Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:37 pm BST

PDB ID	:	6QO1
Title	:	Crystal structure of Borrelia (Borreliella) burgdorferi outer surface protein BBA69
Authors	:	Brangulis, K.; Akopjana, I.; Petrovskis, I.; Kazaks, A.; Tars, K.
Deposited on	:	2019-02-12
Resolution	:	2.25 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 ⓘ symbol.

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

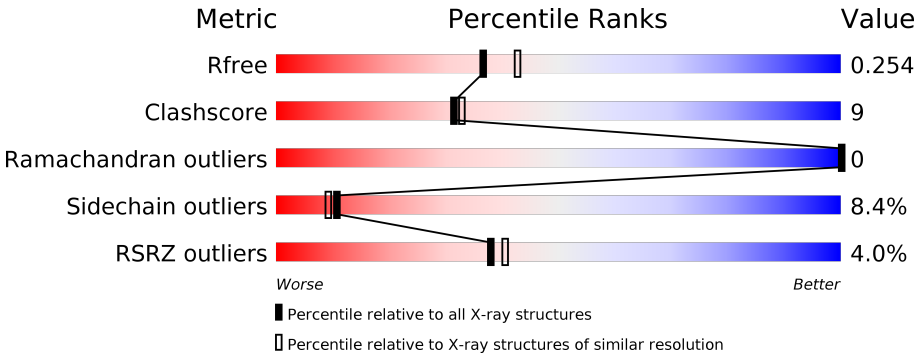
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 >=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	A	192	4% 71% 23%
1	B	192	4% 65% 28%
1	C	192	4% 77% 18%
1	D	192	4% 72% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6201 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 Putative surface protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1534	967	257	309	1			
1	D	186	Total	C	N	O	S	0	0	0
			1534	967	257	309	1			
1	B	186	Total	C	N	O	S	0	0	0
			1534	967	257	309	1			
1	C	186	Total	C	N	O	S	0	0	0
			1534	967	257	309	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O50958
A	2	ALA	-	expression tag	UNP O50958
A	3	MET	-	expression tag	UNP O50958
A	4	GLY	-	expression tag	UNP O50958
D	1	GLY	-	expression tag	UNP O50958
D	2	ALA	-	expression tag	UNP O50958
D	3	MET	-	expression tag	UNP O50958
D	4	GLY	-	expression tag	UNP O50958
B	1	GLY	-	expression tag	UNP O50958
B	2	ALA	-	expression tag	UNP O50958
B	3	MET	-	expression tag	UNP O50958
B	4	GLY	-	expression tag	UNP O50958
C	1	GLY	-	expression tag	UNP O50958
C	2	ALA	-	expression tag	UNP O50958
C	3	MET	-	expression tag	UNP O50958
C	4	GLY	-	expression tag	UNP O50958

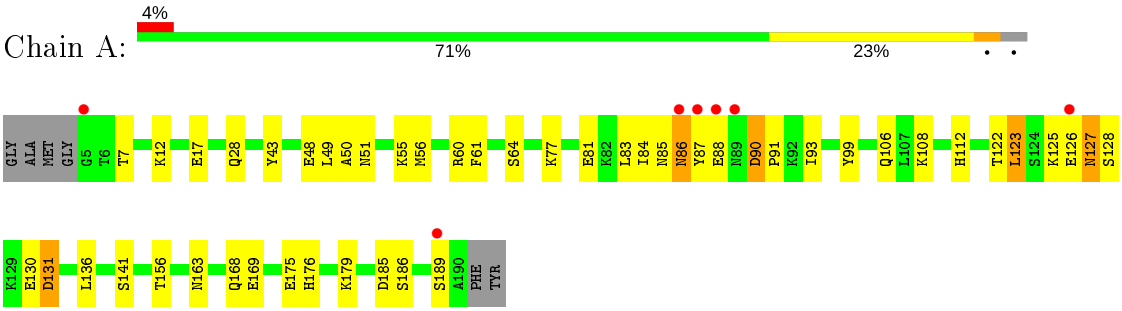
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	D	17	Total O 17 17	0	0
2	B	17	Total O 17 17	0	0
2	C	17	Total O 17 17	0	0

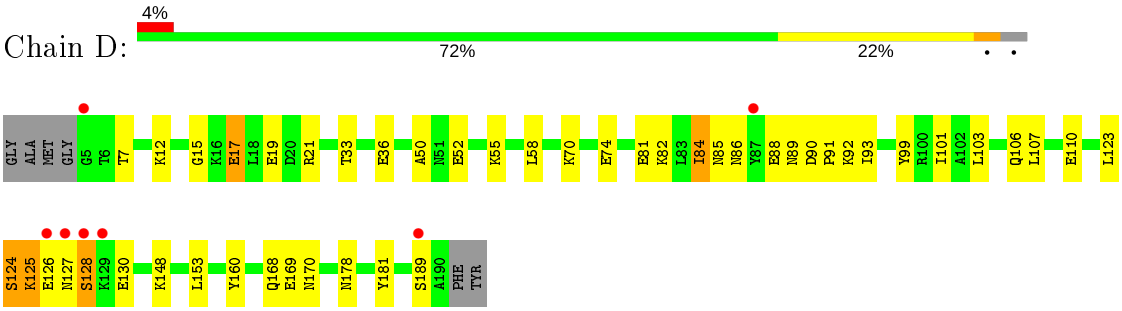
3 Residue-property plots (i)

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

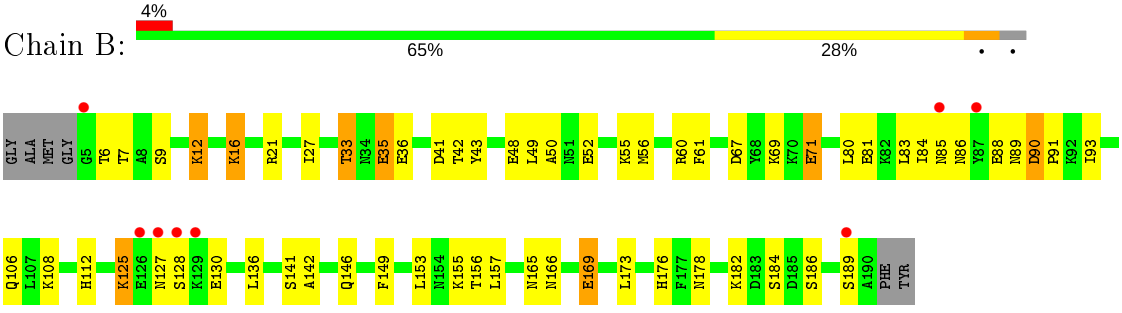
- Molecule 1: Putative surface protein



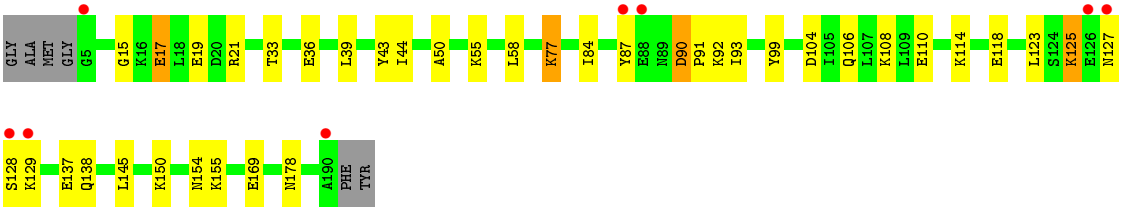
- Molecule 1: Putative surface protein



- Molecule 1: Putative surface protein



- Molecule 1: Putative surface protein


GLY
ALA
MET
GLY
G5
G15
K16
E17
L18
E19
D20
R21
T33
E36
L39
Y43
I44
A50
K55
L58
K77
I84
Y87
E88
N89
D90
P91
K92
I93
Y99
D104
I105
Q106
L107
K108
L109
E110
K114
E118
L123
S124
K125
E126
N127
S128
K129
E137
Q138
L145
K150
N154
K155
E169
N178
A190
PHE
TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.26Å 96.09Å 67.35Å 90.00° 105.83° 90.00°	Depositor
Resolution (Å)	40.62 – 2.25 40.58 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.62-2.25) 99.6 (40.58-2.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.49 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.173 , 0.249 0.186 , 0.254	Depositor DCC
R_{free} test set	1983 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	2.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.299 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6201	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2620e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.05	3/1549 (0.2%)	1.07	8/2076 (0.4%)
1	B	0.95	1/1549 (0.1%)	0.95	0/2076
1	C	0.85	0/1549	0.98	1/2076 (0.0%)
1	D	0.92	0/1549	1.04	4/2076 (0.2%)
All	All	0.95	4/6196 (0.1%)	1.01	13/8304 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	TYR	C-N	-13.11	1.03	1.34
1	B	16	LYS	C-N	-11.89	1.06	1.34
1	A	86	ASN	C-N	-10.71	1.09	1.34
1	A	125	LYS	C-N	8.23	1.52	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	125	LYS	CB-CA-C	-11.68	87.04	110.40
1	A	86	ASN	N-CA-C	-11.36	80.33	111.00
1	A	125	LYS	C-N-CA	-9.33	98.37	121.70
1	A	123	LEU	N-CA-C	-8.20	88.87	111.00
1	A	123	LEU	CB-CA-C	7.60	124.64	110.20
1	A	123	LEU	CA-CB-CG	6.82	131.00	115.30
1	D	124	SER	N-CA-C	5.95	127.05	111.00
1	A	86	ASN	CB-CA-C	5.86	122.12	110.40
1	D	189	SER	CB-CA-C	-5.85	98.99	110.10
1	D	126	GLU	N-CA-C	-5.77	95.42	111.00
1	A	87	TYR	CB-CA-C	-5.75	98.91	110.40
1	C	90	ASP	CB-CA-C	5.62	121.64	110.40
1	A	87	TYR	N-CA-C	5.25	125.17	111.00

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	A	1534	0	1565	29	0
1	B	1534	0	1566	40	0
1	C	1534	0	1567	21	0
1	D	1534	0	1567	26	0
2	A	14	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0
All	All	6201	0	6265	111	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 9.

All (111) 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:81:GLU:O	1:D:85:ASN:ND2	1.66	1.26
1:B:166:ASN:HB3	1:B:169:GLU:OE1	1.47	1.12
1:B:108:LYS:HE2	1:B:112:HIS:NE2	1.75	1.00
1:B:90:ASP:N	1:B:91:PRO:HD2	1.87	0.88
1:A:130:GLU:N	1:A:130:GLU:OE1	2.12	0.82
1:B:21:ARG:HH12	1:B:146:GLN:HE22	1.30	0.77
1:A:108:LYS:HE2	1:A:112:HIS:NE2	2.01	0.75
1:D:86:ASN:ND2	1:D:170:ASN:HB3	2.01	0.75
1:A:81:GLU:HG2	1:A:85:ASN:HD21	1.52	0.74
1:C:33:THR:HG23	1:C:36:GLU:H	1.54	0.73
1:A:81:GLU:HG2	1:A:85:ASN:ND2	2.07	0.69
1:D:82:LYS:HE3	1:D:160:TYR:OH	1.94	0.67
1:D:127:ASN:OD1	1:D:128:SER:N	2.26	0.67
1:B:130:GLU:N	1:B:130:GLU:OE1	2.28	0.67
1:B:7:THR:HG23	1:B:136:LEU:HD22	1.76	0.65
1:B:156:THR:OG1	1:B:176:HIS:HE1	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ILE:HA	1:C:92:LYS:HD3	1.78	0.65
1:B:6:THR:HG23	1:B:9:SER:H	1.61	0.65
1:B:80:LEU:O	1:B:84:ILE:HG12	1.97	0.64
1:C:33:THR:HG22	1:C:36:GLU:CD	2.18	0.64
1:B:21:ARG:HH12	1:B:146:GLN:NE2	1.95	0.64
1:C:17:GLU:OE2	1:C:21:ARG:NE	2.29	0.63
1:C:39:LEU:HG	1:C:77:LYS:HE3	1.80	0.63
1:D:33:THR:HG23	1:D:36:GLU:H	1.63	0.62
1:C:90:ASP:HA	1:C:93:ILE:HD12	1.82	0.61
1:D:17:GLU:OE2	1:D:21:ARG:NE	2.29	0.60
1:B:166:ASN:CB	1:B:169:GLU:OE1	2.37	0.59
1:A:126:GLU:HG2	1:A:127:ASN:N	2.17	0.59
1:A:156:THR:OG1	1:A:176:HIS:HE1	1.87	0.58
1:B:125:LYS:NZ	1:B:125:LYS:HB3	2.18	0.57
1:B:33:THR:CG2	1:B:35:GLU:HG2	2.33	0.57
1:A:28:GLN:HA	1:A:28:GLN:NE2	2.18	0.57
1:B:90:ASP:H	1:B:91:PRO:HD2	1.68	0.57
1:A:128:SER:HB2	1:A:131:ASP:OD1	2.05	0.57
1:D:124:SER:O	1:D:124:SER:OG	2.20	0.57
1:A:7:THR:HG23	1:A:136:LEU:HD22	1.87	0.56
1:C:33:THR:HG22	1:C:36:GLU:CG	2.35	0.56
1:B:90:ASP:HA	1:B:93:ILE:HD12	1.88	0.55
1:A:163:ASN:HB2	1:A:168:GLN:OE1	2.07	0.55
1:B:81:GLU:O	1:B:85:ASN:ND2	2.40	0.55
1:D:153:LEU:HA	1:D:181:TYR:OH	2.07	0.54
1:C:114:LYS:O	1:C:118:GLU:HG3	2.08	0.54
1:B:108:LYS:HD3	1:B:142:ALA:HB2	1.90	0.53
1:B:90:ASP:N	1:B:91:PRO:CD	2.67	0.53
1:A:90:ASP:N	1:A:91:PRO:HD2	2.24	0.52
1:B:33:THR:HG22	1:B:36:GLU:H	1.73	0.52
1:D:70:LYS:NZ	1:D:74:GLU:OE2	2.41	0.52
1:B:125:LYS:HZ2	1:B:125:LYS:HB3	1.73	0.52
1:B:50:ALA:O	1:B:55:LYS:HE3	2.10	0.52
1:B:61:PHE:CD2	1:B:106:GLN:HG2	2.45	0.51
1:C:90:ASP:N	1:C:91:PRO:CD	2.73	0.51
1:C:110:GLU:HA	1:C:110:GLU:OE1	2.10	0.51
1:B:153:LEU:O	1:B:157:LEU:HD13	2.11	0.51
1:A:84:ILE:HG22	1:A:84:ILE:O	2.11	0.51
1:C:43:TYR:HB3	1:C:99:TYR:OH	2.10	0.51
1:D:123:LEU:HD11	1:B:41:ASP:CG	2.32	0.50
1:C:33:THR:HG23	1:C:36:GLU:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:O	1:A:186:SER:HB3	2.10	0.50
1:B:56:MET:HG3	1:B:60:ARG:NH1	2.26	0.49
1:A:28:GLN:HA	1:A:28:GLN:HE21	1.76	0.49
1:C:125:LYS:NZ	1:C:125:LYS:HB3	2.26	0.49
1:B:12:LYS:NZ	1:B:16:LYS:HB2	2.27	0.49
1:D:123:LEU:HG	1:D:123:LEU:O	2.12	0.48
1:D:90:ASP:N	1:D:91:PRO:HD2	2.29	0.48
1:D:15:GLY:O	1:D:19:GLU:HG3	2.14	0.48
1:A:93:ILE:HG12	1:B:48:GLU:O	2.14	0.48
1:C:106:GLN:HA	1:C:106:GLN:OE1	2.13	0.47
1:A:61:PHE:CD2	1:A:106:GLN:HG2	2.48	0.47
1:D:90:ASP:HA	1:D:93:ILE:HD12	1.96	0.47
1:B:43:TYR:OH	1:B:81:GLU:OE1	2.27	0.46
1:B:86:ASN:HB3	1:B:91:PRO:HG3	1.97	0.46
1:A:56:MET:HG3	1:A:60:ARG:NH1	2.31	0.46
1:C:104:ASP:OD2	1:C:108:LYS:HE2	2.15	0.46
1:D:50:ALA:O	1:D:55:LYS:HE3	2.16	0.45
1:B:83:LEU:HD21	1:B:173:LEU:HG	1.98	0.45
1:C:50:ALA:O	1:C:55:LYS:HE3	2.17	0.45
1:D:82:LYS:NZ	1:D:168:GLN:O	2.45	0.45
1:D:106:GLN:OE1	1:D:106:GLN:HA	2.16	0.45
1:A:50:ALA:O	1:A:55:LYS:HE2	2.16	0.45
1:A:83:LEU:O	1:A:91:PRO:HB2	2.17	0.44
1:A:51:ASN:OD1	1:A:51:ASN:C	2.55	0.44
1:D:52:GLU:OE1	1:B:125:LYS:HE2	2.17	0.44
1:B:33:THR:HG21	1:B:35:GLU:HG2	2.01	0.43
1:A:86:ASN:ND2	1:A:91:PRO:HG3	2.33	0.43
1:A:90:ASP:N	1:A:90:ASP:OD1	2.51	0.43
1:C:150:LYS:O	1:C:154:ASN:ND2	2.50	0.43
1:A:48:GLU:O	1:B:93:ILE:HG12	2.18	0.43
1:D:160:TYR:O	1:D:168:GLN:NE2	2.52	0.43
1:A:88:GLU:HG2	1:A:91:PRO:CD	2.49	0.42
1:D:84:ILE:HG22	1:D:84:ILE:O	2.19	0.42
1:D:86:ASN:ND2	1:D:170:ASN:C	2.72	0.42
1:C:44:ILE:HG23	1:C:58:LEU:HD23	2.02	0.42
1:C:17:GLU:OE2	1:C:21:ARG:NH2	2.51	0.42
1:D:90:ASP:N	1:D:91:PRO:CD	2.82	0.42
1:B:149:PHE:C	1:B:149:PHE:CD1	2.93	0.41
1:B:166:ASN:ND2	1:B:169:GLU:OE1	2.53	0.41
1:A:88:GLU:HG2	1:A:91:PRO:HD2	2.02	0.41
1:B:7:THR:HG23	1:B:136:LEU:CD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LEU:HD21	1:D:99:TYR:HB3	2.03	0.41
1:C:137:GLU:HA	1:C:137:GLU:OE1	2.21	0.41
1:D:148:LYS:HA	1:D:148:LYS:HD2	1.89	0.41
1:B:178:ASN:O	1:B:182:LYS:HB2	2.21	0.41
1:C:15:GLY:O	1:C:19:GLU:HG3	2.21	0.41
1:D:110:GLU:OE1	1:D:110:GLU:HA	2.21	0.41
1:A:49:LEU:HD22	1:B:49:LEU:HD22	2.02	0.41
1:A:43:TYR:HB3	1:A:99:TYR:OH	2.21	0.41
1:A:122:THR:C	1:A:123:LEU:O	2.46	0.40
1:B:67:ASP:O	1:B:69:LYS:N	2.54	0.40
1:B:71:GLU:H	1:B:71:GLU:HG3	1.69	0.40
1:A:106:GLN:OE1	1:A:106:GLN:HA	2.21	0.40
1:D:103:LEU:O	1:D:107:LEU:HG	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/192 (96%)	174 (95%)	10 (5%)	0	100	100
1	B	184/192 (96%)	174 (95%)	10 (5%)	0	100	100
1	C	184/192 (96%)	172 (94%)	12 (6%)	0	100	100
1	D	184/192 (96%)	172 (94%)	12 (6%)	0	100	100
All	All	736/768 (96%)	692 (94%)	44 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	172/175 (98%)	160 (93%)	12 (7%)	15 13
1	B	172/175 (98%)	152 (88%)	20 (12%)	5 3
1	C	172/175 (98%)	159 (92%)	13 (8%)	13 12
1	D	172/175 (98%)	159 (92%)	13 (8%)	13 12
All	All	688/700 (98%)	630 (92%)	58 (8%)	11 9

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	17	GLU
1	A	64	SER
1	A	77	LYS
1	A	90	ASP
1	A	127	ASN
1	A	131	ASP
1	A	141	SER
1	A	169	GLU
1	A	175	GLU
1	A	185	ASP
1	A	189	SER
1	D	7	THR
1	D	12	LYS
1	D	17	GLU
1	D	84	ILE
1	D	88	GLU
1	D	89	ASN
1	D	92	LYS
1	D	101	ILE
1	D	125	LYS
1	D	128	SER
1	D	130	GLU
1	D	169	GLU

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Mol	Chain	Res	Type
1	D	178	ASN
1	B	12	LYS
1	B	27	ILE
1	B	33	THR
1	B	35	GLU
1	B	42	THR
1	B	52	GLU
1	B	71	GLU
1	B	88	GLU
1	B	89	ASN
1	B	90	ASP
1	B	125	LYS
1	B	127	ASN
1	B	128	SER
1	B	141	SER
1	B	155	LYS
1	B	165	ASN
1	B	169	GLU
1	B	184	SER
1	B	186	SER
1	B	189	SER
1	C	17	GLU
1	C	77	LYS
1	C	87	TYR
1	C	123	LEU
1	C	125	LYS
1	C	127	ASN
1	C	128	SER
1	C	129	LYS
1	C	138	GLN
1	C	145	LEU
1	C	155	LYS
1	C	169	GLU
1	C	178	ASN

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

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	GLN
1	A	53	ASN
1	A	85	ASN

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Mol	Chain	Res	Type
1	A	127	ASN
1	A	170	ASN
1	A	176	HIS
1	D	86	ASN
1	D	112	HIS
1	D	168	GLN
1	D	176	HIS
1	B	89	ASN
1	B	146	GLN
1	B	176	HIS
1	C	170	ASN
1	C	176	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	86:ASN	C	87:TYR	N	1.09
1	B	16:LYS	C	17:GLU	N	1.06
1	A	87:TYR	C	88:GLU	N	1.03

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^{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	A	186/192 (96%)	-0.04	7 (3%)	40	43	19, 36, 68, 97	0
1	B	186/192 (96%)	0.00	8 (4%)	35	37	20, 37, 72, 124	0
1	C	186/192 (96%)	-0.02	8 (4%)	35	37	18, 33, 79, 126	0
1	D	186/192 (96%)	-0.07	7 (3%)	40	43	19, 35, 70, 112	0
All	All	744/768 (96%)	-0.03	30 (4%)	38	40	18, 35, 73, 126	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	TYR	6.2
1	A	87	TYR	6.1
1	B	87	TYR	5.1
1	D	126	GLU	4.8
1	D	5	GLY	4.3
1	D	127	ASN	4.1
1	D	129	LYS	3.8
1	C	127	ASN	3.8
1	C	126	GLU	3.5
1	C	129	LYS	3.5
1	B	126	GLU	3.5
1	B	128	SER	3.4
1	A	88	GLU	3.4
1	D	128	SER	3.2
1	B	189	SER	3.2
1	B	127	ASN	3.1
1	A	86	ASN	3.1
1	A	126	GLU	3.0
1	C	88	GLU	2.8
1	B	129	LYS	2.8
1	C	5	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	87	TYR	2.6
1	A	89	ASN	2.6
1	A	5	GLY	2.5
1	B	5	GLY	2.5
1	D	189	SER	2.3
1	C	190	ALA	2.2
1	A	189	SER	2.2
1	C	128	SER	2.2
1	B	85	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.