



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:42 AM UTC

PDB ID : 5C59 / pdb_00005c59
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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

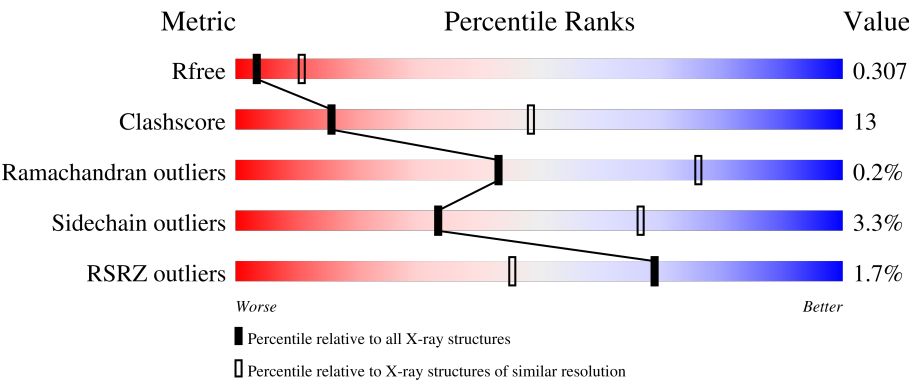
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	

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Mol	Chain	Length	Quality of chain
1	F	226	% 43% 19% 36%
1	G	226	2% 47% 19% 33%

2 Entry composition

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.

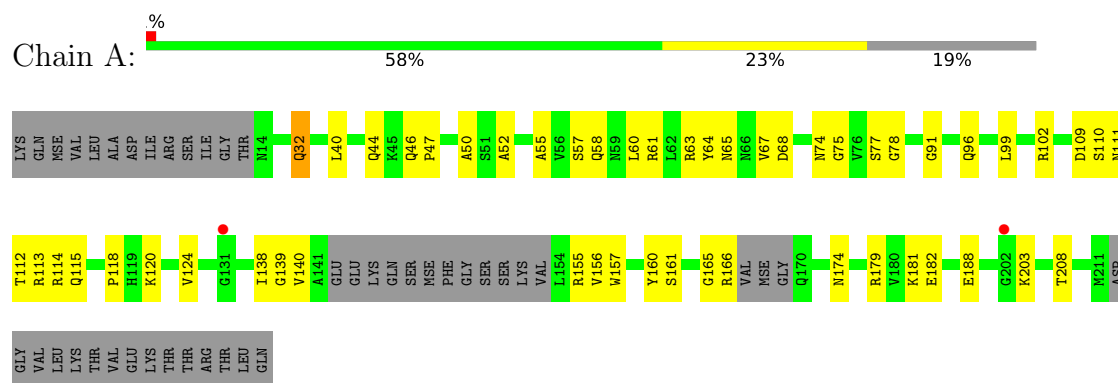
- Molecule 1 is a protein called Macrolide export ATP-binding/permease protein MacB.

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			

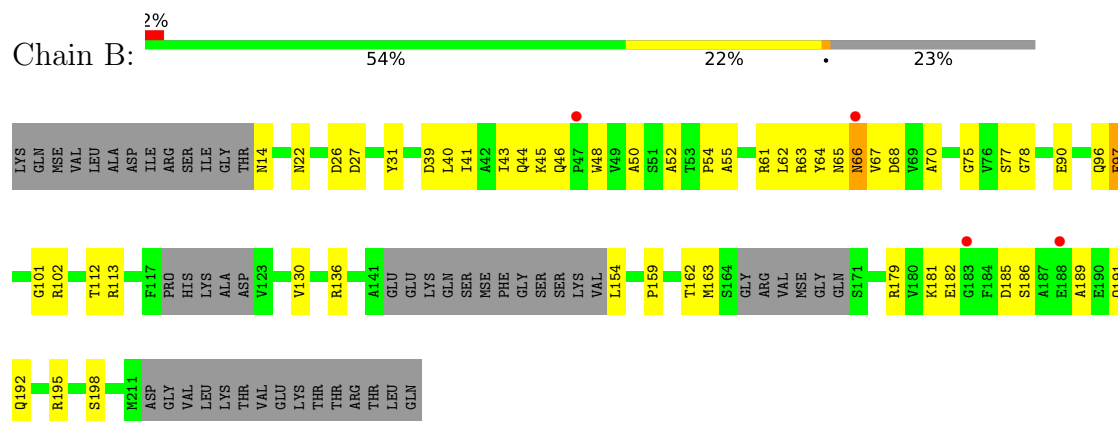
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

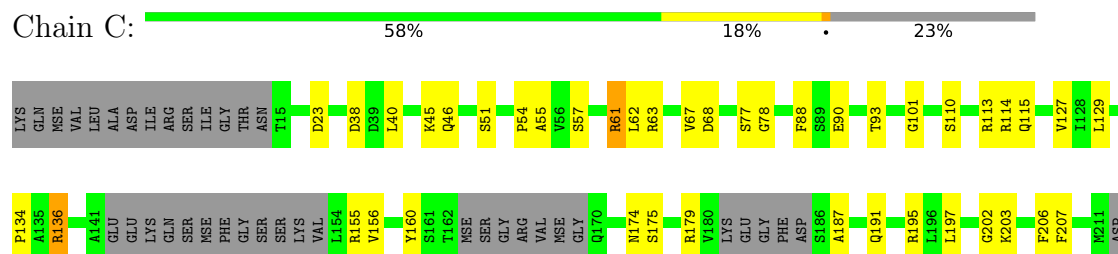
- Molecule 1: Macrolide export ATP-binding/permease protein MacB

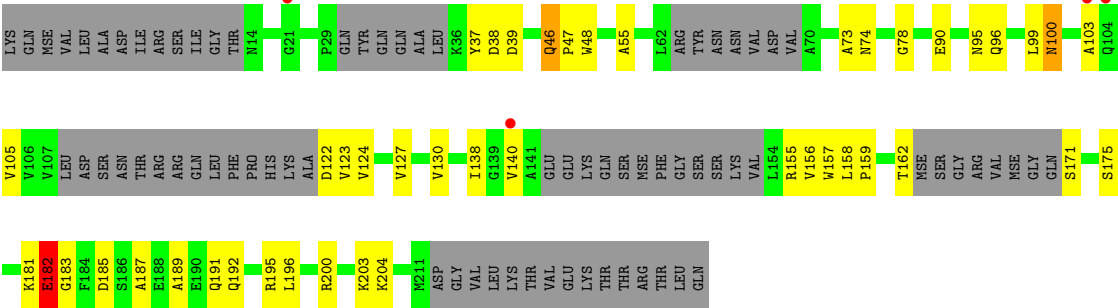


- Molecule 1: Macrolide export ATP-binding/permease protein MacB



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





4 Data and refinement statistics

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 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-3.00) 96.0 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.67 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.247 , 0.306 0.252 , 0.307	Depositor DCC
R_{free} test set	1995 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

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.

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	0.49	0/1474	0.93	1/1994 (0.1%)
1	B	0.41	0/1408	0.91	7/1904 (0.4%)
1	C	0.38	0/1395	0.92	5/1891 (0.3%)
1	D	0.48	0/1443	0.98	2/1952 (0.1%)
1	E	0.39	0/701	0.91	4/939 (0.4%)
1	F	0.46	0/1144	0.95	4/1545 (0.3%)
1	G	0.41	0/1198	1.01	7/1619 (0.4%)
All	All	0.44	0/8763	0.95	30/11844 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	GLY	N-CA-C	-8.63	103.20	114.85
1	D	186	SER	N-CA-C	8.58	123.40	113.19
1	C	101	GLY	N-CA-C	-7.92	104.95	115.32
1	G	183	GLY	N-CA-C	7.04	124.88	115.59
1	G	46	GLN	CA-C-N	6.79	127.06	119.32
1	G	46	GLN	C-N-CA	6.79	127.06	119.32
1	G	103	ALA	CA-C-N	-6.51	113.82	123.00
1	G	103	ALA	C-N-CA	-6.51	113.82	123.00
1	B	66	ASN	N-CA-CB	-6.16	107.14	114.17
1	E	101	GLY	N-CA-C	-6.11	101.60	112.54
1	E	112	THR	N-CA-C	-5.86	105.39	112.54
1	B	96	GLN	N-CA-C	5.86	118.61	111.82
1	F	68	ASP	N-CA-C	5.66	117.62	108.34
1	B	66	ASN	CA-C-N	-5.64	116.19	123.19
1	B	66	ASN	C-N-CA	-5.64	116.19	123.19
1	F	16	ILE	CB-CA-C	-5.58	103.74	110.99
1	B	31	TYR	N-CA-C	5.56	120.05	112.88
1	G	105	VAL	N-CA-C	-5.48	99.91	108.95
1	C	202	GLY	N-CA-C	-5.43	108.14	115.36
1	F	46	GLN	CA-C-N	5.42	124.88	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	GLN	C-N-CA	5.42	124.88	119.24
1	C	155	ARG	N-CA-C	5.36	117.70	109.07
1	G	127	VAL	N-CA-C	5.28	115.46	107.75
1	E	110	SER	N-CA-C	5.21	117.71	111.71
1	A	188	GLU	N-CA-C	-5.17	106.48	112.89
1	C	46	GLN	CA-C-N	5.15	124.60	119.24
1	C	46	GLN	C-N-CA	5.15	124.60	119.24
1	E	92	ASN	N-CA-C	5.08	116.49	110.19
1	B	46	GLN	CA-C-N	5.06	125.09	119.32
1	B	46	GLN	C-N-CA	5.06	125.09	119.32

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	40	2
1	B	1386	0	1341	43	1
1	C	1371	0	1330	22	2
1	D	1419	0	1372	54	0
1	E	697	0	672	15	0
1	F	1130	0	1096	29	1
1	G	1180	0	1137	27	0
All	All	8632	0	8350	225	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 (225) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:B:113:ARG:HG2	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:63:ARG:HG2	1:D:63:ARG:HH11	1.58	0.69
1:D:120:LYS:HD2	1:D:121:ALA:N	2.06	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:HG3	1:B:102:ARG:HH11	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
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:B:48:TRP:CD1	1:B:192:GLN:HE21	2.17	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:HG3	1:A:102:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:D:205:ASP:N	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:N	1:G:100:ASN:HD22	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:G:48:TRP:H	1:G:48:TRP:CD1	2.22	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:A:118:PRO:HD2	1:A:120:LYS:HZ1	1.72	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
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:A:165:GLY:C	1:A:166:ARG:HD3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:14:ASN:CG	1:B:179:ARG:NH1	2.69	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:14:ASN:CG	1:B:179:ARG:HH12	2.21	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:181:LYS:HZ3	1:G:182:GLU:HB2	1.78	0.48
1:G:155:ARG:O	1:G:155:ARG:HG3	2.13	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
1:C:187:ALA:O	1:C:191:GLN:HG3	2.14	0.47
1:D:61:ARG:NH1	1:D:69:VAL:HA	2.29	0.47
1:D:197:LEU:O	1:D:201:HIS:ND1	2.32	0.47
1:E:73:ALA:HB3	1:E:163:MSE:SE	2.64	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: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:E:106:VAL:HG12	1:E:137:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:113:ARG:HE	1:D:113:ARG:HB3	1.46	0.45
1:A:102:ARG:NH1	1:A:102:ARG:CG	2.78	0.45
1:D:59:ASN:C	1:D:60:LEU:HD12	2.41	0.45
1:F:90:GLU:OE2	1:F:122:ASP:CG	2.59	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
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:E:100:ASN:OD1	1:E:100:ASN:C	2.60	0.44
1:A:77:SER:OG	1:A:78:GLY:N	2.51	0.44
1:B:27:ASP:CG	1:F:102:ARG:HH22	2.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:PRO:HA	1:E:206:PHE:HB2	1.99	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:B:102:ARG:C	1:B:162:THR:HG22	2.43	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:48:TRP:CD1	1:B:192:GLN:NE2	2.85	0.43
1:B:185:ASP:OD1	1:B:186:SER:N	2.51	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:F:16:ILE:HG12	1:F:210:ASN:CG	2.43	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:D:48:TRP:H	1:D:48:TRP:CD1	2.36	0.42
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:19:TYR:HB2	1:F:207:PHE:CZ	2.55	0.42
1:F:111:ASN:O	1:F:115:GLN:HG3	2.19	0.42
1:F:37:TYR:O	1:F:41:ILE:HD12	2.20	0.42
1:F:109:ASP:HB3	1:F:157:TRP:CH2	2.55	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:B:77:SER:OG	1:B:78:GLY:N	2.50	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:NH1	1:B:113:ARG:CG	2.79	0.41
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:50:ALA:N	1:F:179:ARG:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:LEU:HD22	1:F:163:MSE:HE3	2.01	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:NH1	1:A:113:ARG:CG	2.74	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:B:102:ARG:HH11	1:B:102:ARG:CG	2.31	0.41
1:D:99:LEU:O	1:D:161:SER:OG	2.21	0.41
1:A:64:TYR:O	1:A:65:ASN:C	2.64	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:HG3	1:B:102:ARG:NH1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	9	38
1	F	132/226 (58%)	126 (96%)	6 (4%)	0	100	100
1	G	139/226 (62%)	133 (96%)	5 (4%)	1 (1%)	18	53
All	All	1028/1582 (65%)	980 (95%)	46 (4%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	182	GLU
1	E	85	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/187 (83%)	153 (98%)	3 (2%)	50	76
1	B	150/187 (80%)	147 (98%)	3 (2%)	48	76
1	C	148/187 (79%)	144 (97%)	4 (3%)	39	71
1	D	153/187 (82%)	145 (95%)	8 (5%)	21	55
1	E	76/187 (41%)	72 (95%)	4 (5%)	20	54
1	F	122/187 (65%)	115 (94%)	7 (6%)	18	52
1	G	127/187 (68%)	125 (98%)	2 (2%)	55	79
All	All	932/1309 (71%)	901 (97%)	31 (3%)	33	67

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	182	GLU
1	B	90	GLU
1	B	97	GLU
1	B	163	MSE
1	C	38	ASP
1	C	45	LYS
1	C	61	ARG
1	C	136	ARG
1	D	22	ASN
1	D	63	ARG
1	D	104	GLN
1	D	110	SER
1	D	195	ARG
1	D	199	LEU
1	D	203	LYS
1	D	205	ASP
1	E	100	ASN
1	E	111	ASN
1	E	163	MSE
1	E	211	MSE
1	F	15	THR
1	F	38	ASP
1	F	49	VAL
1	F	95	ASN
1	F	111	ASN
1	F	132	ASN
1	F	211	MSE
1	G	100	ASN
1	G	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	66	ASN
1	A	104	GLN
1	A	191	GLN
1	A	210	ASN
1	B	66	ASN
1	B	174	ASN
1	C	119	HIS

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Mol	Chain	Res	Type
1	D	59	ASN
1	D	74	ASN
1	D	170	GLN
1	E	74	ASN
1	F	96	GLN
1	F	104	GLN
1	G	22	ASN
1	G	100	ASN
1	G	132	ASN
1	G	192	GLN
1	G	210	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

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, 95th 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%)	0.06	2 (1%) 78 57	33, 66, 98, 109	0
1	B	171/226 (75%)	-0.02	4 (2%) 61 38	37, 60, 90, 104	0
1	C	170/226 (75%)	0.09	0 100 100	44, 72, 101, 117	0
1	D	175/226 (77%)	0.23	4 (2%) 61 38	54, 83, 106, 119	0
1	E	87/226 (38%)	0.31	2 (2%) 61 38	63, 86, 115, 122	0
1	F	140/226 (61%)	0.22	2 (1%) 73 51	47, 81, 103, 108	0
1	G	148/226 (65%)	0.26	4 (2%) 56 33	56, 86, 108, 126	0
All	All	1070/1582 (67%)	0.15	18 (1%) 69 45	33, 76, 104, 126	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	GLY	3.3
1	F	50	ALA	3.2
1	E	74	ASN	2.9
1	G	103	ALA	2.8
1	G	140	VAL	2.7
1	D	182	GLU	2.6
1	D	78	GLY	2.3
1	D	26	ASP	2.3
1	B	47	PRO	2.3
1	B	188	GLU	2.3
1	D	101	GLY	2.3
1	G	104	GLN	2.3
1	E	17	ASP	2.3
1	B	66	ASN	2.2
1	A	202	GLY	2.2
1	F	112	THR	2.1
1	A	131	GLY	2.1
1	G	21	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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.