:C:135:LEU:HD22	2:D:188:VAL:HG11	1.81	0.62
3:L:162:LEU:HD21	3:L:215:LEU:HB2	1.81	0.62
2:D:83:LEU:HB3	2:D:86:LEU:HD21	1.80	0.62
2:B:150:LYS:NZ	2:B:178:GLN:OE1	2.29	0.62
2:D:126:PRO:HB3	2:D:152:TYR:HB3	1.82	0.62
1:E:108:ARG:HG3	1:E:140:TYR:CD2	2.35	0.62
1:E:46:LEU:HD23	1:E:55:ARG:HD3	1.81	0.61
2:H:91:SER:HA	2:H:116:VAL:O	2.01	0.61
2:H:61:ASN:HB3	2:H:64:PHE:HD2	1.65	0.61
2:B:34:MET:HB2	2:B:53:LEU:HD11	1.82	0.61
1:F:78:LEU:HD21	1:F:104:LEU:HD21	1.81	0.61
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.81	0.61
2:H:19:LYS:HG3	2:H:82:GLU:HG3	1.83	0.61
2:D:12:VAL:HG21	2:D:86:LEU:HD12	1.83	0.60
1:E:103:LYS:NZ	4:E:304:HOH:O	2.30	0.60
1:E:151:ASP:OD2	1:E:189:HIS:ND1	2.33	0.60
1:C:33:LEU:HD11	1:C:88:CYS:HB2	1.84	0.59
2:B:126:PRO:HB3	2:B:152:TYR:HB3	1.83	0.59
2:D:155:GLU:HG3	2:D:156:PRO:HA	1.84	0.59
1:E:119:PRO:HB3	1:E:209:PHE:CE2	2.38	0.58
1:E:185:ASP:HA	1:E:188:LYS:HE3	1.85	0.58
3:K:107:TYR:HE2	3:K:110:SER:HB2	1.69	0.58
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.86	0.58
2:H:126:PRO:HB3	2:H:152:TYR:HB3	1.87	0.57
2:D:12:VAL:HG11	2:D:18:VAL:HB	1.87	0.57
2:B:12:VAL:HG11	2:B:18:VAL:HB	1.85	0.57
1:F:186:TYR:HA	1:F:192:TYR:OH	2.04	0.57
2:G:4:LEU:HD22	2:G:22:CYS:SG	2.45	0.57
2:G:166:LEU:HD21	2:G:189:VAL:HG21	1.88	0.56
2:H:103:ASN:ND2	2:H:105:TYR:OH	2.38	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:78:LEU:HD21	1:C:104:LEU:HD21	1.87	0.56
1:C:135:LEU:HD13	2:D:188:VAL:HG21	1.88	0.56
3:K:94:TYR:OH	3:K:130:GLN:NE2	2.37	0.56
3:K:103:ASN:OD1	3:K:106:GLU:N	2.38	0.56
2:B:170:VAL:HG22	2:B:189:VAL:HG22	1.88	0.55
1:C:132:VAL:HG13	1:C:179:LEU:HB3	1.86	0.55
3:K:125:TRP:CZ3	3:K:129:PHE:HE2	2.24	0.55
2:B:76:SER:OG	2:B:78:THR:OG1	2.22	0.55
1:C:27:GLN:NE2	4:C:303:HOH:O	2.34	0.55
2:H:208:LYS:HG3	4:H:301:HOH:O	2.06	0.55
1:C:136:LEU:HB2	1:C:175:LEU:HB3	1.88	0.55
3:J:101:TYR:O	3:J:218:SER:OG	2.20	0.55
3:I:205:HIS:HD2	3:I:206:HIS:HD2	1.54	0.54
3:J:144:PRO:HD3	3:J:164:VAL:HB	1.88	0.54
3:K:118:PHE:HE2	3:K:215:LEU:HD13	1.72	0.54
2:D:38:LYS:HB2	2:D:48:ILE:HD11	1.89	0.54
1:E:4:MET:CE	1:E:90:GLN:HB3	2.38	0.54
3:I:88:PHE:CE2	3:I:90:VAL:HG22	2.42	0.53
1:C:121:SER:HB3	1:C:123:GLU:HG2	1.89	0.53
1:C:15:LEU:HD21	1:C:80:GLN:HG2	1.91	0.53
3:K:189:GLY:HA3	3:K:204:SER:CB	2.39	0.53
3:L:196:SER:H	3:L:199:SER:HB2	1.73	0.53
2:H:6:GLN:HE22	2:H:95:TYR:HA	1.73	0.53
2:G:145:LEU:HB2	2:G:218:VAL:HG11	1.90	0.53
1:E:140:TYR:CD1	1:E:141:PRO:HA	2.43	0.53
3:K:94:TYR:CE2	3:K:129:PHE:HB3	2.44	0.53
2:D:34:MET:HB2	2:D:53:LEU:HD21	1.91	0.52
2:D:48:ILE:HD13	2:D:81:MET:HE1	1.92	0.52
1:E:138:ASN:ND2	1:E:172:THR:OG1	2.41	0.52
3:K:163:TRP:CZ3	3:K:192:CYS:HB2	2.44	0.52
3:L:118:PHE:HE1	3:L:215:LEU:HD13	1.75	0.52
1:F:6:GLN:HE21	1:F:99:GLY:HA3	1.75	0.52
2:D:74:ASN:ND2	4:D:304:HOH:O	2.40	0.52
2:G:148:LEU:HD22	2:G:150:LYS:HB2	1.90	0.52
1:E:78:LEU:HD11	1:E:104:LEU:HD21	1.92	0.52
3:I:163:TRP:CE2	3:I:212:LYS:HD2	2.45	0.52
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.90	0.52
3:I:191:HIS:ND1	3:I:208:CYS:SG	2.82	0.52
1:A:135:LEU:HD22	2:B:188:VAL:HG11	1.91	0.51
1:E:103:LYS:HD3	1:E:104:LEU:N	2.26	0.51
3:K:207:GLU:CD	3:K:209:SER:H	2.13	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
3:K:162:LEU:HD21	3:K:215:LEU:HB2	1.92	0.51
1:C:186:TYR:CE2	1:C:211:ARG:HD2	2.45	0.51
2:D:97:ALA:HB1	2:D:107:MET:HB3	1.93	0.51
1:F:19:VAL:HG21	1:F:104:LEU:HD11	1.92	0.51
1:C:2:ILE:HD13	1:C:29:ILE:HG22	1.93	0.51
2:D:170:VAL:HG22	2:D:189:VAL:HG22	1.91	0.50
2:H:171:HIS:NE2	4:H:303:HOH:O	2.29	0.50
3:L:176:SER:OG	3:L:177:LEU:N	2.44	0.50
1:E:140:TYR:HD1	1:E:141:PRO:CA	2.24	0.50
2:H:148:LEU:HD22	2:H:150:LYS:HB2	1.93	0.50
1:A:6:GLN:HE22	1:A:87:PHE:HA	1.75	0.50
1:E:80:GLN:O	1:E:83:ILE:HG13	2.11	0.50
1:E:4:MET:HE1	1:E:90:GLN:HB3	1.94	0.50
2:B:91:SER:HA	2:B:116:VAL:O	2.12	0.50
1:F:125:LEU:O	1:F:183:LYS:HD2	2.12	0.50
2:G:105:TYR:HB3	3:K:185:TYR:CZ	2.47	0.50
2:H:178:GLN:HG3	2:H:180:SER:OG	2.12	0.49
1:C:125:LEU:HD21	1:C:130:ALA:HB2	1.94	0.49
2:G:163:SER:O	2:G:163:SER:OG	2.28	0.49
3:J:130:GLN:O	3:J:130:GLN:NE2	2.46	0.49
1:E:125:LEU:O	1:E:183:LYS:HD2	2.13	0.49
1:A:78:LEU:HD11	1:A:104:LEU:HD21	1.95	0.49
2:B:98:ARG:NH2	2:B:109:TYR:CE2	2.81	0.48
2:D:48:ILE:HG21	2:D:81:MET:HE3	1.95	0.48
1:F:6:GLN:HE22	1:F:87:PHE:HA	1.79	0.48
2:G:32:TYR:CE2	2:G:101:TYR:HB2	2.48	0.48
1:C:96:PHE:HB2	2:D:47:TRP:CG	2.48	0.48
2:B:139:SER:O	2:B:142:THR:OG1	2.29	0.48
1:E:186:TYR:CE2	1:E:211:ARG:NH1	2.81	0.48
1:E:211:ARG:HH11	1:E:211:ARG:HB2	1.79	0.48
3:I:205:HIS:CD2	3:I:206:HIS:HD2	2.31	0.48
3:L:114:CYS:SG	3:L:219:GLN:NE2	2.82	0.48
1:C:33:LEU:HG	1:C:34:ASN:N	2.29	0.48
1:C:116:PHE:CD1	1:C:135:LEU:HD23	2.48	0.47
1:F:136:LEU:HD21	1:F:196:VAL:HG21	1.96	0.47
2:H:11:LEU:HD22	2:H:154:PRO:HG3	1.95	0.47
1:C:33:LEU:HD22	1:C:71:TYR:CB	2.44	0.47
2:H:191:VAL:HG11	2:H:201:TYR:CE1	2.50	0.47
2:H:206:ASN:HB3	2:H:213:LYS:NZ	2.29	0.47
1:A:135:LEU:CD2	2:B:188:VAL:HG11	2.45	0.47
1:C:134:CYS:HB2	1:C:148:TRP:CH2	2.50	0.47



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:H:105:TYR:HB3	3:L:185:TYR:CZ	2.49	0.47	
3:I:183:LYS:HD3	3:I:201:VAL:HG11	1.97	0.47	
2:D:60:TYR:CE1	2:D:70:LEU:HG	2.50	0.47	
2:B:3:GLN:OE1	2:B:26:GLY:HA3	2.14	0.46	
1:C:36:TYR:HE1	1:C:89:GLN:HB3	1.79	0.46	
1:E:83:ILE:HG22	1:E:103:LYS:NZ	2.30	0.46	
1:A:118:PHE:HB3	2:B:131:LEU:HD22	1.96	0.46	
1:E:134:CYS:HB2	1:E:148:TRP:CH2	2.51	0.46	
2:B:150:LYS:HG2	2:B:151:ASP:OD1	2.15	0.46	
2:G:38:LYS:HB2	2:G:48:ILE:HD11	1.97	0.46	
1:E:50:TYR:HB3	1:E:53:ARG:HG2	1.98	0.46	
2:G:83:LEU:HB3	2:G:86:LEU:HD11	1.97	0.46	
2:H:34:MET:HB2	2:H:53:LEU:HD21	1.97	0.46	
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.97	0.46	
3:K:191:HIS:O	3:K:191:HIS:ND1	2.49	0.46	
3:L:196:SER:H	3:L:199:SER:CB	2.29	0.45	
1:C:78:LEU:HD12	1:C:78:LEU:HA	1.77	0.45	
2:G:87:THR:O	2:G:118:VAL:HG11	2.16	0.45	
3:J:186:GLN:HA	3:J:204:SER:OG	2.17	0.45	
1:C:141:PRO:HB2	1:C:143:GLU:OE2	2.17	0.45	
1:C:80:GLN:HA	1:C:106:ILE:HD11	1.99	0.45	
3:I:192:CYS:O	3:I:204:SER:HA	2.16	0.45	
1:A:96:PHE:HB2	2:B:47:TRP:CG	2.51	0.45	
2:B:138:THR:HA	2:B:142:THR:O	2.17	0.45	
2:D:44:ASN:N	2:D:44:ASN:HD22	2.15	0.45	
1:E:186:TYR:HE2	1:E:211:ARG:NH1	2.15	0.45	
2:G:126:PRO:HB3	2:G:152:TYR:HB3	1.99	0.45	
3:I:166:VAL:HG12	3:I:174:TRP:HB3	1.98	0.44	
2:G:37:VAL:HG22	2:G:47:TRP:HA	1.99	0.44	
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.99	0.44	
3:J:101:TYR:HE2	3:J:136:TYR:HB3	1.82	0.44	
3:I:162:LEU:HD12	3:I:213:PRO:HB2	1.99	0.44	
3:K:163:TRP:CE3	3:K:194:TYR:HB3	2.53	0.44	
2:B:129:PHE:HD2	2:B:148:LEU:HD23	1.83	0.44	
1:E:155:GLN:OE1	1:E:158:ASN:ND2	2.51	0.44	
2:G:34:MET:HB2	2:G:53:LEU:HD21	2.00	0.44	
2:H:145:LEU:HD13	2:H:218:VAL:HB	1.99	0.44	
2:B:32:TYR:CE2	2:B:101:TYR:HB2	2.52	0.44	
2:B:150:LYS:HZ3	2:B:150:LYS:HG3	1.59	0.44	
2:D:150:LYS:HE2	2:D:151:ASP:OD1	2.18	0.44	
2:G:61:ASN:HB3	2:G:64:PHE:HD1	1.82	0.44	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:K:139:THR:HG22	3:K:216:CYS:HB3	2.00	0.44
1:E:124:GLN:O	1:E:127:SER:OG	2.24	0.43
3:L:153:THR:HB	3:L:197:LYS:O	2.18	0.43
2:D:87:THR:HG22	2:D:88:SER:H	1.83	0.43
3:J:186:GLN:HA	3:J:204:SER:HG	1.82	0.43
2:H:37:VAL:HG22	2:H:95:TYR:HB2	2.00	0.43
1:E:186:TYR:HA	1:E:192:TYR:OH	2.19	0.43
2:B:137:SER:OG	2:B:138:THR:N	2.51	0.43
3:L:197:LYS:NZ	4:L:302:HOH:O	2.52	0.43
2:G:126:PRO:HD2	2:G:212:THR:HG21	2.00	0.43
3:J:219:GLN:H	3:J:219:GLN:HG2	1.61	0.43
2:H:2:VAL:HA	2:H:25:SER:O	2.18	0.43
1:A:158:ASN:OD1	1:A:158:ASN:N	2.51	0.42
2:G:29:PHE:CE1	2:G:53:LEU:HD13	2.54	0.42
3:J:107:TYR:HA	3:J:117:TYR:CD2	2.53	0.42
3:J:163:TRP:CD1	3:J:212:LYS:HB2	2.54	0.42
1:E:211:ARG:NH1	1:E:211:ARG:HB2	2.33	0.42
3:I:119:THR:O	3:I:213:PRO:HB3	2.19	0.42
3:I:144:PRO:HD3	3:I:164:VAL:HB	2.00	0.42
3:K:191:HIS:O	3:K:191:HIS:CG	2.72	0.42
1:E:108:ARG:HG3	1:E:140:TYR:HD2	1.84	0.42
1:C:145:LYS:HE3	1:C:145:LYS:HB3	1.69	0.42
1:E:114:SER:HB3	1:E:116:PHE:CE1	2.55	0.42
1:A:46:LEU:HD23	1:A:55:ARG:HD2	2.01	0.42
1:E:80:GLN:HE21	1:E:80:GLN:HB2	1.53	0.42
3:I:107:TYR:HA	3:I:117:TYR:CD2	2.54	0.42
1:F:24:ARG:HG3	1:F:70:ASP:OD2	2.19	0.42
2:H:206:ASN:HB3	2:H:213:LYS:HZ1	1.84	0.42
3:J:96:LYS:HG3	3:J:140:TYR:CE1	2.54	0.42
2:B:37:VAL:HG22	2:B:95:TYR:HB2	2.01	0.42
1:F:61:ARG:HB3	1:F:76:ASN:O	2.20	0.42
2:D:166:LEU:HD21	2:D:189:VAL:HG11	2.01	0.41
2:G:91:SER:HA	2:G:116:VAL:O	2.19	0.41
2:B:126:PRO:HD2	2:B:212:THR:HG21	2.02	0.41
2:D:37:VAL:HG22	2:D:95:TYR:HB2	2.02	0.41
1:F:18:ARG:HH11	1:F:76:ASN:ND2	2.17	0.41
1:F:135:LEU:HD13	2:G:188:VAL:HG21	2.02	0.41
2:H:178:GLN:HG2	2:H:182:LEU:O	2.20	0.41
2:G:30:THR:HG21	2:G:74:ASN:HD21	1.86	0.41
2:G:204:ASN:ND2	2:G:215:ASP:OD2	2.53	0.41
2:H:67:LYS:O	2:H:83:LEU:HA	2.19	0.41



A + 1	A + a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:J:101:TYR:CE2	3:J:136:TYR:HB3	2.56	0.41
1:A:108:ARG:NH2	1:A:111:ALA:HB2	2.36	0.41
1:C:187:GLU:HA	1:C:211:ARG:CZ	2.50	0.41
2:H:32:TYR:CE2	2:H:101:TYR:HB2	2.55	0.41
2:H:149:VAL:HG11	2:H:157:VAL:HG11	2.01	0.41
3:I:139:THR:HG22	3:I:216:CYS:HB3	2.02	0.41
1:A:160:GLN:HB3	2:B:176:VAL:HG11	2.02	0.41
1:E:107:LYS:HG2	1:E:140:TYR:OH	2.20	0.41
1:A:161:GLU:OE2	1:A:175:LEU:HD11	2.21	0.41
1:A:41:ASP:OD2	1:A:43:THR:OG1	2.24	0.41
1:A:120:PRO:HB2	1:A:125:LEU:HD21	2.03	0.41
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.79	0.41
1:F:54:LEU:HD11	1:F:58:VAL:HB	2.03	0.41
3:I:101:TYR:CE2	3:I:136:TYR:HB3	2.55	0.41
3:I:196:SER:H	3:I:199:SER:HG	1.60	0.41
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.56	0.41
2:H:104:PRO:HG2	3:L:185:TYR:CE2	2.56	0.40
2:B:166:LEU:HD21	2:B:189:VAL:HG11	2.04	0.40
2:B:100:TYR:HB3	2:B:103:ASN:HB2	2.03	0.40
2:D:208:LYS:HE2	2:G:199:GLN:HE21	1.87	0.40
1:F:164:THR:HG23	1:F:165:GLU:O	2.21	0.40
3:J:187:ILE:HD13	3:J:187:ILE:HA	1.89	0.40
3:L:205:HIS:HD2	3:L:212:LYS:NZ	2.19	0.40
2:B:34:MET:CB	2:B:53:LEU:HD11	2.49	0.40
1:E:4:MET:HE2	1:E:90:GLN:HB3	2.03	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	Percer	ntiles
1	А	209/214~(98%)	198 (95%)	11 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	С	209/214~(98%)	199~(95%)	10~(5%)	0	100	100
1	Ε	209/214~(98%)	200 (96%)	8 (4%)	1 (0%)	29	52
1	F	209/214~(98%)	200 (96%)	9~(4%)	0	100	100
2	В	218/234~(93%)	197 (90%)	15 (7%)	6 (3%)	5	7
2	D	218/234~(93%)	203 (93%)	14 (6%)	1 (0%)	29	52
2	G	218/234~(93%)	207~(95%)	10 (5%)	1 (0%)	29	52
2	Н	218/234~(93%)	205 (94%)	12 (6%)	1 (0%)	29	52
3	Ι	134/139~(96%)	126 (94%)	7 (5%)	1 (1%)	22	43
3	J	134/139~(96%)	128 (96%)	5 (4%)	1 (1%)	22	43
3	Κ	134/139~(96%)	127~(95%)	6 (4%)	1 (1%)	22	43
3	L	134/139~(96%)	125 (93%)	9 (7%)	0	100	100
All	All	2244/2348~(96%)	2115 (94%)	116 (5%)	13 (1%)	25	47

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All (13) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
2	D	2	VAL
2	В	26	GLY
2	В	133	PRO
3	Ι	191	HIS
3	J	171	GLU
2	В	138	THR
2	В	25	SER
2	В	2	VAL
2	В	134	SER
2	G	41	HIS
3	Κ	190	SER
1	Е	138	ASN
2	Н	197	GLY

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	А	177/191~(93%)	167 (94%)	10 (6%)	21 42
1	С	175/191~(92%)	163 (93%)	12 (7%)	15 31
1	Ε	179/191 (94%)	172 (96%)	7 (4%)	32 58
1	F	174/191 (91%)	166 (95%)	8 (5%)	27 51
2	В	172/200~(86%)	163 (95%)	9 (5%)	23 46
2	D	170/200~(85%)	163 (96%)	7 (4%)	30 56
2	G	176/200~(88%)	164 (93%)	12 (7%)	16 32
2	Н	179/200~(90%)	170~(95%)	9~(5%)	24 47
3	Ι	109/126~(86%)	102 (94%)	7~(6%)	17 35
3	J	110/126~(87%)	105~(96%)	5(4%)	27 52
3	Κ	113/126~(90%)	101 (89%)	12 (11%)	6 12
3	L	115/126 (91%)	104 (90%)	11 (10%)	8 16
All	All	1849/2068 (89%)	1740 (94%)	109 (6%)	19 39

All (109) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	9	SER
1	А	17	ASP
1	А	18	ARG
1	А	19	VAL
1	А	26	SER
1	А	126	LYS
1	А	142	ARG
1	А	185	ASP
1	А	203	SER
1	А	206	THR
2	В	74	ASN
2	В	78	THR
2	В	100	TYR
2	В	135	SER
2	В	139	SER
2	В	178	GLN
2	В	186	SER
2	В	200	THR
2	В	204	ASN
1	С	8	THR
1	С	17	ASP
1	С	19	VAL



Mol	Chain	Res	Type
1	С	26	SER
1	С	39	LYS
1	С	45	LYS
1	С	55	ARG
1	С	114	SER
1	С	121	SER
1	С	123	GLU
1	С	203	SER
1	С	207	LYS
2	D	7	SER
2	D	25	SER
2	D	66	SER
2	D	100	TYR
2	D	160	SER
2	D	193	SER
2	D	204	ASN
1	Е	4	MET
1	Е	76	ASN
1	Е	80	GLN
1	Е	100	SER
1	Е	114	SER
1	Е	140	TYR
1	Е	211	ARG
1	F	17	ASP
1	F	26	SER
1	F	33	LEU
1	F	80	GLN
1	F	121	SER
1	F	150	VAL
1	F	182	SER
1	F	185	ASP
2	G	3	GLN
2	G	19	LYS
2	G	21	SER
2	G	25	SER
2	G	40	SER
2	G	100	TYR
2	G	135	SER
2	G	142	THR
2	G	163	SER
2	G	167	THR
2	G	198	THR



Mol	Chain	Res	Type
2	G	215	ASP
2	Н	7	SER
2	Н	25	SER
2	Н	76	SER
2	Н	100	TYR
2	Н	179	SER
2	Н	193	SER
2	Н	194	SER
2	Н	203	CYS
2	Н	204	ASN
3	Ι	85	LEU
3	Ι	96	LYS
3	Ι	107	TYR
3	Ι	141	PHE
3	Ι	178	ASP
3	Ι	192	CYS
3	Ι	205	HIS
3	J	85	LEU
3	J	192	CYS
3	J	205	HIS
3	J	218	SER
3	J	219	GLN
3	Κ	85	LEU
3	K	86	HIS
3	K	100	THR
3	K	107	TYR
3	K	110	SER
3	K	123	HIS
3	K	147	ASP
3	K	159	ILE
3	K	169	VAL
3	K	186	GLN
3	K	192	CYS
3	K	199	SER
3	L	111	TYR
3	L	117	TYR
3	L	123	HIS
3	L	141	PHE
3	L	157	ASN
3	L	173	ASN
3	L	178	ASP
3	L	192	CYS



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Mol	Chain	Res	Type
3	L	193	THR
3	L	199	SER
3	L	205	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	155	GLN
2	D	44	ASN
1	F	6	GLN
1	F	76	ASN
2	G	44	ASN
2	G	74	ASN
2	G	178	GLN
2	Н	6	GLN
2	Н	33	ASN
2	Н	103	ASN
3	Ι	205	HIS
3	Ι	206	HIS
3	J	206	HIS
3	Κ	130	GLN
3	Κ	191	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (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^{th} 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	$OWAB(Å^2)$	Q<0.9
1	А	211/214~(98%)	-0.01	4 (1%) 66 62	28, 47, 78, 102	0
1	С	211/214~(98%)	0.01	3 (1%) 75 71	26, 47, 77, 101	0
1	Ε	211/214~(98%)	-0.07	0 100 100	27, 46, 77, 92	0
1	\mathbf{F}	211/214~(98%)	-0.08	5 (2%) 59 53	28, 47, 71, 100	0
2	В	220/234~(94%)	0.19	4 (1%) 68 64	29, 47, 83, 98	0
2	D	220/234~(94%)	0.17	7 (3%) 47 40	27, 45, 83, 108	0
2	G	220/234~(94%)	0.17	6 (2%) 54 48	30, 46, 82, 105	0
2	Н	220/234~(94%)	0.09	6 (2%) 54 48	28, 46, 78, 114	0
3	Ι	136/139~(97%)	0.30	6 (4%) 34 27	31, 51, 82, 107	0
3	J	136/139~(97%)	0.31	2 (1%) 73 70	32, 51, 82, 103	0
3	Κ	136/139~(97%)	0.54	11 (8%) 12 8	30, 55, 84, 98	0
3	L	136/139~(97%)	0.37	10 (7%) 14 10	31, 56, 85, 99	0
All	All	2268/2348~(96%)	0.14	64 (2%) 53 46	26, 48, 80, 114	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	137	SER	5.4
3	L	111	TYR	5.0
3	Κ	180	GLY	5.0
2	G	140	GLY	5.0
2	D	2	VAL	4.9
2	G	139	SER	4.7
3	Κ	144	PRO	4.4
2	G	163	SER	4.4
3	Ι	152	VAL	4.0
1	С	205	VAL	3.9
3	L	135	LEU	3.9



Mol	Chain	Res	Type	RSRZ
3	L	144	PRO	3.8
2	D	197	GLY	3.8
2	Н	139	SER	3.6
3	Ι	144	PRO	3.6
2	D	138	THR	3.6
3	Κ	143	GLY	3.5
2	G	29	PHE	3.5
2	Н	196	LEU	3.4
3	L	180	GLY	3.3
2	Н	144	ALA	3.3
3	J	148	ILE	3.1
2	В	27	TYR	3.1
1	С	154	LEU	2.9
3	K	159	ILE	2.9
1	F	21	ILE	2.8
3	L	215	LEU	2.8
2	Н	163	SER	2.7
1	F	196	VAL	2.7
2	G	66	SER	2.6
1	F	78	LEU	2.6
2	Н	29	PHE	2.6
3	L	85	LEU	2.5
3	L	139	THR	2.5
3	Ι	165	GLY	2.5
3	L	118	PHE	2.4
3	Κ	111	TYR	2.4
2	В	26	GLY	2.4
3	Κ	139	THR	2.4
2	D	29	PHE	2.4
3	K	118	PHE	2.3
2	D	163	SER	2.3
1	А	192	TYR	2.3
3	J	188	PHE	2.3
1	А	199	GLN	2.2
1	А	11	LEU	2.2
2	D	133	PRO	2.2
3	Ι	172	GLY	2.2
2	Н	198	THR	2.2
3	L	141	PHE	2.2
3	K	142	TYR	2.2
3	K	87	THR	2.2
2	В	76	SER	2.1



7 7 1		- D	<u> </u>	DODZ
Mol	Chain	Res	Type	RSRZ
1	F	144	ALA	2.1
3	L	142	TYR	2.1
3	Κ	141	PHE	2.1
3	Κ	210	PHE	2.1
2	G	220	PRO	2.1
1	А	205	VAL	2.0
3	Ι	141	PHE	2.0
2	В	131	LEU	2.0
1	F	135	LEU	2.0
3	Ι	148	ILE	2.0
1	С	192	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

