Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2016 – 12:25 AM EDT

PDB ID	:	5C59
Title	:	Crystal structure of the periplasmic region of MacB from E. coli
Authors	:	Ha, N.C.; Kim, J.S.
Deposited on	:	2015-06-19
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

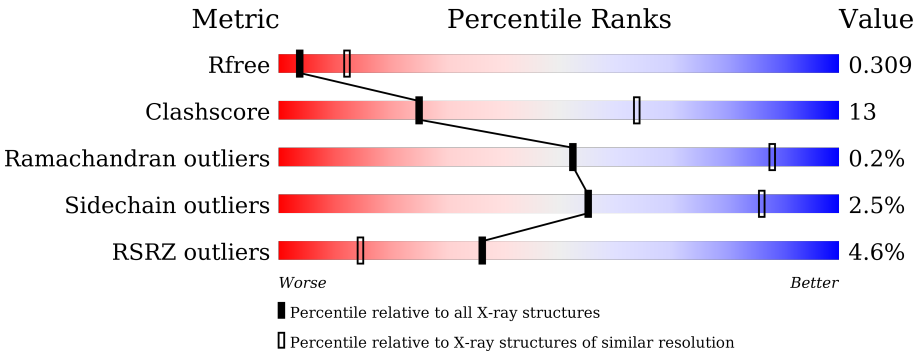
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	226	58% 23% 19%
1	B	226	3% 56% 21% 23%
1	C	226	60% 15% 23%
1	D	226	4% 49% 29% 21%
1	E	226	3% 29% 11% 60%
1	F	226	5% 44% 19% 36%

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Mol	Chain	Length	Quality of chain
1	G	226	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8632 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 Macrolide export ATP-binding/permease protein MacB.

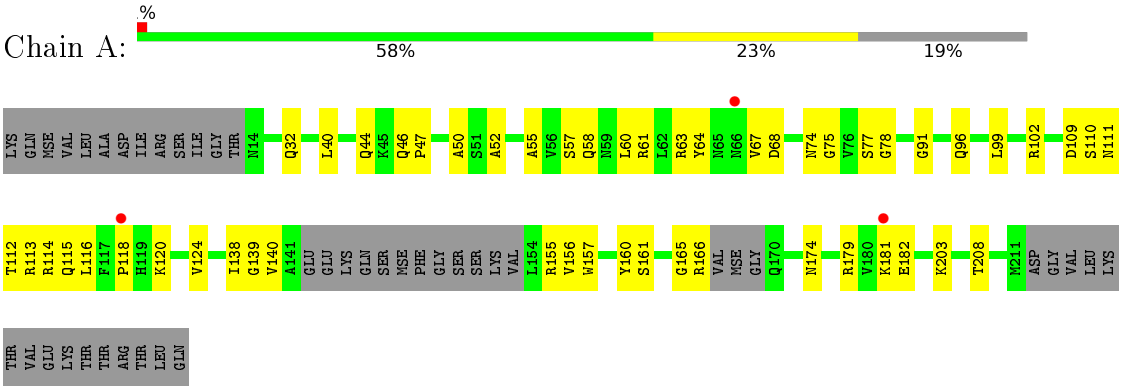
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	Se	0	0	0
			1449	912	257	276	4			
1	B	175	Total	C	N	O	Se	0	0	0
			1386	875	242	265	4			
1	C	173	Total	C	N	O	Se	0	0	0
			1371	866	242	260	3			
1	D	179	Total	C	N	O	Se	0	0	0
			1419	896	249	270	4			
1	E	91	Total	C	N	O	Se	0	0	0
			697	441	120	132	4			
1	F	144	Total	C	N	O	Se	0	0	0
			1130	716	196	214	4			
1	G	151	Total	C	N	O	Se	0	0	0
			1180	748	202	227	3			

3 Residue-property plots

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

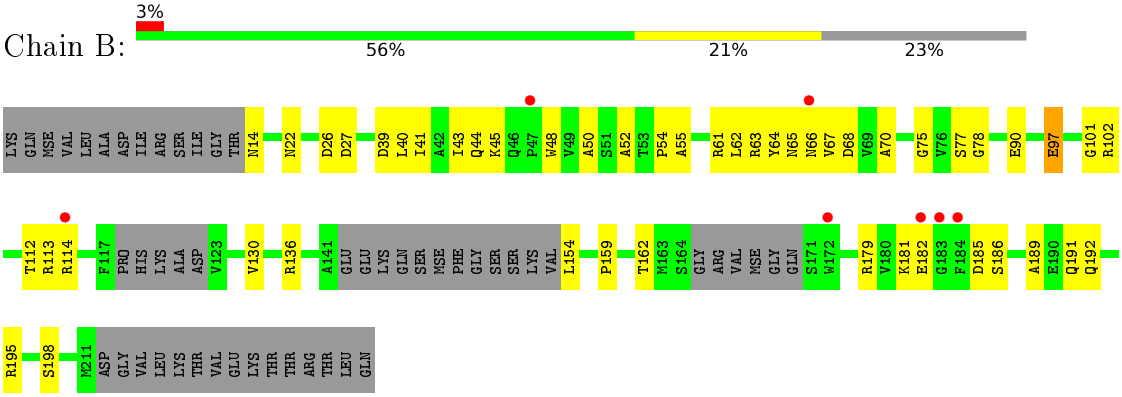
- Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain A:



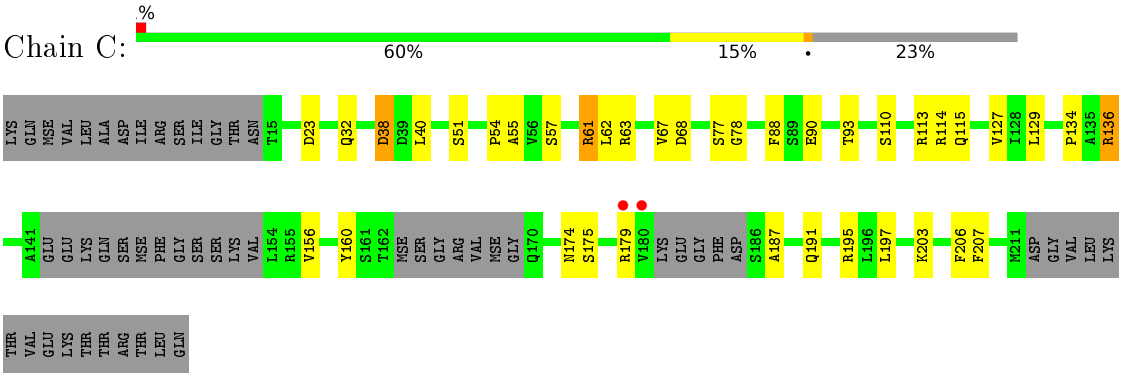
- Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain B:



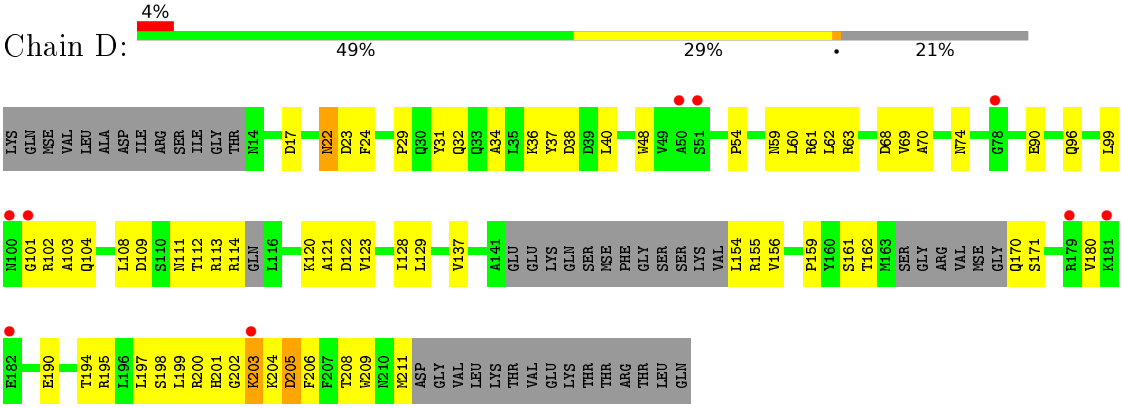
- Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain C:



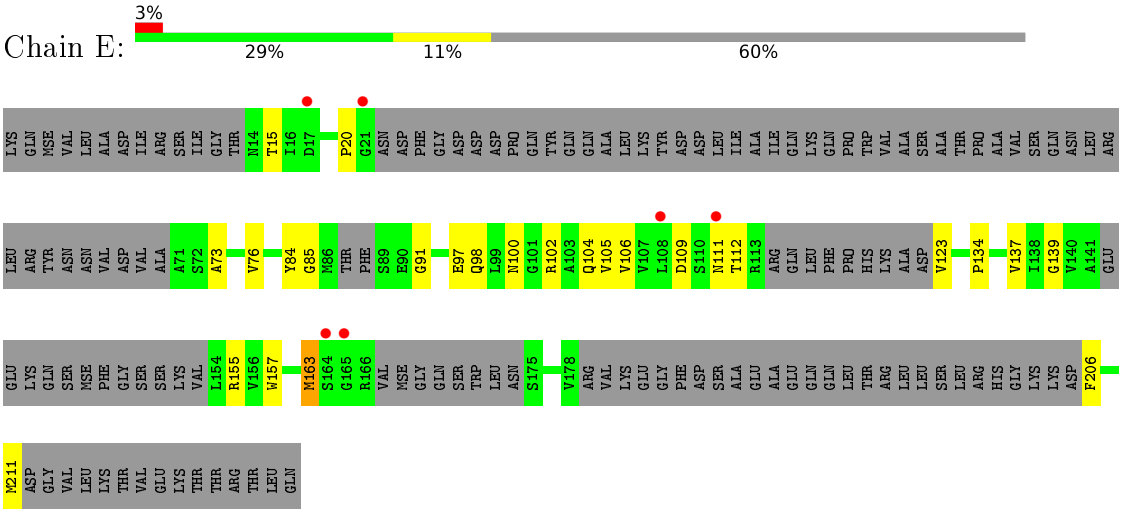
• Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain D:



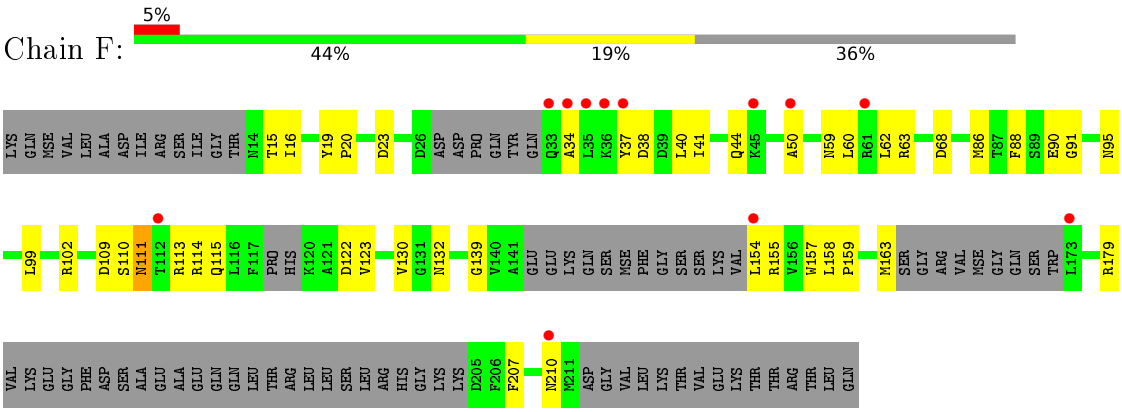
• Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain E:



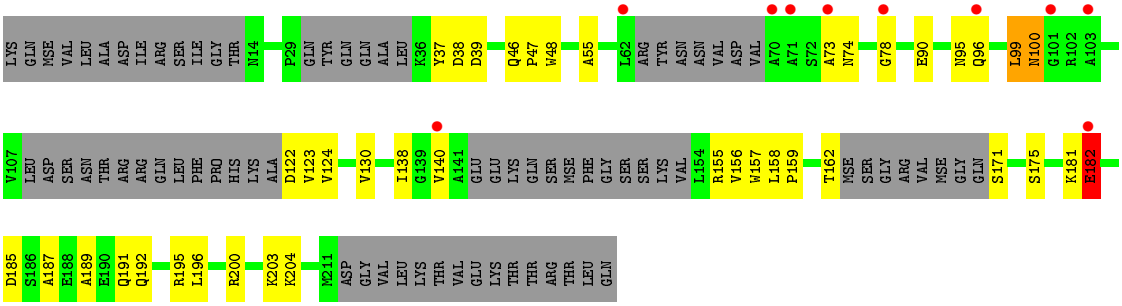
• Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain F:



• Molecule 1: Macrolide export ATP-binding/permease protein MacB

Chain G:


LYS GLN MSE VAL LEU ALA ASP ILE ARG SER ILE GLY THR N14 P29 GLN TYR GLN GLN ALA LEU K36 Y37 D38 D39 Q46 P47 W48 A55 L62 ARG TYR ASN ASN VAL ASP VAL A70 A71 S72 A73 N74 G78 E90 N95 Q96 L99 N100 G101 R102 A103
V107 LEU ASP SER ASN THR ARG ARG GLN LEU PHE PRO HIS LYS ALA D122 V123 V124 V130 I138 G139 V140 A141 GLU GLU LYS GLN SER MSE PHE GLY SER SER LYS VAL L154 R155 V156 W157 L158 P159 T162 MSE SER GLY ARG VAL MSE GLY GLN S171 S175 K181 E182
D185 S186 A187 E188 A189 E190 Q191 Q192 R195 L196 R200 K203 K204 M211 ASP GLY VAL LEU LYS THR VAL GLU LYS THR THR ARG THR LEU GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.14Å 78.56Å 137.92Å 90.00° 99.72° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 33.46 – 2.99	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-3.00) 96.0 (33.46-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.89 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.247 , 0.306 0.255 , 0.309	Depositor DCC
R_{free} test set	1988 reflections (7.05%)	DCC
Wilson B-factor (Å^2)	70.7	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	0/1474	0.67	1/1994 (0.1%)
1	B	0.33	0/1408	0.64	1/1904 (0.1%)
1	C	0.31	0/1395	0.60	0/1891
1	D	0.39	0/1443	0.67	0/1952
1	E	0.31	0/701	0.59	0/939
1	F	0.36	0/1144	0.63	0/1545
1	G	0.32	0/1198	0.66	1/1619 (0.1%)
All	All	0.35	0/8763	0.64	3/11844 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	LEU	CA-CB-CG	7.72	133.06	115.30
1	G	99	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	114	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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	1449	0	1402	38	2
1	B	1386	0	1341	40	1
1	C	1371	0	1330	23	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1419	0	1372	53	0
1	E	697	0	672	14	0
1	F	1130	0	1096	27	1
1	G	1180	0	1137	25	0
All	All	8632	0	8350	216	3

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 13.

All (216) 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:C:90:GLU:OE1	1:C:113:ARG:NH1	2.03	0.91
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.36	0.90
1:A:61:ARG:NH1	1:A:68:ASP:OD2	2.05	0.90
1:C:63:ARG:HE	1:C:129:LEU:HD13	1.40	0.87
1:D:120:LYS:HD2	1:D:121:ALA:H	1.39	0.87
1:G:55:ALA:HB3	1:G:175:SER:HB3	1.60	0.83
1:B:113:ARG:HG2	1:B:113:ARG:HH11	1.45	0.81
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.46	0.81
1:B:61:ARG:NH1	1:B:68:ASP:OD2	2.15	0.79
1:A:63:ARG:HE	1:A:68:ASP:HB2	1.49	0.76
1:D:62:LEU:HD11	1:D:156:VAL:HG21	1.68	0.74
1:D:74:ASN:HD21	1:D:155:ARG:HD2	1.51	0.74
1:F:63:ARG:HH11	1:F:68:ASP:HB2	1.54	0.72
1:A:113:ARG:HG2	1:A:113:ARG:NH1	2.04	0.72
1:D:99:LEU:HD23	1:D:159:PRO:HB3	1.70	0.71
1:D:37:TYR:OH	1:D:171:SER:OG	2.08	0.71
1:G:37:TYR:OH	1:G:171:SER:OG	2.10	0.70
1:F:122:ASP:OD1	1:F:123:VAL:N	2.25	0.70
1:D:111:ASN:OD1	1:D:114:ARG:NH2	2.25	0.70
1:D:120:LYS:HD2	1:D:121:ALA:N	2.06	0.69
1:D:63:ARG:HH11	1:D:63:ARG:HG2	1.58	0.69
1:E:155:ARG:HH21	1:E:157:TRP:HZ2	1.41	0.69
1:D:38:ASP:CB	1:D:200:ARG:HH12	2.06	0.69
1:A:63:ARG:NE	1:A:68:ASP:HB2	2.08	0.69
1:B:27:ASP:OD2	1:F:102:ARG:NH2	2.26	0.68
1:D:103:ALA:O	1:D:162:THR:OG1	2.10	0.68
1:B:102:ARG:HH11	1:B:102:ARG:HG3	1.60	0.67
1:B:41:ILE:HG23	1:B:45:LYS:HE2	1.78	0.66
1:B:22:ASN:N	1:B:26:ASP:OD2	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ASN:OD1	1:D:170:GLN:NE2	2.28	0.65
1:E:104:GLN:NE2	1:E:134:PRO:O	2.30	0.65
1:G:130:VAL:HG21	1:G:158:LEU:HD21	1.78	0.65
1:A:50:ALA:HA	1:A:181:LYS:HE2	1.80	0.64
1:F:63:ARG:NH1	1:F:68:ASP:HB2	2.13	0.64
1:G:90:GLU:HG2	1:G:140:VAL:HG12	1.79	0.64
1:A:110:SER:O	1:A:114:ARG:HG3	1.98	0.63
1:C:136:ARG:NH2	1:D:208:THR:O	2.31	0.63
1:A:99:LEU:HD21	1:A:160:TYR:CZ	2.34	0.62
1:G:73:ALA:HA	1:G:156:VAL:HG23	1.81	0.62
1:E:20:PRO:O	1:E:84:TYR:OH	2.13	0.61
1:A:102:ARG:NH1	1:A:102:ARG:HG3	2.18	0.59
1:D:38:ASP:HB2	1:D:200:ARG:HH12	1.68	0.58
1:F:99:LEU:HD23	1:F:159:PRO:HB3	1.86	0.58
1:A:208:THR:O	1:B:136:ARG:NH2	2.33	0.58
1:B:14:ASN:ND2	1:B:179:ARG:HH12	2.02	0.58
1:D:205:ASP:N	1:D:205:ASP:OD1	2.36	0.58
1:E:123:VAL:HG12	1:E:137:VAL:HG11	1.86	0.57
1:F:20:PRO:HB3	1:F:34:ALA:HB3	1.86	0.57
1:A:113:ARG:HD2	1:A:140:VAL:HG21	1.86	0.57
1:A:58:GLN:HB2	1:A:60:LEU:HD11	1.87	0.56
1:C:67:VAL:HG11	1:C:115:GLN:O	2.05	0.56
1:D:70:ALA:O	1:D:154:LEU:HD23	2.06	0.56
1:G:100:ASN:HD22	1:G:100:ASN:N	2.03	0.56
1:A:112:THR:HG21	1:A:156:VAL:HG13	1.87	0.56
1:D:36:LYS:HE3	1:D:38:ASP:OD2	2.06	0.56
1:G:181:LYS:NZ	1:G:182:GLU:HB2	2.21	0.55
1:F:86:MSE:HE1	1:F:155:ARG:HH22	1.71	0.55
1:B:14:ASN:OD1	1:B:179:ARG:NH1	2.40	0.55
1:D:108:LEU:HB3	1:D:112:THR:OG1	2.07	0.54
1:G:95:ASN:OD1	1:G:96:GLN:N	2.41	0.54
1:D:29:PRO:HA	1:D:32:GLN:HB2	1.88	0.54
1:F:91:GLY:HA3	1:F:139:GLY:HA2	1.87	0.54
1:C:61:ARG:CZ	1:C:68:ASP:OD2	2.56	0.54
1:D:120:LYS:HE3	1:D:122:ASP:O	2.07	0.54
1:A:64:TYR:O	1:A:67:VAL:HG12	2.07	0.54
1:B:97:GLU:O	1:B:101:GLY:N	2.39	0.54
1:A:32:GLN:HE22	1:A:155:ARG:NH1	2.06	0.54
1:D:112:THR:HG21	1:D:156:VAL:HG23	1.90	0.54
1:B:159:PRO:HB2	1:B:162:THR:HG23	1.89	0.54
1:B:181:LYS:HD2	1:B:182:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:CZ	1:A:68:ASP:OD2	2.56	0.53
1:G:192:GLN:HA	1:G:195:ARG:HD2	1.90	0.53
1:D:209:TRP:CD2	1:D:211:MSE:HE2	2.43	0.53
1:C:62:LEU:HD11	1:C:156:VAL:HG11	1.90	0.53
1:B:113:ARG:HG2	1:B:113:ARG:NH1	2.18	0.53
1:F:111:ASN:O	1:F:114:ARG:HG3	2.09	0.53
1:G:38:ASP:OD1	1:G:39:ASP:N	2.42	0.53
1:D:32:GLN:HE21	1:D:155:ARG:HD3	1.75	0.52
1:G:185:ASP:OD1	1:G:187:ALA:N	2.36	0.52
1:G:159:PRO:HB2	1:G:162:THR:HG23	1.92	0.52
1:C:61:ARG:NH2	1:C:68:ASP:OD2	2.43	0.52
1:A:50:ALA:HA	1:A:181:LYS:CE	2.40	0.52
1:B:61:ARG:HE	1:B:63:ARG:HH21	1.57	0.51
1:A:32:GLN:HE22	1:A:155:ARG:HH11	1.58	0.51
1:A:55:ALA:HB1	1:A:75:GLY:O	2.11	0.51
1:C:57:SER:OG	1:C:174:ASN:ND2	2.36	0.51
1:B:64:TYR:O	1:B:67:VAL:HG12	2.11	0.51
1:D:96:GLN:HG3	1:D:99:LEU:HD12	1.93	0.51
1:D:40:LEU:HD22	1:D:54:PRO:HB3	1.92	0.51
1:F:40:LEU:O	1:F:44:GLN:HG3	2.11	0.50
1:D:109:ASP:OD1	1:D:112:THR:HG23	2.12	0.50
1:B:55:ALA:HB1	1:B:75:GLY:O	2.12	0.49
1:A:91:GLY:HA3	1:A:139:GLY:HA2	1.93	0.49
1:D:38:ASP:HB3	1:D:200:ARG:HH12	1.76	0.49
1:F:16:ILE:HA	1:F:210:ASN:HA	1.94	0.49
1:G:122:ASP:OD2	1:G:123:VAL:N	2.45	0.49
1:A:124:VAL:HG13	1:A:138:ILE:HA	1.95	0.49
1:C:77:SER:OG	1:C:78:GLY:N	2.45	0.49
1:A:118:PRO:HD2	1:A:120:LYS:NZ	2.27	0.49
1:G:181:LYS:HD2	1:G:182:GLU:H	1.77	0.49
1:B:41:ILE:O	1:B:45:LYS:HG2	2.13	0.49
1:F:90:GLU:OE2	1:F:122:ASP:OD1	2.31	0.49
1:G:78:GLY:H	1:G:99:LEU:HD21	1.78	0.48
1:G:155:ARG:O	1:G:155:ARG:HG3	2.13	0.48
1:A:165:GLY:C	1:A:166:ARG:HD3	2.33	0.48
1:D:63:ARG:HH11	1:D:63:ARG:CG	2.26	0.48
1:B:61:ARG:CZ	1:B:68:ASP:OD2	2.62	0.48
1:C:127:VAL:HG22	1:C:136:ARG:HG3	1.96	0.48
1:D:23:ASP:OD1	1:D:24:PHE:N	2.39	0.48
1:D:74:ASN:ND2	1:D:155:ARG:HD2	2.27	0.47
1:A:50:ALA:N	1:A:179:ARG:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ALA:O	1:C:191:GLN:HG3	2.14	0.47
1:D:197:LEU:O	1:D:201:HIS:ND1	2.32	0.47
1:D:61:ARG:NH1	1:D:69:VAL:HA	2.29	0.47
1:E:73:ALA:HB3	1:E:163:MSE:SE	2.64	0.47
1:B:70:ALA:O	1:B:154:LEU:HD23	2.14	0.47
1:C:88:PHE:CZ	1:C:93:THR:HB	2.49	0.47
1:A:40:LEU:HD11	1:A:52:ALA:O	2.15	0.47
1:B:40:LEU:HD11	1:B:52:ALA:O	2.14	0.47
1:E:106:VAL:HG12	1:E:137:VAL:HA	1.96	0.47
1:G:48:TRP:NE1	1:G:192:GLN:NE2	2.62	0.47
1:B:40:LEU:HD22	1:B:54:PRO:HB3	1.96	0.47
1:E:91:GLY:HA3	1:E:139:GLY:HA2	1.96	0.47
1:C:55:ALA:HB3	1:C:175:SER:HB3	1.97	0.47
1:D:101:GLY:O	1:D:102:ARG:HB3	2.15	0.47
1:A:102:ARG:HG2	1:A:161:SER:HB2	1.97	0.46
1:B:61:ARG:HH21	1:B:63:ARG:CZ	2.27	0.46
1:G:203:LYS:HG3	1:G:204:LYS:H	1.80	0.46
1:B:50:ALA:HB2	1:B:181:LYS:HA	1.97	0.46
1:D:62:LEU:O	1:D:68:ASP:HA	2.15	0.46
1:D:203:LYS:HB3	1:D:205:ASP:OD1	2.16	0.46
1:A:111:ASN:O	1:A:115:GLN:HG3	2.16	0.46
1:B:14:ASN:CG	1:B:179:ARG:NH1	2.69	0.46
1:B:191:GLN:O	1:B:195:ARG:HG3	2.15	0.46
1:A:57:SER:OG	1:A:174:ASN:ND2	2.43	0.46
1:D:209:TRP:CE3	1:D:211:MSE:HE2	2.51	0.46
1:G:46:GLN:HA	1:G:47:PRO:HD3	1.85	0.46
1:B:61:ARG:HE	1:B:63:ARG:NH2	2.14	0.45
1:D:113:ARG:HE	1:D:113:ARG:HB3	1.46	0.45
1:D:34:ALA:HB1	1:D:205:ASP:HB2	1.98	0.45
1:D:96:GLN:HA	1:D:99:LEU:HB2	1.98	0.45
1:A:102:ARG:NH1	1:A:102:ARG:CG	2.78	0.45
1:F:110:SER:O	1:F:114:ARG:HG2	2.17	0.45
1:A:32:GLN:NE2	1:A:155:ARG:NH1	2.63	0.45
1:G:191:GLN:O	1:G:195:ARG:HG3	2.16	0.45
1:A:166:ARG:HD3	1:A:166:ARG:N	2.31	0.45
1:B:65:ASN:O	1:B:66:ASN:HB3	2.17	0.45
1:D:63:ARG:HB2	1:D:129:LEU:HB2	1.99	0.45
1:E:98:GLN:NE2	1:E:105:VAL:HG11	2.32	0.45
1:A:58:GLN:HB2	1:A:60:LEU:CD1	2.47	0.44
1:C:40:LEU:HD22	1:C:54:PRO:HB3	1.99	0.44
1:E:76:VAL:HG11	1:E:157:TRP:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ASN:HA	1:F:114:ARG:NE	2.32	0.44
1:G:196:LEU:O	1:G:200:ARG:HG3	2.17	0.44
1:D:190:GLU:OE2	1:D:208:THR:OG1	2.32	0.44
1:F:111:ASN:HB2	1:F:154:LEU:HD12	2.00	0.44
1:D:198:SER:O	1:D:202:GLY:N	2.44	0.44
1:A:77:SER:OG	1:A:78:GLY:N	2.51	0.44
1:E:20:PRO:HA	1:E:206:PHE:HB2	1.99	0.44
1:B:14:ASN:CG	1:B:179:ARG:HH12	2.21	0.44
1:D:90:GLU:OE1	1:D:123:VAL:HG12	2.17	0.44
1:F:86:MSE:HE1	1:F:155:ARG:NH2	2.32	0.44
1:E:15:THR:HG23	1:E:211:MSE:HB2	1.99	0.44
1:G:74:ASN:HB2	1:G:157:TRP:CD1	2.53	0.44
1:C:110:SER:O	1:C:114:ARG:HG3	2.18	0.44
1:D:194:THR:O	1:D:206:PHE:HZ	2.01	0.44
1:C:197:LEU:HB2	1:C:206:PHE:CZ	2.53	0.43
1:B:185:ASP:OD1	1:B:186:SER:N	2.51	0.43
1:B:48:TRP:CD1	1:B:192:GLN:NE2	2.85	0.43
1:D:17:ASP:OD2	1:D:211:MSE:HE3	2.18	0.43
1:G:124:VAL:HG13	1:G:138:ILE:HA	2.00	0.43
1:G:96:GLN:HA	1:G:99:LEU:HD13	1.99	0.43
1:D:203:LYS:HG2	1:D:204:LYS:H	1.84	0.43
1:B:39:ASP:O	1:B:43:ILE:HG13	2.19	0.43
1:B:77:SER:OG	1:B:78:GLY:N	2.50	0.43
1:F:62:LEU:HD23	1:F:130:VAL:HA	2.00	0.43
1:F:90:GLU:OE1	1:F:113:ARG:NH1	2.52	0.43
1:C:114:ARG:HE	1:C:114:ARG:HB3	1.49	0.43
1:A:109:ASP:HB3	1:A:157:TRP:CZ3	2.54	0.43
1:C:23:ASP:HA	1:C:207:PHE:CG	2.54	0.43
1:D:61:ARG:HH11	1:D:69:VAL:HA	1.84	0.43
1:F:23:ASP:HA	1:F:207:PHE:CG	2.53	0.42
1:E:109:ASP:OD2	1:E:112:THR:HB	2.19	0.42
1:F:111:ASN:O	1:F:115:GLN:HG3	2.19	0.42
1:F:19:TYR:HB2	1:F:207:PHE:CZ	2.55	0.42
1:F:109:ASP:HB3	1:F:157:TRP:CH2	2.55	0.42
1:F:37:TYR:O	1:F:41:ILE:HD12	2.20	0.42
1:G:48:TRP:CE3	1:G:189:ALA:HB1	2.54	0.42
1:B:40:LEU:O	1:B:44:GLN:HG3	2.20	0.42
1:E:102:ARG:O	1:E:102:ARG:HG2	2.20	0.42
1:C:63:ARG:HG2	1:C:129:LEU:HB2	2.01	0.42
1:D:123:VAL:HG13	1:D:137:VAL:HG11	2.02	0.41
1:B:113:ARG:CG	1:B:113:ARG:NH1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:SER:HB2	1:C:160:TYR:HE2	1.85	0.41
1:E:97:GLU:OE2	1:E:100:ASN:ND2	2.52	0.41
1:B:181:LYS:HD2	1:B:182:GLU:N	2.36	0.41
1:F:158:LEU:HD22	1:F:163:MSE:HE3	2.01	0.41
1:F:50:ALA:N	1:F:179:ARG:O	2.52	0.41
1:A:74:ASN:HB2	1:A:157:TRP:CD1	2.55	0.41
1:D:48:TRP:CZ3	1:D:180:VAL:HG12	2.55	0.41
1:F:59:ASN:O	1:F:60:LEU:HD23	2.21	0.41
1:D:62:LEU:HD22	1:D:128:ILE:HD12	2.03	0.41
1:A:113:ARG:CG	1:A:113:ARG:NH1	2.74	0.41
1:B:102:ARG:CG	1:B:102:ARG:HH11	2.31	0.41
1:C:38:ASP:OD1	1:C:38:ASP:N	2.52	0.41
1:B:48:TRP:CE3	1:B:189:ALA:HB1	2.56	0.41
1:B:62:LEU:HD23	1:B:130:VAL:HA	2.02	0.41
1:D:59:ASN:C	1:D:60:LEU:HD12	2.41	0.41
1:D:99:LEU:O	1:D:161:SER:OG	2.21	0.41
1:F:90:GLU:OE2	1:F:122:ASP:CG	2.59	0.41
1:D:22:ASN:OD1	1:D:31:TYR:HE2	2.04	0.41
1:A:46:GLN:HA	1:A:47:PRO:HD3	1.93	0.40
1:C:134:PRO:HB3	1:D:209:TRP:CH2	2.55	0.40
1:B:112:THR:HA	1:B:154:LEU:HD11	2.02	0.40
1:B:102:ARG:NH1	1:B:102:ARG:HG3	2.32	0.40
1:C:51:SER:OG	1:C:179:ARG:NH2	2.54	0.40

All (3) 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:A:44:GLN:OE1	1:B:198:SER:OG[1_655]	2.13	0.07
1:A:203:LYS:O	1:C:203:LYS:NZ[2_656]	2.16	0.04
1:C:195:ARG:NE	1:F:88:PHE:O[2_546]	2.18	0.02

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	177/226 (78%)	170 (96%)	7 (4%)	0	100	100
1	B	167/226 (74%)	161 (96%)	6 (4%)	0	100	100
1	C	165/226 (73%)	158 (96%)	7 (4%)	0	100	100
1	D	171/226 (76%)	162 (95%)	9 (5%)	0	100	100
1	E	77/226 (34%)	70 (91%)	6 (8%)	1 (1%)	15	53
1	F	132/226 (58%)	126 (96%)	6 (4%)	0	100	100
1	G	139/226 (62%)	133 (96%)	5 (4%)	1 (1%)	26	70
All	All	1028/1582 (65%)	980 (95%)	46 (4%)	2 (0%)	52	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	182	GLU
1	E	85	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	A	156/187 (83%)	154 (99%)	2 (1%)	76	93
1	B	150/187 (80%)	148 (99%)	2 (1%)	76	93
1	C	148/187 (79%)	144 (97%)	4 (3%)	52	85
1	D	153/187 (82%)	147 (96%)	6 (4%)	39	77
1	E	76/187 (41%)	74 (97%)	2 (3%)	54	85
1	F	122/187 (65%)	117 (96%)	5 (4%)	37	76
1	G	127/187 (68%)	125 (98%)	2 (2%)	70	92
All	All	932/1309 (71%)	909 (98%)	23 (2%)	55	86

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	182	GLU
1	B	90	GLU
1	B	97	GLU
1	C	32	GLN
1	C	38	ASP
1	C	61	ARG
1	C	136	ARG
1	D	22	ASN
1	D	104	GLN
1	D	195	ARG
1	D	199	LEU
1	D	203	LYS
1	D	205	ASP
1	E	111	ASN
1	E	163	MSE
1	F	15	THR
1	F	38	ASP
1	F	95	ASN
1	F	111	ASN
1	F	132	ASN
1	G	100	ASN
1	G	182	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	B	66	ASN
1	D	59	ASN
1	D	74	ASN
1	D	170	GLN
1	F	104	GLN
1	G	100	ASN
1	G	132	ASN
1	G	192	GLN

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

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^{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	179/226 (79%)	0.10	3 (1%) 73 45	33, 66, 98, 109	0
1	B	171/226 (75%)	0.16	7 (4%) 41 16	37, 60, 90, 104	0
1	C	170/226 (75%)	0.02	2 (1%) 81 55	44, 72, 101, 117	0
1	D	175/226 (77%)	0.33	9 (5%) 32 12	54, 83, 106, 119	0
1	E	87/226 (38%)	0.46	6 (6%) 20 7	63, 86, 115, 122	0
1	F	140/226 (61%)	0.47	12 (8%) 13 4	47, 81, 103, 108	0
1	G	148/226 (65%)	0.48	10 (6%) 20 7	56, 87, 108, 126	0
All	All	1070/1582 (67%)	0.26	49 (4%) 36 14	33, 76, 104, 126	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	173	LEU	4.9
1	B	183	GLY	4.9
1	F	112	THR	4.8
1	G	140	VAL	4.6
1	G	78	GLY	4.5
1	D	101	GLY	4.5
1	G	96	GLN	4.3
1	G	103	ALA	4.2
1	F	33	GLN	4.1
1	E	17	ASP	3.7
1	D	51	SER	3.7
1	D	182	GLU	3.6
1	G	62	LEU	3.6
1	C	180	VAL	3.4
1	G	71	ALA	3.3
1	E	108	LEU	3.3
1	D	100	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	111	ASN	3.1
1	F	50	ALA	3.1
1	B	66	ASN	3.0
1	B	184	PHE	3.0
1	D	50	ALA	2.9
1	F	45	LYS	2.8
1	F	34	ALA	2.8
1	E	164	SER	2.7
1	B	114	ARG	2.7
1	D	181	LYS	2.7
1	B	182	GLU	2.7
1	F	36	LYS	2.6
1	D	179	ARG	2.6
1	F	210	ASN	2.6
1	F	154	LEU	2.6
1	C	179	ARG	2.5
1	G	70	ALA	2.5
1	G	73	ALA	2.4
1	G	182	GLU	2.3
1	A	66	ASN	2.3
1	A	181	LYS	2.3
1	E	165	GLY	2.2
1	G	101	GLY	2.2
1	D	203	LYS	2.2
1	F	35	LEU	2.2
1	A	118	PRO	2.2
1	D	78	GLY	2.2
1	E	21	GLY	2.1
1	F	37	TYR	2.1
1	B	172	TRP	2.1
1	F	61	ARG	2.1
1	B	47	PRO	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.