



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:00 AM UTC

PDB ID : 6GAV / pdb_00006gav
Title : Extremely 'open' clamp structure of DNA gyrase: role of the Corynebacteriales GyrB specific insert
Authors : Petrella, S.; Capton, E.; Alzari, P.M.; Aubry, A.; MAyer, C.
Deposited on : 2018-04-12
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 ⓘ 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

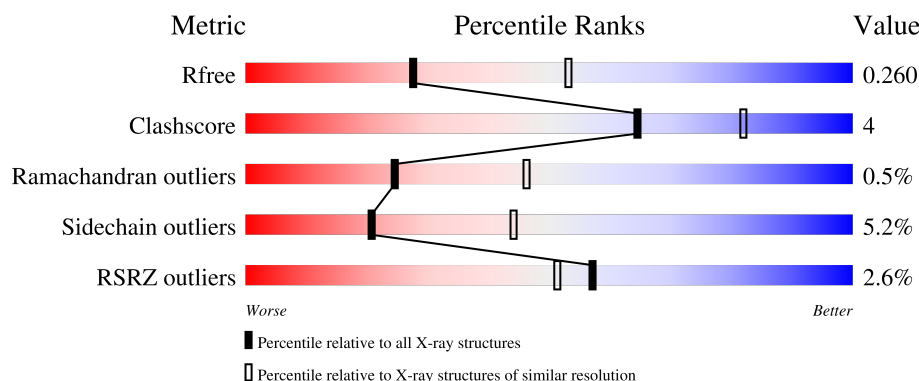
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	1179	
1	B	1179	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17544 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 DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1119	Total	C	N	O	S	0	0	0
			8723	5442	1574	1681	26			
1	B	1117	Total	C	N	O	S	0	0	0
			8714	5437	1571	1680	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP F6N7X0
A	676	GLY	-	linker	UNP F6N7X0
A	677	ASP	-	linker	UNP F6N7X0
A	678	LEU	-	linker	UNP F6N7X0
B	0	MET	-	initiating methionine	UNP F6N7X0
B	676	GLY	-	linker	UNP F6N7X0
B	677	ASP	-	linker	UNP F6N7X0
B	678	LEU	-	linker	UNP F6N7X0

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).

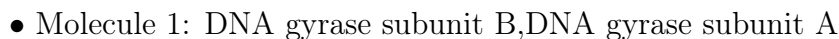


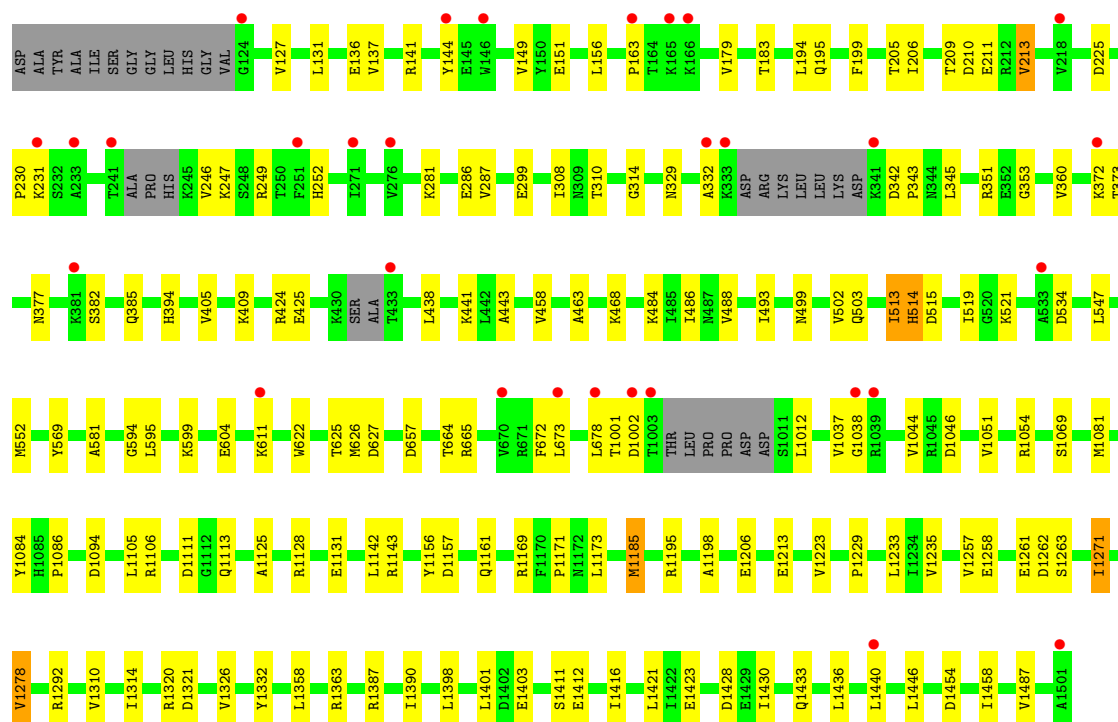
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	25	Total	O	0	0
			25	25		

- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.51Å 157.62Å 103.50Å 90.00° 98.11° 90.00°	Depositor
Resolution (Å)	46.15 – 2.60 46.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.15-2.60) 99.4 (46.15-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.197 , 0.240 0.218 , 0.260	Depositor DCC
R_{free} test set	4733 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17544	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MES

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	0.76	0/8864	1.35	17/11994 (0.1%)
1	B	0.77	1/8851 (0.0%)	1.35	26/11971 (0.2%)
All	All	0.77	1/17715 (0.0%)	1.35	43/23965 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1081	MET	SD-CE	-5.45	1.66	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1222	ARG	N-CA-C	-7.73	103.69	113.43
1	B	1320	ARG	CA-C-N	7.60	130.47	120.28
1	B	1320	ARG	C-N-CA	7.60	130.47	120.28
1	A	586	GLU	N-CA-C	-7.17	103.54	111.36
1	A	1278	VAL	N-CA-CB	6.64	118.58	111.00
1	B	1332	TYR	CA-C-N	6.63	129.07	120.44
1	B	1332	TYR	C-N-CA	6.63	129.07	120.44
1	B	1038	GLY	N-CA-C	6.26	120.46	112.83
1	B	1428	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	1278	VAL	N-CA-CB	6.19	118.06	111.00
1	B	513	ILE	CA-C-N	6.17	133.33	121.54
1	B	513	ILE	C-N-CA	6.17	133.33	121.54
1	A	1157	ASP	CA-CB-CG	6.17	118.77	112.60
1	B	1037	VAL	CA-C-N	6.14	126.90	120.03
1	B	1037	VAL	C-N-CA	6.14	126.90	120.03
1	B	314	GLY	CA-C-N	5.88	128.44	120.38
1	B	314	GLY	C-N-CA	5.88	128.44	120.38
1	B	1262	ASP	CA-CB-CG	5.84	118.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1223	VAL	CA-C-N	5.75	127.99	120.28
1	A	1223	VAL	C-N-CA	5.75	127.99	120.28
1	B	1046	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	1321	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	1171	PRO	CA-C-N	5.43	127.56	120.28
1	A	1171	PRO	C-N-CA	5.43	127.56	120.28
1	B	627	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	330	LYS	N-CA-C	-5.36	105.60	111.82
1	A	1262	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	1263	SER	CA-C-N	5.33	128.16	120.38
1	B	1263	SER	C-N-CA	5.33	128.16	120.38
1	A	314	GLY	CA-C-N	5.26	127.33	120.28
1	A	314	GLY	C-N-CA	5.26	127.33	120.28
1	B	1157	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	1171	PRO	CA-C-N	5.23	127.28	120.28
1	B	1171	PRO	C-N-CA	5.23	127.28	120.28
1	A	532	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	199	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	1223	VAL	N-CA-CB	5.14	117.77	111.60
1	A	1044	VAL	CA-C-N	5.11	127.08	120.44
1	A	1044	VAL	C-N-CA	5.11	127.08	120.44
1	B	195	GLN	CA-C-N	5.09	127.51	120.29
1	B	195	GLN	C-N-CA	5.09	127.51	120.29
1	A	199	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	1111	ASP	CA-CB-CG	5.01	117.61	112.60

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	8723	0	8713	80	1
1	B	8714	0	8707	61	1
2	A	36	0	39	2	0
2	B	24	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	0	0	0
3	B	25	0	0	0	0
All	All	17544	0	17485	136	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:TYR:OH	1:A:584:ASP:OD1	1.87	0.91
1:B:329:ASN:HD21	1:B:345:LEU:H	1.15	0.89
1:A:177:PRO:HB3	1:A:675:VAL:HG12	1.53	0.89
1:A:567:PRO:HA	1:A:582:TYR:CE2	2.21	0.76
1:A:567:PRO:HA	1:A:582:TYR:CD2	2.20	0.75
1:A:68:VAL:HG13	1:A:209:THR:HG23	1.68	0.73
1:A:1072:LYS:HD3	1:A:1131:GLU:HG2	1.71	0.71
1:B:29:ARG:HG2	1:B:29:ARG:O	1.91	0.70
1:A:567:PRO:CA	1:A:582:TYR:CE2	2.78	0.67
1:B:664:THR:HG23	1:B:1185:MET:HE1	1.76	0.66
1:A:1040:ALA:HB2	1:A:1182:ALA:HB3	1.79	0.65
1:B:499:ASN:HD22	1:B:502:VAL:H	1.47	0.62
1:A:499:ASN:HD22	1:A:502:VAL:H	1.47	0.61
1:A:1445:ALA:HB3	1:B:1412:GLU:HA	1.83	0.61
1:A:569:TYR:CZ	1:A:584:ASP:OD1	2.55	0.60
1:A:659:ARG:HD2	1:A:1028:TYR:OH	2.04	0.58
1:A:177:PRO:CB	1:A:675:VAL:HG12	2.28	0.58
1:A:281:LYS:HG2	1:A:286:GLU:HG3	1.86	0.58
1:A:585:ARG:NH1	1:A:585:ARG:HB3	2.19	0.57
1:B:1001:THR:O	1:B:1002:ASP:OD1	2.21	0.57
1:A:678:LEU:C	1:A:678:LEU:HD23	2.30	0.57
1:B:31:GLY:C	1:B:33:TYR:H	2.13	0.56
1:A:569:TYR:CE2	1:A:584:ASP:OD1	2.58	0.56
1:A:567:PRO:N	1:A:582:TYR:HE2	2.04	0.56
1:B:1387:ARG:HH11	1:B:1458:ILE:HD11	1.71	0.56
1:B:281:LYS:HG2	1:B:286:GLU:HG3	1.87	0.55
1:A:1002:ASP:O	1:A:1003:THR:HG22	2.05	0.55
1:A:1387:ARG:HH11	1:A:1458:ILE:HD11	1.70	0.55
1:A:497:LEU:HD21	1:A:513:ILE:HD11	1.87	0.55
1:A:678:LEU:HD23	1:A:678:LEU:O	2.06	0.55
1:A:1107:TYR:HB3	1:A:1137:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PRO:HB2	1:B:1213:GLU:HG3	1.88	0.55
1:A:64:THR:HG22	1:A:205:THR:HB	1.89	0.55
1:A:291:MET:HB2	1:A:354:LEU:HD11	1.88	0.54
1:B:1113:GLN:HB3	1:B:1131:GLU:HB2	1.90	0.54
1:A:188:GLU:HB3	1:A:192:ARG:NH2	2.22	0.54
1:B:443:ALA:HB2	1:B:468:LYS:HE3	1.90	0.54
1:B:458:VAL:HG21	1:B:463:ALA:HB3	1.89	0.54
1:A:1136:PRO:HB2	1:A:1490:HIS:HE1	1.74	0.52
1:B:30:PRO:HG2	1:B:37:THR:CG2	2.39	0.52
1:A:461:ASP:O	1:B:1125:ALA:HA	2.10	0.52
1:A:585:ARG:NH1	1:A:585:ARG:CB	2.73	0.52
1:B:1390:ILE:HD11	1:B:1430:ILE:HG22	1.91	0.52
1:B:622:TRP:HA	1:B:626:MET:HB2	1.90	0.52
1:B:31:GLY:O	1:B:33:TYR:N	2.44	0.51
1:A:177:PRO:HB3	1:A:675:VAL:CG1	2.35	0.51
1:B:136:GLU:HG2	1:B:149:VAL:HG22	1.92	0.51
1:A:323:ALA:HB2	1:A:385:GLN:HG3	1.92	0.51
1:A:585:ARG:CB	1:A:585:ARG:HH11	2.23	0.51
1:A:1454:ASP:O	1:A:1458:ILE:HG12	2.12	0.50
1:B:1454:ASP:O	1:B:1458:ILE:HG12	2.12	0.49
1:B:1143:ARG:HD3	1:B:1169:ARG:HG3	1.95	0.49
1:A:1323:VAL:HB	1:A:1326:VAL:HG12	1.94	0.49
1:A:1136:PRO:HB2	1:A:1490:HIS:CE1	2.48	0.49
1:B:594:GLY:O	1:B:599:LYS:HB2	2.13	0.49
1:B:31:GLY:C	1:B:33:TYR:N	2.66	0.49
1:B:1398:LEU:HA	1:B:1401:LEU:HG	1.95	0.49
1:A:1190:PRO:HB2	1:A:1226:PRO:HB3	1.95	0.49
1:A:1065:ARG:HD2	1:A:1068:ARG:HH21	1.78	0.49
1:B:438:LEU:HB3	1:B:441:LYS:HB3	1.94	0.49
1:A:233:ALA:HA	1:A:236:ARG:HH11	1.77	0.48
1:B:1054:ARG:HG2	1:B:1084:TYR:HB3	1.94	0.48
1:A:276:VAL:HB	1:A:291:MET:HG2	1.95	0.48
1:B:151:GLU:HB2	1:B:156:LEU:HD11	1.96	0.48
1:A:1105:LEU:HD21	2:A:1601:MES:H32	1.96	0.48
1:A:144:TYR:HA	1:A:163:PRO:HA	1.95	0.48
1:A:177:PRO:HB2	1:A:1001:THR:HG21	1.96	0.48
1:B:1411:SER:HB2	1:B:1416:ILE:HG23	1.95	0.48
1:A:1040:ALA:HB2	1:A:1182:ALA:CB	2.44	0.48
1:A:1056:LEU:HD11	1:A:1109:LEU:HD13	1.95	0.47
1:B:299:GLU:HG3	1:B:351:ARG:HB3	1.96	0.47
1:A:1002:ASP:OD1	1:A:1003:THR:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PRO:HB2	1:A:1213:GLU:HG2	1.96	0.47
1:A:1349:VAL:HB	1:A:1354:ARG:HD3	1.96	0.47
1:B:1257:VAL:HG22	1:B:1271:ILE:HD12	1.96	0.47
1:A:481:LEU:HD13	1:A:485:ILE:HD11	1.96	0.47
1:B:353:GLY:HA3	1:B:409:LYS:HE2	1.97	0.47
1:B:569:TYR:HB2	1:B:581:ALA:HB3	1.96	0.46
1:A:568:LEU:HD13	1:A:582:TYR:O	2.16	0.46
1:A:1113:GLN:HB3	1:A:1131:GLU:HB2	1.97	0.46
1:A:1433:GLN:HA	1:A:1436:LEU:HD12	1.97	0.46
1:A:621:LEU:HG	1:A:626:MET:HE2	1.98	0.46
1:A:569:TYR:HB2	1:A:581:ALA:HB3	1.97	0.46
1:A:137:VAL:HG12	1:A:171:VAL:HG22	1.97	0.45
1:B:213:VAL:HG21	1:B:247:LYS:HB2	1.97	0.45
1:A:647:LEU:HD11	1:A:1025:GLN:HG3	1.99	0.45
1:A:1086:PRO:HB2	1:B:1128:ARG:HB3	1.98	0.45
1:A:1449:GLN:HA	1:A:1452:ILE:HD12	1.98	0.45
1:B:86:VAL:HG22	1:B:141:ARG:HD3	1.98	0.45
1:B:205:THR:HG23	1:B:252:HIS:HB2	1.98	0.45
1:B:1105:LEU:HD21	2:B:1601:MES:H32	1.99	0.45
1:A:1441:ARG:HB3	1:B:1436:LEU:HB3	1.98	0.45
1:A:567:PRO:N	1:A:582:TYR:CE2	2.83	0.45
1:B:1198:ALA:HB2	1:B:1487:VAL:HG21	1.99	0.45
1:B:595:LEU:HD23	1:B:595:LEU:HA	1.41	0.44
1:B:131:LEU:HD22	1:B:179:VAL:HG11	2.00	0.44
1:B:211:GLU:HA	1:B:246:VAL:HG22	1.98	0.44
1:A:1425:LEU:HB2	1:A:1427:ILE:HG12	1.99	0.44
1:B:194:LEU:HD22	1:B:206:ILE:HG21	2.00	0.44
1:A:1119:PRO:HD2	2:A:1603:MES:H72	2.00	0.44
1:A:1376:ARG:HD3	1:A:1380:ARG:CZ	2.48	0.44
1:A:1391:LEU:HA	1:A:1394:LEU:HD12	1.99	0.44
1:A:458:VAL:HG21	1:A:463:ALA:HB3	2.00	0.44
1:A:678:LEU:O	1:A:678:LEU:HG	2.16	0.44
1:A:1036:ILE:HA	1:A:1040:ALA:HB3	2.00	0.43
1:B:1106:ARG:HA	1:B:1229:PRO:HB3	1.99	0.43
1:A:287:VAL:HG23	1:A:360:VAL:HG12	2.00	0.43
1:B:1044:VAL:HA	1:B:1173:LEU:HD22	2.01	0.43
1:B:64:THR:HG22	1:B:205:THR:HB	2.01	0.42
1:B:488:VAL:HG21	1:B:547:LEU:HA	2.02	0.42
1:B:287:VAL:HG23	1:B:360:VAL:HG12	2.00	0.42
1:A:286:GLU:HB3	1:A:361:LYS:HB2	2.01	0.42
1:A:591:LEU:HD13	1:A:607:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:VAL:HG22	1:A:356:ALA:HB3	2.01	0.42
1:A:42:LEU:HG	1:A:185:TYR:CE1	2.55	0.42
1:B:26:VAL:HG11	1:B:127:VAL:HG13	2.01	0.42
1:B:342:ASP:HB3	1:B:343:PRO:CD	2.50	0.42
1:B:552:MET:HE3	1:B:552:MET:HB2	1.98	0.42
1:B:210:ASP:HB3	1:B:247:LYS:HB3	2.02	0.41
1:A:454:GLU:HG2	1:A:526:LYS:HB2	2.02	0.41
1:B:1271:ILE:HB	1:B:1314:ILE:HB	2.01	0.41
1:A:1413:THR:HG22	1:B:1446:LEU:HD22	2.02	0.41
1:B:144:TYR:HA	1:B:163:PRO:HA	2.02	0.41
1:A:622:TRP:HA	1:A:626:MET:HB2	2.02	0.41
1:A:1143:ARG:HD3	1:A:1169:ARG:HG3	2.02	0.41
1:B:310:THR:HA	1:B:373:THR:HB	2.02	0.41
1:A:177:PRO:CB	1:A:675:VAL:CG1	2.97	0.41
1:A:1054:ARG:HG2	1:A:1084:TYR:HB3	2.03	0.41
1:B:183:THR:HG23	1:B:672:PHE:HE2	1.85	0.41
1:B:1086:PRO:HG3	1:B:1156:TYR:CD2	2.56	0.41
1:A:211:GLU:HA	1:A:246:VAL:HG12	2.04	0.40
1:B:249:ARG:HH22	1:B:665:ARG:HD2	1.87	0.40
1:A:1070:HIS:HB3	1:A:1131:GLU:HB3	2.03	0.40
1:A:71:GLU:HA	1:A:212:ARG:HG2	2.02	0.40
1:B:1223:VAL:CG1	1:B:1358:LEU:HD21	2.51	0.40
1:B:32:MET:SD	1:B:32:MET:O	2.79	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ARG:NH2	1:B:604:GLU:OE2[2_8511]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	1111/1179 (94%)	1063 (96%)	44 (4%)	4 (0%)	30	51
1	B	1105/1179 (94%)	1047 (95%)	51 (5%)	7 (1%)	21	42
All	All	2216/2358 (94%)	2110 (95%)	95 (4%)	11 (0%)	24	46

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1003	THR
1	B	514	HIS
1	A	514	HIS
1	B	31	GLY
1	A	283	THR
1	B	32	MET
1	B	377	ASN
1	B	332	ALA
1	B	372	LYS
1	A	493	ILE
1	B	493	ILE

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	931/976 (95%)	889 (96%)	42 (4%)	24	50
1	B	931/976 (95%)	876 (94%)	55 (6%)	18	38
All	All	1862/1952 (95%)	1765 (95%)	97 (5%)	21	44

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	213	VAL
1	A	245	LYS
1	A	248	SER
1	A	271	ILE

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Mol	Chain	Res	Type
1	A	350	ILE
1	A	370	GLN
1	A	405	VAL
1	A	409	LYS
1	A	426	LEU
1	A	434	ASP
1	A	435	ILE
1	A	484	LYS
1	A	486	ILE
1	A	513	ILE
1	A	515	ASP
1	A	519	ILE
1	A	521	LYS
1	A	534	ASP
1	A	552	MET
1	A	568	LEU
1	A	571	LEU
1	A	605	ASP
1	A	625	THR
1	A	1001	THR
1	A	1003	THR
1	A	1004	THR
1	A	1015	ILE
1	A	1016	GLU
1	A	1043	GLU
1	A	1051	VAL
1	A	1069	SER
1	A	1094	ASP
1	A	1147	GLU
1	A	1185	MET
1	A	1223	VAL
1	A	1250	SER
1	A	1258	GLU
1	A	1278	VAL
1	A	1403	GLU
1	A	1430	ILE
1	A	1459	GLU
1	B	32	MET
1	B	34	ILE
1	B	84	ILE
1	B	96	VAL
1	B	103	LEU

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Mol	Chain	Res	Type
1	B	137	VAL
1	B	209	THR
1	B	213	VAL
1	B	225	ASP
1	B	231	LYS
1	B	308	ILE
1	B	382	SER
1	B	385	GLN
1	B	394	HIS
1	B	405	VAL
1	B	424	ARG
1	B	425	GLU
1	B	484	LYS
1	B	486	ILE
1	B	503	GLN
1	B	513	ILE
1	B	514	HIS
1	B	515	ASP
1	B	519	ILE
1	B	521	LYS
1	B	534	ASP
1	B	611	LYS
1	B	625	THR
1	B	657	ASP
1	B	673	LEU
1	B	678	LEU
1	B	1012	LEU
1	B	1051	VAL
1	B	1069	SER
1	B	1094	ASP
1	B	1142	LEU
1	B	1161	GLN
1	B	1185	MET
1	B	1195	ARG
1	B	1206	GLU
1	B	1233	LEU
1	B	1235	VAL
1	B	1258	GLU
1	B	1261	GLU
1	B	1271	ILE
1	B	1278	VAL
1	B	1292	ARG

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Mol	Chain	Res	Type
1	B	1310	VAL
1	B	1326	VAL
1	B	1363	ARG
1	B	1403	GLU
1	B	1421	LEU
1	B	1423	GLU
1	B	1433	GLN
1	B	1440	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	285	HIS
1	A	370	GLN
1	A	391	GLN
1	A	499	ASN
1	A	503	GLN
1	A	558	ASN
1	A	602	ASN
1	A	1113	GLN
1	A	1115	ASN
1	A	1207	ASN
1	A	1208	HIS
1	A	1238	GLN
1	A	1475	GLN
1	B	52	ASN
1	B	329	ASN
1	B	344	ASN
1	B	499	ASN
1	B	503	GLN
1	B	574	GLN
1	B	1052	HIS
1	B	1113	GLN
1	B	1207	ASN
1	B	1208	HIS
1	B	1280	HIS
1	B	1334	HIS
1	B	1449	GLN
1	B	1475	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MES	A	1602	-	12,12,12	0.71	0	15,16,16	0.32	0
2	MES	A	1601	-	12,12,12	0.67	0	15,16,16	0.41	0
2	MES	A	1603	-	12,12,12	0.75	0	15,16,16	0.38	0
2	MES	B	1601	-	12,12,12	0.69	0	15,16,16	0.31	0
2	MES	B	1602	-	12,12,12	0.71	0	15,16,16	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	A	1602	-	-	0/6/14/14	0/1/1/1
2	MES	A	1601	-	-	6/6/14/14	0/1/1/1
2	MES	A	1603	-	-	0/6/14/14	0/1/1/1
2	MES	B	1601	-	-	3/6/14/14	0/1/1/1
2	MES	B	1602	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1601	MES	C7-C8-S-O1S
2	B	1601	MES	C7-C8-S-O2S
2	B	1601	MES	C7-C8-S-O3S
2	A	1601	MES	N4-C7-C8-S
2	A	1601	MES	C8-C7-N4-C3
2	A	1601	MES	C8-C7-N4-C5
2	A	1601	MES	C7-C8-S-O1S
2	A	1601	MES	C7-C8-S-O2S
2	A	1601	MES	C7-C8-S-O3S

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	MES	1	0
2	A	1603	MES	1	0
2	B	1601	MES	1	0

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	1119/1179 (94%)	0.10	20 (1%) 67 63	26, 82, 129, 163	0
1	B	1117/1179 (94%)	0.22	39 (3%) 47 41	54, 93, 170, 211	0
All	All	2236/2358 (94%)	0.16	59 (2%) 57 51	26, 86, 146, 211	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1003	THR	6.5
1	A	1004	THR	6.4
1	B	1002	ASP	5.3
1	B	1003	THR	5.1
1	A	25	ALA	4.5
1	A	1002	ASP	4.4
1	B	25	ALA	4.0
1	B	372	LYS	3.9
1	A	343	PRO	3.7
1	B	251	PHE	3.5
1	B	32	MET	3.3
1	B	165	LYS	3.2
1	B	1440	LEU	3.0
1	B	332	ALA	3.0
1	B	218	VAL	2.9
1	A	333	LYS	2.9
1	B	163	PRO	2.9
1	A	406	VAL	2.9
1	B	333	LYS	2.9
1	B	678	LEU	2.8
1	B	124	GLY	2.8
1	B	241	THR	2.7
1	B	611	LYS	2.6
1	A	435	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	276	VAL	2.5
1	A	271	ILE	2.5
1	B	1039	ARG	2.5
1	A	35	GLY	2.5
1	B	75	VAL	2.5
1	B	99	VAL	2.5
1	A	1501	ALA	2.5
1	A	332	ALA	2.4
1	A	433	THR	2.4
1	B	341	LYS	2.4
1	B	233	ALA	2.4
1	B	103	LEU	2.3
1	B	673	LEU	2.3
1	A	153	SER	2.3
1	B	381	LYS	2.2
1	B	1501	ALA	2.2
1	B	231	LYS	2.2
1	B	146	TRP	2.2
1	B	84	ILE	2.2
1	A	33	TYR	2.1
1	B	67	VAL	2.1
1	B	533	ALA	2.1
1	B	166	LYS	2.1
1	B	104	HIS	2.1
1	A	667	ALA	2.1
1	B	33	TYR	2.1
1	B	1038	GLY	2.1
1	A	164	THR	2.1
1	A	98	VAL	2.0
1	B	670	VAL	2.0
1	B	433	THR	2.0
1	A	369	GLY	2.0
1	B	271	ILE	2.0
1	A	219	VAL	2.0
1	B	144	TYR	2.0

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

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	A	1602	12/12	0.67	0.20	160,162,167,168	0
2	MES	B	1602	12/12	0.73	0.19	118,121,133,134	0
2	MES	A	1603	12/12	0.74	0.32	156,158,164,164	0
2	MES	B	1601	12/12	0.83	0.18	108,113,125,126	0
2	MES	A	1601	12/12	0.89	0.15	87,91,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.