



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 12:27 AM EDT

PDB ID : 6GAV
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

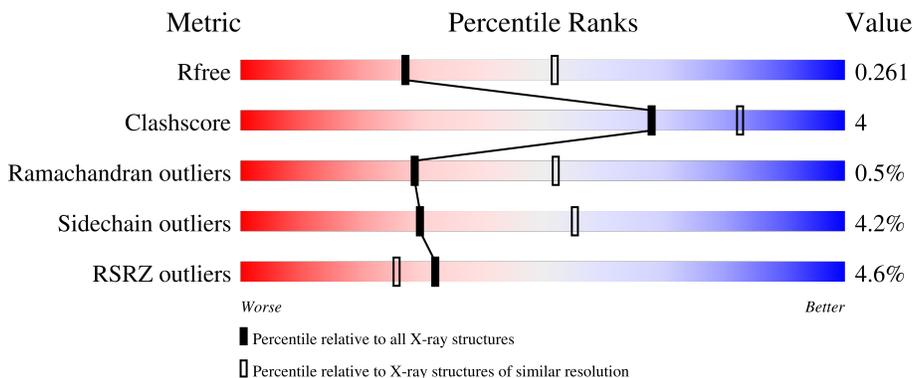
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MES	A	1603	-	-	-	X

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.

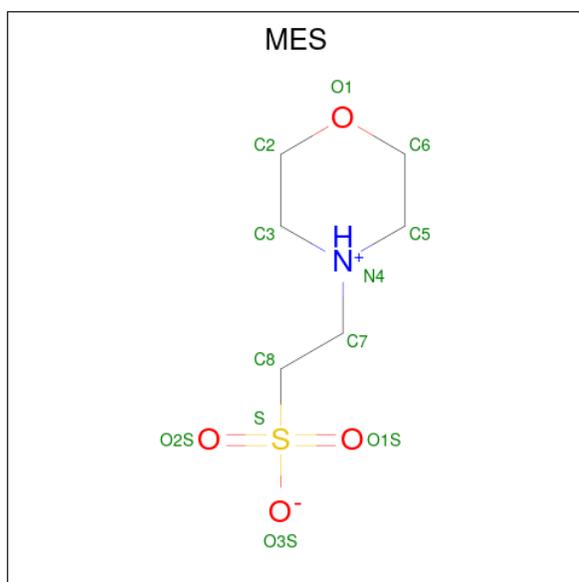
- Molecule 1 is a protein called DNA gyrase subunit B,DNA gyrase subunit A.

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

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 (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
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		

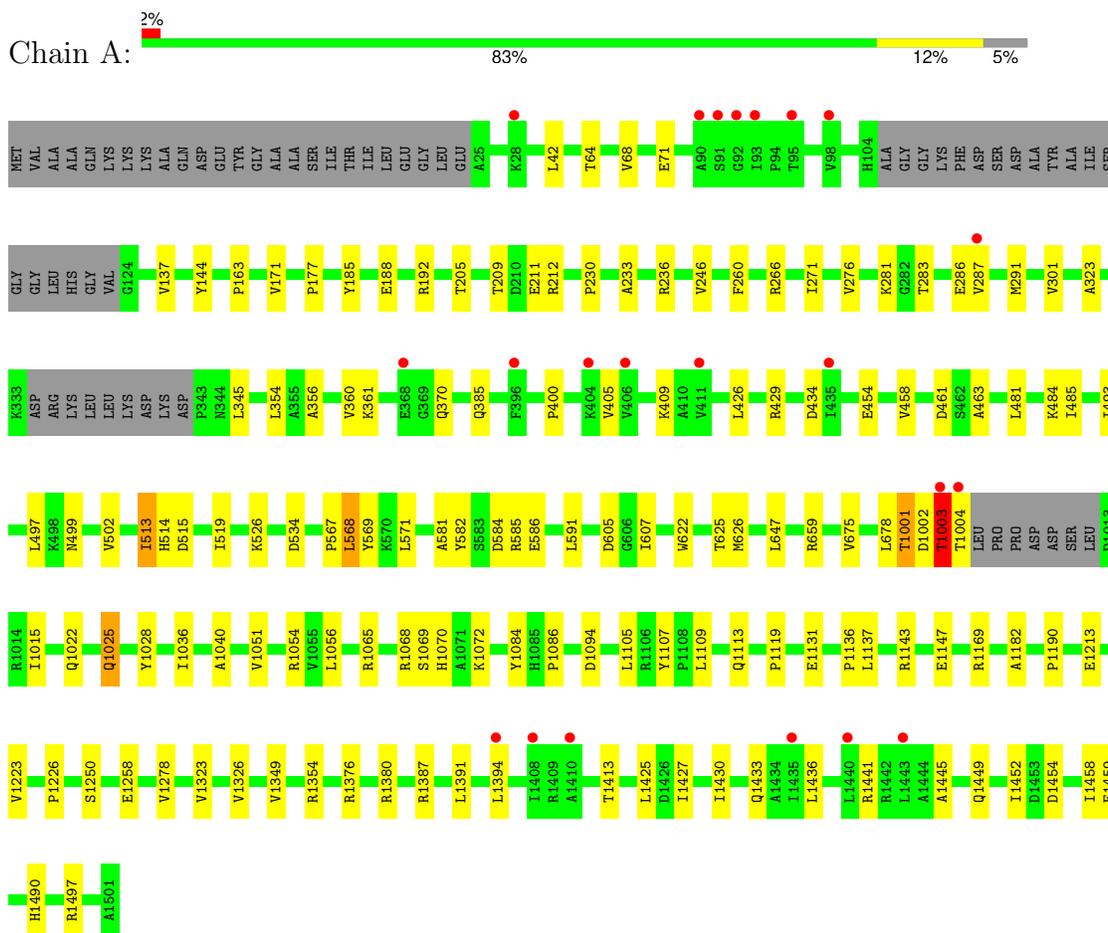
- Molecule 3 is water.

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

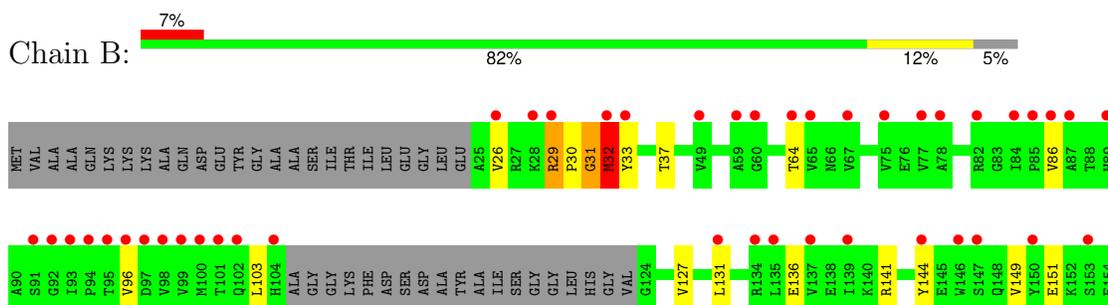
3 Residue-property plots i

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

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



- 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) 99.5 (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)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.197 , 0.240 0.219 , 0.261	Depositor DCC
R_{free} test set	4733 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtrriage
Anisotropy	0.841	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.42	0/8864	0.63	0/11994
1	B	0.42	0/8851	0.62	1/11971 (0.0%)
All	All	0.42	0/17715	0.63	1/23965 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1002	ASP	CB-CG-OD2	5.22	123.00	118.30

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	8723	0	8713	79	1
1	B	8714	0	8707	59	1
2	A	36	0	39	2	0
2	B	24	0	26	1	0
3	A	22	0	0	0	0
3	B	25	0	0	0	0
All	All	17544	0	17485	133	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 (133) 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: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: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:O	1:A:678:LEU:HD23	2.06	0.55
1:A:1107:TYR:HB3	1:A:1137:LEU:HD13	1.89	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:GLY:C	1:B:33:TYR:H	2.13	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:A:678:LEU:HD23	1:A:678:LEU:C	2.30	0.51
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:31:GLY:C	1:B:33:TYR:N	2.66	0.49
1:B:594:GLY:O	1:B:599:LYS:HB2	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	1111/1179 (94%)	1063 (96%)	44 (4%)	4 (0%)	34 57
1	B	1105/1179 (94%)	1047 (95%)	51 (5%)	7 (1%)	25 47
All	All	2216/2358 (94%)	2110 (95%)	95 (4%)	11 (0%)	29 52

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 [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	931/976 (95%)	894 (96%)	37 (4%)	31 57
1	B	931/976 (95%)	889 (96%)	42 (4%)	27 52
All	All	1862/1952 (95%)	1783 (96%)	79 (4%)	30 55

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	PHE
1	A	266	ARG
1	A	271	ILE
1	A	345	LEU
1	A	370	GLN
1	A	400	PRO
1	A	405	VAL
1	A	409	LYS
1	A	426	LEU
1	A	434	ASP
1	A	484	LYS
1	A	513	ILE
1	A	515	ASP

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Mol	Chain	Res	Type
1	A	519	ILE
1	A	534	ASP
1	A	568	LEU
1	A	571	LEU
1	A	586	GLU
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	1022	GLN
1	A	1025	GLN
1	A	1051	VAL
1	A	1069	SER
1	A	1094	ASP
1	A	1147	GLU
1	A	1223	VAL
1	A	1250	SER
1	A	1258	GLU
1	A	1278	VAL
1	A	1430	ILE
1	A	1459	GLU
1	A	1497	ARG
1	B	29	ARG
1	B	32	MET
1	B	96	VAL
1	B	103	LEU
1	B	209	THR
1	B	225	ASP
1	B	231	LYS
1	B	260	PHE
1	B	285	HIS
1	B	372	LYS
1	B	382	SER
1	B	385	GLN
1	B	394	HIS
1	B	405	VAL
1	B	425	GLU
1	B	486	ILE
1	B	494	ASP
1	B	503	GLN

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Mol	Chain	Res	Type
1	B	514	HIS
1	B	515	ASP
1	B	519	ILE
1	B	534	ASP
1	B	625	THR
1	B	657	ASP
1	B	671	ARG
1	B	673	LEU
1	B	1012	LEU
1	B	1051	VAL
1	B	1069	SER
1	B	1094	ASP
1	B	1185	MET
1	B	1206	GLU
1	B	1222	ARG
1	B	1233	LEU
1	B	1235	VAL
1	B	1292	ARG
1	B	1310	VAL
1	B	1326	VAL
1	B	1363	ARG
1	B	1423	GLU
1	B	1433	GLN
1	B	1497	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS
1	A	499	ASN
1	A	1490	HIS
1	B	329	ASN
1	B	385	GLN
1	B	499	ASN
1	B	514	HIS
1	B	1052	HIS
1	B	1280	HIS
1	B	1490	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1601	-	12,12,12	0.69	0	15,16,16	0.31	0
2	MES	A	1602	-	12,12,12	0.71	0	15,16,16	0.32	0
2	MES	A	1603	-	12,12,12	0.75	0	15,16,16	0.38	0
2	MES	A	1601	-	12,12,12	0.67	0	15,16,16	0.41	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	B	1601	-	-	3/6/14/14	0/1/1/1
2	MES	A	1602	-	-	0/6/14/14	0/1/1/1
2	MES	A	1603	-	-	0/6/14/14	0/1/1/1
2	MES	A	1601	-	-	6/6/14/14	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	B	1601	MES	1	0
2	A	1603	MES	1	0
2	A	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%)	0.04	22 (1%) 65 60	26, 82, 129, 163	0
1	B	1117/1179 (94%)	0.28	81 (7%) 15 11	54, 93, 170, 211	0
All	All	2236/2358 (94%)	0.16	103 (4%) 32 26	26, 86, 146, 211	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	VAL	7.8
1	B	158	LEU	7.5
1	B	93	ILE	6.7
1	B	95	THR	6.3
1	B	29	ARG	5.1
1	B	144	TYR	5.0
1	B	99	VAL	5.0
1	B	28	LYS	4.9
1	B	157	GLY	4.9
1	B	146	TRP	4.8
1	B	139	ILE	4.7
1	B	32	MET	4.6
1	B	85	PRO	4.5
1	B	163	PRO	4.5
1	B	75	VAL	4.4
1	B	94	PRO	4.3
1	A	1003	THR	4.3
1	B	673	LEU	4.3
1	B	135	LEU	4.3
1	B	91	SER	4.0
1	B	180	PHE	3.9
1	B	84	ILE	3.9
1	B	96	VAL	3.9
1	A	406	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	162	ALA	3.8
1	B	150	TYR	3.7
1	B	1440	LEU	3.7
1	B	173	PHE	3.7
1	A	1004	THR	3.7
1	B	26	VAL	3.6
1	B	98	VAL	3.6
1	B	137	VAL	3.6
1	B	164	THR	3.6
1	A	90	ALA	3.5
1	B	87	ALA	3.5
1	B	100	MET	3.4
1	B	1003	THR	3.4
1	B	147	SER	3.4
1	B	159	LYS	3.4
1	B	251	PHE	3.3
1	B	134	ARG	3.3
1	B	1012	LEU	3.3
1	B	92	GLY	3.2
1	B	156	LEU	3.2
1	B	33	TYR	3.1
1	B	59	ALA	3.1
1	B	401	THR	3.1
1	B	1002	ASP	3.0
1	B	78	ALA	3.0
1	B	328	VAL	2.9
1	A	368	GLU	2.9
1	B	101	THR	2.8
1	A	91	SER	2.8
1	B	155	PRO	2.8
1	B	276	VAL	2.8
1	B	675	VAL	2.8
1	B	1408	ILE	2.8
1	A	98	VAL	2.8
1	B	167	THR	2.8
1	A	93	ILE	2.7
1	B	179	VAL	2.7
1	A	92	GLY	2.6
1	B	153	SER	2.6
1	B	241	THR	2.6
1	B	289	ILE	2.6
1	B	77	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	160	GLN	2.6
1	B	64	THR	2.6
1	B	67	VAL	2.6
1	A	1408	ILE	2.5
1	A	404	LYS	2.5
1	B	411	VAL	2.5
1	B	170	THR	2.5
1	A	396	PHE	2.5
1	B	394	HIS	2.4
1	B	89	HIS	2.4
1	B	172	ARG	2.4
1	B	104	HIS	2.4
1	A	435	ILE	2.4
1	A	287	VAL	2.4
1	B	82	ARG	2.3
1	A	1435	ILE	2.3
1	B	426	LEU	2.3
1	B	60	GLY	2.3
1	A	1394	LEU	2.3
1	B	49	VAL	2.3
1	B	65	VAL	2.3
1	A	411	VAL	2.2
1	B	165	LYS	2.2
1	B	672	PHE	2.2
1	B	97	ASP	2.2
1	B	283	THR	2.2
1	A	1443	LEU	2.1
1	B	1011	SER	2.1
1	B	131	LEU	2.1
1	B	404	LYS	2.1
1	B	315	THR	2.1
1	A	1410	ALA	2.1
1	A	95	THR	2.1
1	B	1184	GLY	2.1
1	A	28	LYS	2.0
1	B	102	GLN	2.0
1	A	1440	LEU	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 monosaccharides 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(\AA^2)	Q<0.9
2	MES	A	1603	12/12	0.56	0.45	156,158,164,164	0
2	MES	A	1602	12/12	0.70	0.32	160,162,167,168	0
2	MES	B	1602	12/12	0.82	0.21	118,121,133,134	0
2	MES	B	1601	12/12	0.84	0.29	108,113,125,126	0
2	MES	A	1601	12/12	0.93	0.20	87,91,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.