



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:30 PM GMT

PDB ID : 3ZM7
Title : CRYSTAL STRUCTURE OF THE ATPASE REGION OF Mycobacterium tuberculosis GyrB WITH AMPPCP
Authors : Agrawal, A.; Roue, M.; Spitzfaden, C.; Petrella, S.; Aubry, A.; Volker, C.; Mossakowska, D.; Hann, M.; Bax, B.; Mayer, C.
Deposited on : 2013-02-05
Resolution : 3.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

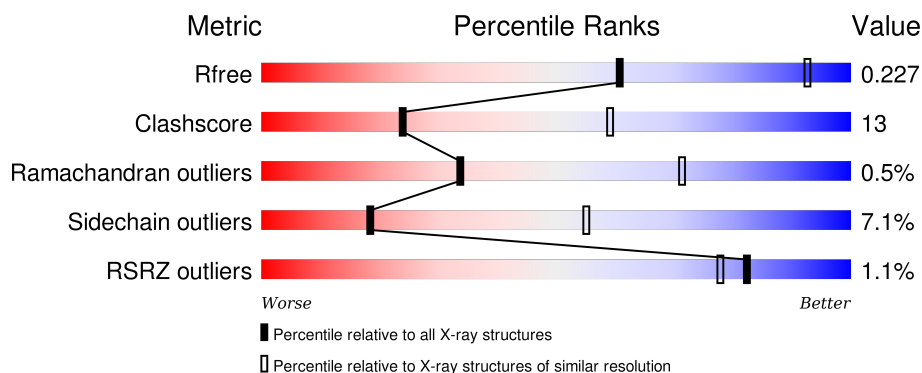
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 $\leq 5\%$. 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	442	<div> <div>2%</div> <div>58%</div> <div>20%</div> <div>•</div> <div>19%</div> </div>
1	B	442	<div> <div>2%</div> <div>62%</div> <div>17%</div> <div>•</div> <div>19%</div> </div>
1	C	442	<div> <div>2%</div> <div>58%</div> <div>18%</div> <div>•</div> <div>22%</div> </div>
1	D	442	<div> <div>2%</div> <div>56%</div> <div>22%</div> <div>•</div> <div>19%</div> </div>
1	E	442	<div> <div>2%</div> <div>61%</div> <div>15%</div> <div>•</div> <div>23%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	442	

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	ACP	F	525	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16295 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2714	1699	479	530	6			
1	B	356	Total	C	N	O	S	0	0	0
			2680	1679	472	523	6			
1	C	346	Total	C	N	O	S	0	0	0
			2622	1639	464	513	6			
1	D	357	Total	C	N	O	S	0	0	0
			2684	1677	469	532	6			
1	E	342	Total	C	N	O	S	0	0	0
			2609	1635	459	509	6			
1	F	357	Total	C	N	O	S	0	0	0
			2703	1690	476	531	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP I6WX66
A	-12	ALA	-	EXPRESSION TAG	UNP I6WX66
A	-11	HIS	-	EXPRESSION TAG	UNP I6WX66
A	-10	HIS	-	EXPRESSION TAG	UNP I6WX66
A	-9	HIS	-	EXPRESSION TAG	UNP I6WX66
A	-8	HIS	-	EXPRESSION TAG	UNP I6WX66
A	-7	HIS	-	EXPRESSION TAG	UNP I6WX66
A	-6	HIS	-	EXPRESSION TAG	UNP I6WX66
A	-5	VAL	-	EXPRESSION TAG	UNP I6WX66
A	-4	ASP	-	EXPRESSION TAG	UNP I6WX66
A	-3	ASP	-	EXPRESSION TAG	UNP I6WX66
A	-2	ASP	-	EXPRESSION TAG	UNP I6WX66
A	-1	ASP	-	EXPRESSION TAG	UNP I6WX66
A	0	LYS	-	EXPRESSION TAG	UNP I6WX66
B	-13	MET	-	EXPRESSION TAG	UNP I6WX66
B	-12	ALA	-	EXPRESSION TAG	UNP I6WX66
B	-11	HIS	-	EXPRESSION TAG	UNP I6WX66

Continued on next page...

Continued from previous page...

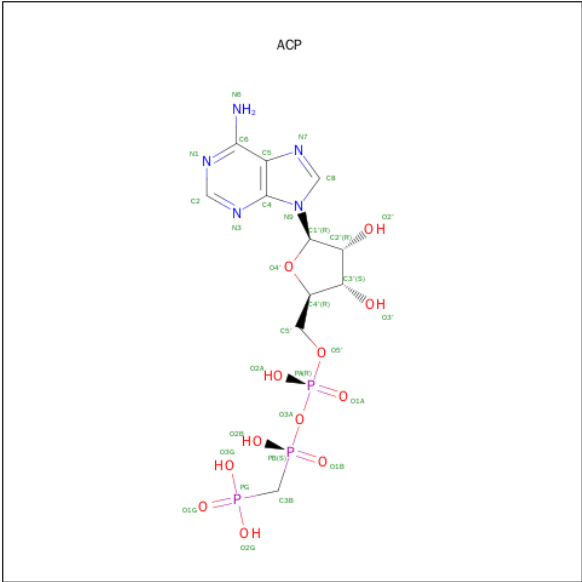
Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP I6WX66
B	-9	HIS	-	EXPRESSION TAG	UNP I6WX66
B	-8	HIS	-	EXPRESSION TAG	UNP I6WX66
B	-7	HIS	-	EXPRESSION TAG	UNP I6WX66
B	-6	HIS	-	EXPRESSION TAG	UNP I6WX66
B	-5	VAL	-	EXPRESSION TAG	UNP I6WX66
B	-4	ASP	-	EXPRESSION TAG	UNP I6WX66
B	-3	ASP	-	EXPRESSION TAG	UNP I6WX66
B	-2	ASP	-	EXPRESSION TAG	UNP I6WX66
B	-1	ASP	-	EXPRESSION TAG	UNP I6WX66
B	0	LYS	-	EXPRESSION TAG	UNP I6WX66
C	-13	MET	-	EXPRESSION TAG	UNP I6WX66
C	-12	ALA	-	EXPRESSION TAG	UNP I6WX66
C	-11	HIS	-	EXPRESSION TAG	UNP I6WX66
C	-10	HIS	-	EXPRESSION TAG	UNP I6WX66
C	-9	HIS	-	EXPRESSION TAG	UNP I6WX66
C	-8	HIS	-	EXPRESSION TAG	UNP I6WX66
C	-7	HIS	-	EXPRESSION TAG	UNP I6WX66
C	-6	HIS	-	EXPRESSION TAG	UNP I6WX66
C	-5	VAL	-	EXPRESSION TAG	UNP I6WX66
C	-4	ASP	-	EXPRESSION TAG	UNP I6WX66
C	-3	ASP	-	EXPRESSION TAG	UNP I6WX66
C	-2	ASP	-	EXPRESSION TAG	UNP I6WX66
C	-1	ASP	-	EXPRESSION TAG	UNP I6WX66
C	0	LYS	-	EXPRESSION TAG	UNP I6WX66
D	-13	MET	-	EXPRESSION TAG	UNP I6WX66
D	-12	ALA	-	EXPRESSION TAG	UNP I6WX66
D	-11	HIS	-	EXPRESSION TAG	UNP I6WX66
D	-10	HIS	-	EXPRESSION TAG	UNP I6WX66
D	-9	HIS	-	EXPRESSION TAG	UNP I6WX66
D	-8	HIS	-	EXPRESSION TAG	UNP I6WX66
D	-7	HIS	-	EXPRESSION TAG	UNP I6WX66
D	-6	HIS	-	EXPRESSION TAG	UNP I6WX66
D	-5	VAL	-	EXPRESSION TAG	UNP I6WX66
D	-4	ASP	-	EXPRESSION TAG	UNP I6WX66
D	-3	ASP	-	EXPRESSION TAG	UNP I6WX66
D	-2	ASP	-	EXPRESSION TAG	UNP I6WX66
D	-1	ASP	-	EXPRESSION TAG	UNP I6WX66
D	0	LYS	-	EXPRESSION TAG	UNP I6WX66
E	-13	MET	-	EXPRESSION TAG	UNP I6WX66
E	-12	ALA	-	EXPRESSION TAG	UNP I6WX66
E	-11	HIS	-	EXPRESSION TAG	UNP I6WX66

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP I6WX66
E	-9	HIS	-	EXPRESSION TAG	UNP I6WX66
E	-8	HIS	-	EXPRESSION TAG	UNP I6WX66
E	-7	HIS	-	EXPRESSION TAG	UNP I6WX66
E	-6	HIS	-	EXPRESSION TAG	UNP I6WX66
E	-5	VAL	-	EXPRESSION TAG	UNP I6WX66
E	-4	ASP	-	EXPRESSION TAG	UNP I6WX66
E	-3	ASP	-	EXPRESSION TAG	UNP I6WX66
E	-2	ASP	-	EXPRESSION TAG	UNP I6WX66
E	-1	ASP	-	EXPRESSION TAG	UNP I6WX66
E	0	LYS	-	EXPRESSION TAG	UNP I6WX66
F	-13	MET	-	EXPRESSION TAG	UNP I6WX66
F	-12	ALA	-	EXPRESSION TAG	UNP I6WX66
F	-11	HIS	-	EXPRESSION TAG	UNP I6WX66
F	-10	HIS	-	EXPRESSION TAG	UNP I6WX66
F	-9	HIS	-	EXPRESSION TAG	UNP I6WX66
F	-8	HIS	-	EXPRESSION TAG	UNP I6WX66
F	-7	HIS	-	EXPRESSION TAG	UNP I6WX66
F	-6	HIS	-	EXPRESSION TAG	UNP I6WX66
F	-5	VAL	-	EXPRESSION TAG	UNP I6WX66
F	-4	ASP	-	EXPRESSION TAG	UNP I6WX66
F	-3	ASP	-	EXPRESSION TAG	UNP I6WX66
F	-2	ASP	-	EXPRESSION TAG	UNP I6WX66
F	-1	ASP	-	EXPRESSION TAG	UNP I6WX66
F	0	LYS	-	EXPRESSION TAG	UNP I6WX66

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

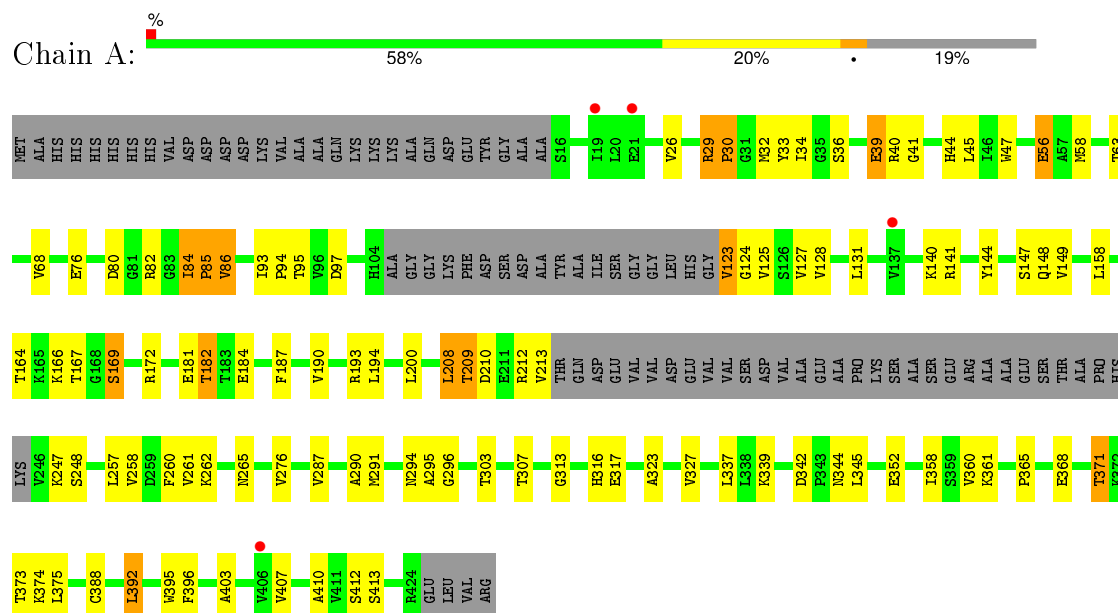
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total 16	O 16	0	0
4	B	20	Total 20	O 20	0	0
4	C	13	Total 13	O 13	0	0
4	D	14	Total 14	O 14	0	0
4	E	14	Total 14	O 14	0	0
4	F	14	Total 14	O 14	0	0

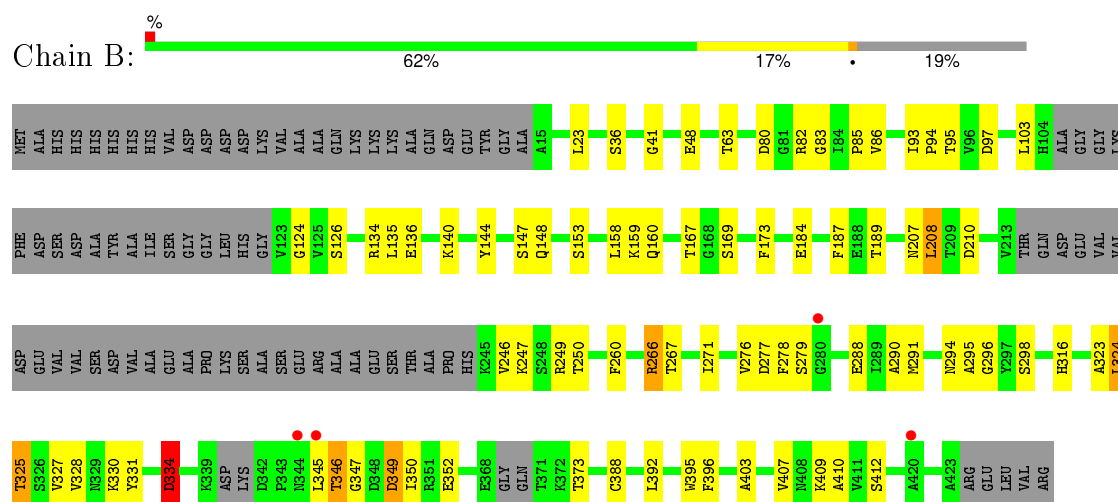
3 Residue-property plots

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: DNA GYRASE SUBUNIT B

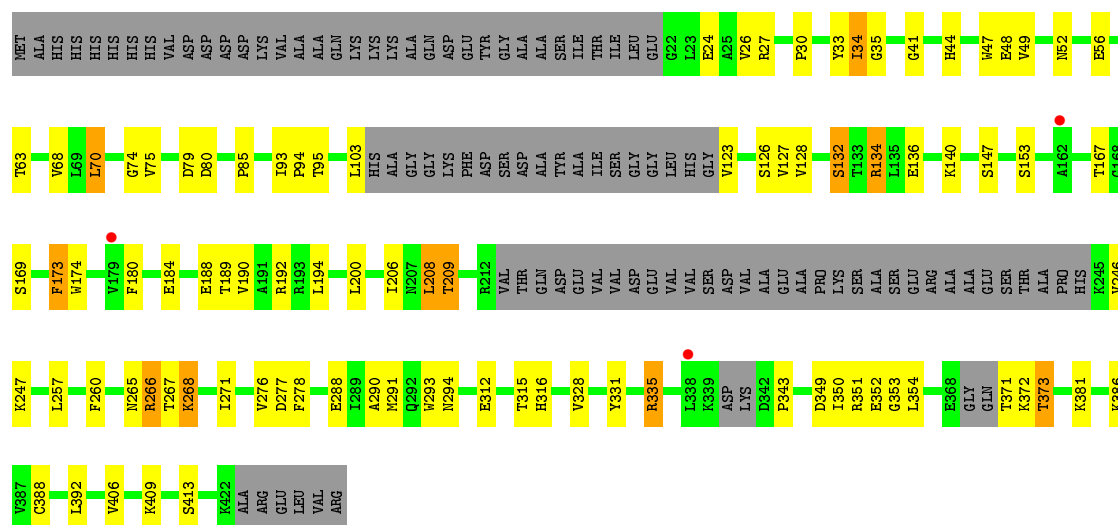


• Molecule 1: DNA GYRASE SUBUNIT B

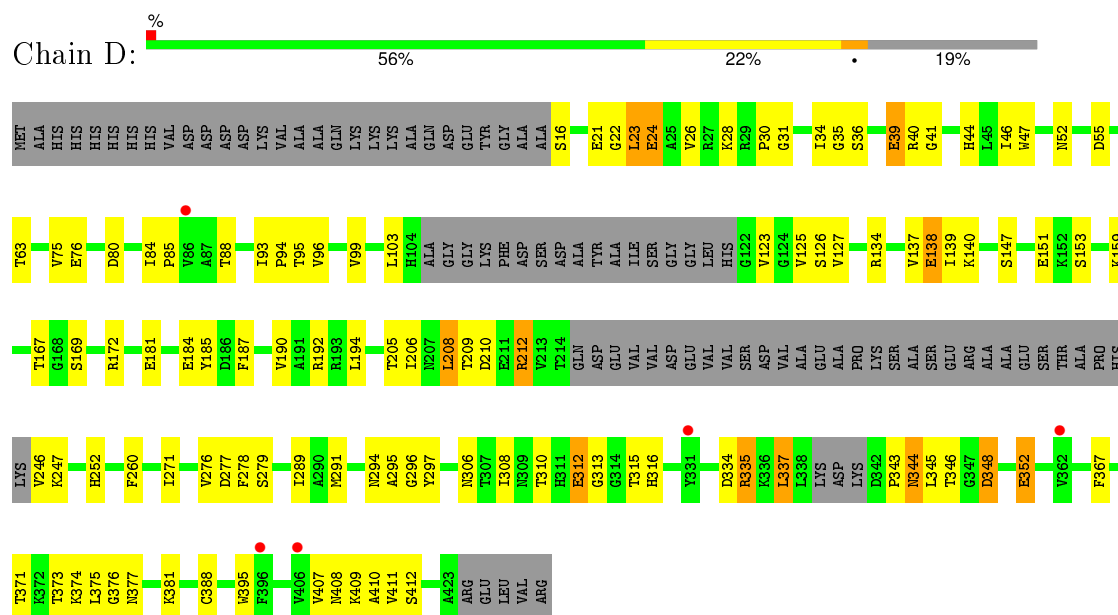


• Molecule 1: DNA GYRASE SUBUNIT B

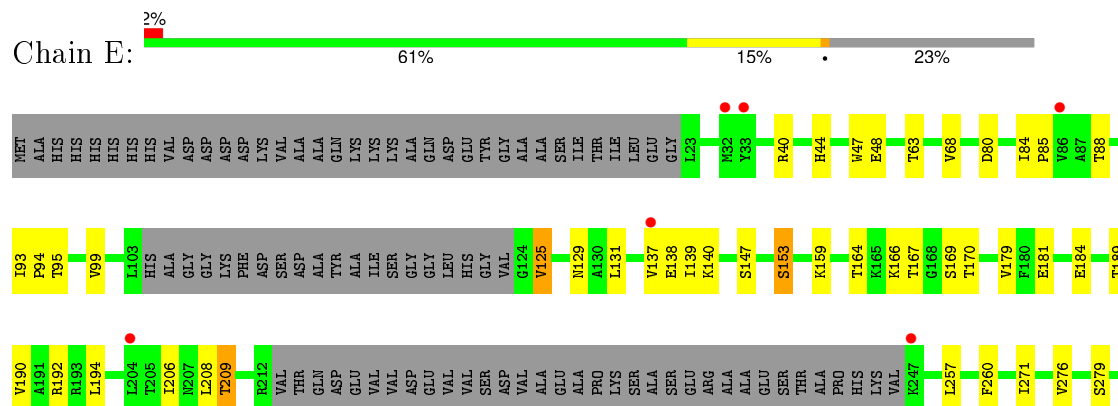


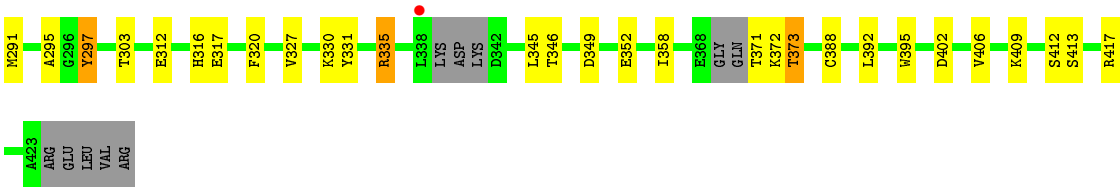


• Molecule 1: DNA GYRASE SUBUNIT B

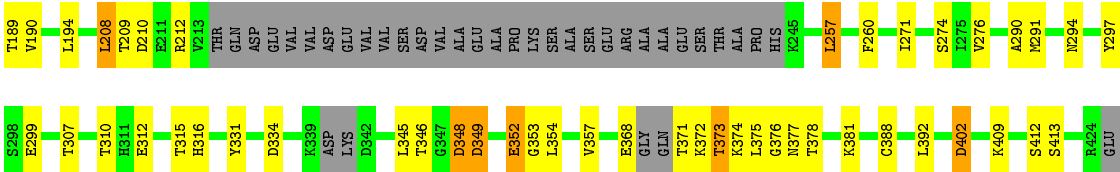
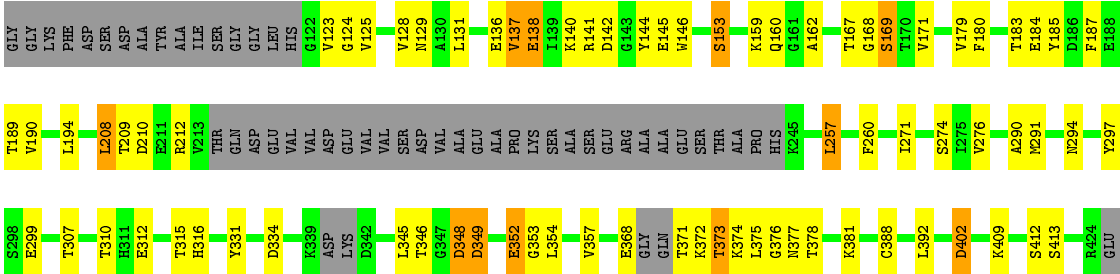
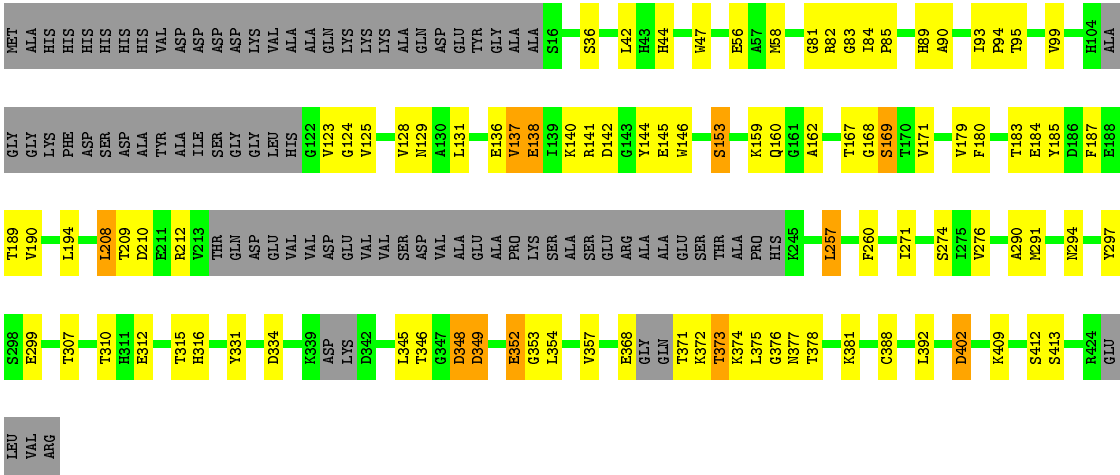


• Molecule 1: DNA GYRASE SUBUNIT B





• Molecule 1: DNA GYRASE SUBUNIT B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.61Å 171.92Å 109.23Å 90.00° 110.22° 90.00°	Depositor
Resolution (Å)	25.00 – 3.30 24.92 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-3.30) 99.7 (24.92-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.30Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.196 , 0.223 0.197 , 0.227	Depositor DCC
R_{free} test set	2055 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	106.2	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.4	EDS
Estimated twinning fraction	0.100 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 40735 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16295	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ACP

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	0.56	2/2762 (0.1%)	0.69	2/3751 (0.1%)
1	B	0.48	0/2726	0.65	1/3702 (0.0%)
1	C	0.44	0/2667	0.63	0/3619
1	D	0.51	1/2730 (0.0%)	0.66	0/3711
1	E	0.52	1/2655 (0.0%)	0.66	0/3601
1	F	0.53	0/2748	0.67	0/3727
All	All	0.51	4/16288 (0.0%)	0.66	3/22111 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	LEU	N-CA	-7.20	1.31	1.46
1	E	297	TYR	CE1-CZ	-5.61	1.31	1.38
1	A	85	PRO	N-CD	5.60	1.55	1.47
1	A	30	PRO	N-CD	5.03	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ASP	C-N-CA	-5.80	107.19	121.70
1	A	29	ARG	C-N-CD	5.63	140.22	128.40
1	A	84	ILE	C-N-CD	5.42	139.78	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	123	VAL	Peptide

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	2714	0	2620	79	0
1	B	2680	0	2580	61	0
1	C	2622	0	2517	68	0
1	D	2684	0	2557	89	0
1	E	2609	0	2532	46	0
1	F	2703	0	2604	87	0
2	A	31	0	14	1	0
2	B	31	0	14	1	0
2	C	31	0	14	3	0
2	D	31	0	14	2	0
2	E	31	0	14	8	0
2	F	31	0	14	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	16	0	0	0	0
4	B	20	0	0	0	0
4	C	13	0	0	0	0
4	D	14	0	0	0	0
4	E	14	0	0	1	0
4	F	14	0	0	0	0
All	All	16295	0	15494	414	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (414) 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:34:ILE:HD11	1:C:41:GLY:O	1.17	1.26
1:F:352:GLU:OE1	1:F:413:SER:HB2	1.09	1.24
1:F:352:GLU:OE1	1:F:413:SER:CB	1.90	1.20
1:D:210:ASP:OD1	1:D:212:ARG:HG3	1.46	1.15
1:C:34:ILE:HD11	1:C:41:GLY:C	1.70	1.10
1:F:99:VAL:HG13	2:F:525:ACP:H5'2	1.28	1.08
1:F:99:VAL:CG1	2:F:525:ACP:H5'2	1.85	1.07
1:E:352:GLU:OE1	1:F:159:LYS:NZ	1.87	1.06
1:D:185:TYR:O	1:D:212:ARG:NH2	1.88	1.05
1:D:352:GLU:OE1	1:E:159:LYS:NZ	1.87	1.05
1:C:34:ILE:CD1	1:C:41:GLY:O	2.04	1.04
1:D:138:GLU:OE1	1:D:172:ARG:NH2	1.93	1.00
1:B:346:THR:HB	1:B:349:ASP:OD2	1.62	1.00
1:D:76:GLU:OE1	1:D:172:ARG:NH1	1.94	1.00
1:A:164:THR:HG22	1:A:166:LYS:H	1.28	0.99
1:B:346:THR:CB	1:B:349:ASP:OD2	2.11	0.98
1:A:76:GLU:OE1	1:A:172:ARG:NH1	1.99	0.96
1:B:403:ALA:O	1:B:407:VAL:HG23	1.66	0.96
1:F:312:GLU:HG3	1:F:373:THR:HG23	1.46	0.95
1:F:312:GLU:HG3	1:F:373:THR:CG2	2.00	0.92
1:E:125:VAL:HG12	2:E:525:ACP:O1A	1.70	0.91
1:F:210:ASP:OD1	1:F:212:ARG:HG3	1.69	0.91
1:C:349:ASP:OD1	1:C:413:SER:OG	1.89	0.91
1:F:294:ASN:OD1	1:F:353:GLY:O	1.91	0.88
1:B:347:GLY:HA2	1:B:350:ILE:HD12	1.55	0.88
1:E:349:ASP:OD1	1:E:413:SER:OG	1.91	0.88
2:C:525:ACP:O2B	2:C:525:ACP:H5'1	1.73	0.87
1:E:125:VAL:HG12	2:E:525:ACP:PA	2.15	0.87
1:C:128:VAL:O	1:C:132:SER:OG	1.93	0.86
1:C:75:VAL:HB	1:C:173:PHE:CE1	2.11	0.85
1:D:26:VAL:HG11	1:D:127:VAL:HG13	1.58	0.85
1:A:84:ILE:HD12	1:A:169:SER:HB3	1.59	0.84
1:D:36:SER:O	1:D:41:GLY:HA3	1.77	0.84
1:F:99:VAL:HG13	2:F:525:ACP:C5'	2.06	0.84
2:D:525:ACP:O1B	2:D:525:ACP:H5'1	1.78	0.82
1:D:184:GLU:HG3	1:F:189:THR:HG22	1.63	0.81
1:F:346:THR:HB	1:F:349:ASP:OD2	1.81	0.80
1:D:184:GLU:CG	1:F:189:THR:HG22	2.10	0.80
1:C:48:GLU:O	1:C:52:ASN:ND2	2.16	0.79
1:C:24:GLU:OE1	1:C:27:ARG:NH1	2.14	0.79
1:A:164:THR:HG22	1:A:166:LYS:N	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:GLY:O	1:D:103:LEU:HD12	1.84	0.77
1:F:375:LEU:HD12	1:F:376:GLY:H	1.49	0.77
1:B:135:LEU:HD12	1:B:173:PHE:HB3	1.67	0.77
1:B:324:LEU:O	1:B:324:LEU:HD12	1.82	0.77
1:D:184:GLU:HG3	1:F:189:THR:CG2	2.15	0.77
1:D:408:ASN:HA	1:D:411:VAL:HG22	1.66	0.76
1:D:99:VAL:CG1	1:D:125:VAL:HG11	2.15	0.76
1:E:312:GLU:HB2	1:E:373:THR:O	1.85	0.76
1:C:70:LEU:HD12	1:C:74:GLY:C	2.06	0.75
1:C:276:VAL:HB	1:C:291:MET:HG2	1.68	0.75
1:D:63:THR:HG22	1:D:80:ASP:OD2	1.86	0.74
1:D:334:ASP:HB2	1:D:335:ARG:HH21	1.53	0.74
1:B:134:ARG:NH1	1:B:136:GLU:OE2	2.20	0.73
1:E:189:THR:HG22	1:F:184:GLU:HG3	1.71	0.73
1:C:371:THR:OG1	1:C:372:LYS:N	2.20	0.73
1:C:34:ILE:HD11	1:C:41:GLY:CA	2.17	0.73
1:A:403:ALA:O	1:A:407:VAL:HG23	1.89	0.73
1:D:334:ASP:CB	1:D:335:ARG:HH21	2.02	0.73
1:A:86:VAL:HG12	1:A:158:LEU:HD21	1.72	0.72
1:C:352:GLU:HG2	1:C:409:LYS:HE3	1.69	0.72
2:C:525:ACP:PB	2:C:525:ACP:H5'1	2.29	0.72
1:F:312:GLU:CG	1:F:373:THR:HG23	2.20	0.71
1:D:99:VAL:HG12	1:D:125:VAL:HG11	1.71	0.71
1:A:164:THR:CG2	1:A:166:LYS:H	2.03	0.69
1:F:375:LEU:HD11	1:F:377:ASN:OD1	1.92	0.69
1:C:63:THR:HG22	1:C:80:ASP:OD2	1.93	0.69
1:E:131:LEU:HD22	1:E:179:VAL:HG11	1.74	0.69
1:F:276:VAL:HB	1:F:291:MET:HG2	1.74	0.68
1:A:63:THR:HG22	1:A:80:ASP:OD2	1.94	0.68
1:B:63:THR:HG22	1:B:80:ASP:OD2	1.92	0.68
1:F:388:CYS:O	1:F:392:LEU:HB2	1.94	0.68
1:E:327:VAL:HA	1:E:330:LYS:HE2	1.76	0.68
1:D:277:ASP:OD1	1:D:278:PHE:N	2.27	0.67
1:A:210:ASP:OD1	1:A:212:ARG:HG3	1.94	0.67
1:A:164:THR:CG2	1:A:166:LYS:HB2	2.25	0.67
1:E:63:THR:HG22	1:E:80:ASP:OD2	1.95	0.67
1:D:306:ASN:O	1:D:308:ILE:CD1	2.42	0.67
1:F:124:GLY:N	2:F:525:ACP:O3G	2.27	0.67
1:D:31:GLY:O	1:D:35:GLY:N	2.27	0.67
1:B:276:VAL:HB	1:B:291:MET:HG2	1.75	0.66
1:B:345:LEU:HD13	1:B:410:ALA:CB	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:THR:HG21	1:A:166:LYS:HB2	1.76	0.66
1:D:34:ILE:O	1:D:34:ILE:HG22	1.93	0.66
1:F:144:TYR:CG	1:F:160:GLN:NE2	2.64	0.66
2:B:525:ACP:O3'	2:B:525:ACP:O2B	2.03	0.65
1:D:306:ASN:O	1:D:308:ILE:HD12	1.96	0.65
1:C:26:VAL:HA	1:C:33:TYR:CE2	2.32	0.65
1:B:330:LYS:O	1:B:334:ASP:HB3	1.97	0.65
1:A:313:GLY:O	1:A:374:LYS:HG3	1.97	0.64
1:C:265:ASN:OD1	1:C:294:ASN:ND2	2.27	0.64
1:F:124:GLY:HA3	2:F:525:ACP:O2A	1.98	0.63
1:D:123:VAL:CB	1:D:127:VAL:HG21	2.29	0.63
1:E:276:VAL:HB	1:E:291:MET:HG2	1.80	0.63
1:B:325:THR:HG23	1:B:350:ILE:CD1	2.29	0.63
1:B:325:THR:HG23	1:B:350:ILE:HD13	1.81	0.63
1:A:84:ILE:CD1	1:A:169:SER:HB3	2.28	0.63
1:A:276:VAL:HB	1:A:291:MET:HG2	1.80	0.63
1:B:324:LEU:HD12	1:B:328:VAL:HG23	1.80	0.63
1:C:70:LEU:HD12	1:C:74:GLY:CA	2.29	0.62
1:F:124:GLY:CA	2:F:525:ACP:O2A	2.47	0.62
1:A:36:SER:O	1:A:41:GLY:HA3	2.00	0.62
1:A:39:GLU:OE2	1:C:184:GLU:HG3	1.99	0.61
1:D:276:VAL:HB	1:D:291:MET:HG2	1.82	0.61
1:B:347:GLY:CA	1:B:350:ILE:HD12	2.27	0.61
1:E:48:GLU:HG3	4:E:2003:HOH:O	1.99	0.61
1:F:183:THR:HG22	1:F:183:THR:O	2.00	0.61
1:F:352:GLU:OE1	1:F:413:SER:CA	2.49	0.61
1:D:308:ILE:HD12	1:D:308:ILE:N	2.15	0.61
1:C:312:GLU:HB2	1:C:373:THR:O	2.01	0.60
1:C:47:TRP:HH2	1:C:190:VAL:HA	1.66	0.60
1:B:144:TYR:CD2	1:B:160:GLN:NE2	2.70	0.60
1:A:371:THR:HB	1:A:373:THR:OG1	2.01	0.60
1:A:29:ARG:NH1	1:A:29:ARG:HG2	2.15	0.60
1:A:352:GLU:OE1	1:A:413:SER:OG	2.16	0.60
1:F:402:ASP:OD1	1:F:402:ASP:N	2.34	0.60
1:D:276:VAL:HG22	1:D:395:TRP:CE2	2.36	0.60
1:D:39:GLU:OE1	1:D:40:ARG:N	2.34	0.60
1:B:345:LEU:HD13	1:B:410:ALA:HB1	1.83	0.60
1:D:335:ARG:N	1:D:335:ARG:HE	1.98	0.60
1:F:83:GLY:HA2	1:F:169:SER:OG	2.02	0.59
1:B:140:LYS:O	1:B:167:THR:HA	2.02	0.59
1:F:348:ASP:OD1	1:F:348:ASP:N	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:GLY:HA2	2:F:525:ACP:O3G	2.01	0.59
1:B:23:LEU:CD1	1:B:153:SER:HB3	2.33	0.59
1:B:346:THR:OG1	1:B:349:ASP:OD2	2.20	0.59
1:D:312:GLU:HB2	1:D:373:THR:OG1	2.02	0.59
1:C:134:ARG:NH1	1:C:136:GLU:OE2	2.36	0.59
1:E:44:HIS:NE2	1:E:48:GLU:OE1	2.35	0.58
1:A:29:ARG:HH11	1:A:29:ARG:HG2	1.68	0.58
1:C:49:VAL:HA	1:C:52:ASN:HD22	1.67	0.58
1:D:46:ILE:HD11	1:D:185:TYR:CD1	2.39	0.58
1:F:375:LEU:HD12	1:F:376:GLY:N	2.17	0.58
1:F:140:LYS:O	1:F:167:THR:HA	2.03	0.58
1:E:125:VAL:CG1	2:E:525:ACP:O1A	2.50	0.58
1:D:313:GLY:O	1:D:374:LYS:HA	2.04	0.58
1:F:99:VAL:HG11	2:F:525:ACP:H5'2	1.82	0.58
1:E:371:THR:O	1:E:371:THR:HG22	2.03	0.58
1:D:184:GLU:HG2	1:F:189:THR:HG22	1.82	0.57
1:E:164:THR:HG22	1:E:166:LYS:H	1.69	0.57
1:F:185:TYR:O	1:F:212:ARG:NH2	2.25	0.57
1:E:125:VAL:CG1	2:E:525:ACP:PA	2.92	0.56
1:F:371:THR:O	1:F:372:LYS:HB2	2.04	0.56
1:B:396:PHE:CD1	1:B:403:ALA:HB1	2.40	0.56
1:C:24:GLU:CD	1:C:27:ARG:NH1	2.58	0.56
1:A:47:TRP:HH2	1:A:190:VAL:HA	1.69	0.56
1:F:124:GLY:CA	2:F:525:ACP:O3G	2.54	0.56
1:E:47:TRP:HH2	1:E:190:VAL:HA	1.70	0.56
1:E:99:VAL:HG13	2:E:525:ACP:H5'1	1.87	0.56
1:C:271:ILE:HD13	1:C:409:LYS:HG3	1.88	0.56
1:F:81:GLY:O	1:F:83:GLY:N	2.39	0.56
1:B:396:PHE:HD1	1:B:403:ALA:HB1	1.70	0.56
1:C:26:VAL:HA	1:C:33:TYR:CD2	2.41	0.56
1:B:93:ILE:HG12	1:B:94:PRO:HD2	1.87	0.55
1:D:348:ASP:N	1:D:348:ASP:OD1	2.38	0.55
1:F:371:THR:OG1	1:F:372:LYS:N	2.39	0.55
1:A:316:HIS:ND1	1:A:375:LEU:HD23	2.22	0.55
1:B:48:GLU:OE1	1:B:124:GLY:N	2.38	0.55
1:B:97:ASP:OD1	1:B:148:GLN:NE2	2.39	0.55
1:F:144:TYR:CD2	1:F:160:GLN:NE2	2.74	0.55
1:D:205:THR:HG23	1:D:252:HIS:HB2	1.88	0.55
1:C:24:GLU:CD	1:C:27:ARG:HH12	2.09	0.55
1:A:323:ALA:O	1:A:327:VAL:HG23	2.07	0.55
1:A:213:VAL:HA	1:B:249:ARG:HH22	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:ILE:HD13	1:E:409:LYS:HG3	1.88	0.55
1:D:375:LEU:HD12	1:D:376:GLY:H	1.71	0.54
2:F:525:ACP:O1B	2:F:525:ACP:O2G	2.26	0.54
1:D:371:THR:OG1	1:D:373:THR:HG23	2.07	0.54
1:E:194:LEU:HB3	1:E:206:ILE:HG21	1.89	0.54
1:D:93:ILE:HG12	1:D:94:PRO:HD2	1.88	0.54
1:C:140:LYS:O	1:C:167:THR:HA	2.07	0.54
1:A:33:TYR:N	1:A:33:TYR:CD1	2.76	0.54
1:A:93:ILE:HG12	1:A:94:PRO:HD2	1.89	0.54
1:A:34:ILE:HD13	1:A:131:LEU:CD1	2.37	0.54
1:A:287:VAL:HG23	1:A:360:VAL:HG12	1.90	0.54
2:E:525:ACP:O2B	2:E:525:ACP:O3'	2.22	0.54
1:C:70:LEU:HD12	1:C:74:GLY:HA3	1.88	0.53
2:C:525:ACP:PB	2:C:525:ACP:C5'	2.96	0.53
1:A:30:PRO:O	1:A:34:ILE:HG12	2.08	0.53
1:A:247:LYS:O	1:A:247:LYS:HG3	2.07	0.53
1:E:140:LYS:O	1:E:167:THR:HA	2.07	0.53
1:B:323:ALA:O	1:B:327:VAL:HG23	2.09	0.53
1:B:345:LEU:HD13	1:B:410:ALA:HB3	1.90	0.53
1:C:173:PHE:CD1	1:C:173:PHE:N	2.76	0.53
1:D:26:VAL:CG1	1:D:127:VAL:HG13	2.34	0.53
1:F:274:SER:HB3	1:F:402:ASP:OD2	2.09	0.53
1:E:189:THR:CG2	1:F:184:GLU:HG3	2.38	0.52
1:B:352:GLU:HG2	1:B:409:LYS:HE3	1.90	0.52
1:D:52:ASN:O	1:D:55:ASP:HB2	2.09	0.52
1:F:312:GLU:HG3	1:F:373:THR:HG21	1.86	0.52
1:B:23:LEU:HD12	1:B:153:SER:HB3	1.90	0.52
1:C:188:GLU:HG3	1:C:192:ARG:HH21	1.74	0.52
1:A:47:TRP:CZ3	1:A:193:ARG:HG2	2.45	0.52
1:E:129:ASN:OD1	1:E:153:SER:HA	2.09	0.52
1:B:324:LEU:C	1:B:324:LEU:HD12	2.29	0.52
1:A:276:VAL:O	1:A:290:ALA:HA	2.10	0.52
1:C:351:ARG:O	1:C:354:LEU:HB3	2.09	0.52
1:D:276:VAL:HG22	1:D:395:TRP:CD2	2.44	0.52
1:C:265:ASN:HA	1:C:268:LYS:HG3	1.92	0.52
1:B:277:ASP:O	1:B:278:PHE:HB3	2.10	0.52
1:A:34:ILE:HG22	1:A:44:HIS:ND1	2.25	0.52
1:C:93:ILE:HG12	1:C:94:PRO:HD2	1.92	0.51
1:D:22:GLY:O	1:D:103:LEU:CD1	2.57	0.51
1:B:266:ARG:HG3	1:B:267:THR:N	2.24	0.51
1:C:34:ILE:CD1	1:C:41:GLY:CA	2.88	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:LEU:CD1	1:F:377:ASN:OD1	2.58	0.51
1:C:293:TRP:HA	1:C:353:GLY:O	2.10	0.51
1:F:81:GLY:O	1:F:168:GLY:HA2	2.10	0.51
1:D:140:LYS:O	1:D:167:THR:HA	2.11	0.51
1:D:294:ASN:O	1:D:296:GLY:N	2.42	0.51
1:D:159:LYS:NZ	1:F:352:GLU:HG3	2.26	0.50
1:B:276:VAL:HG22	1:B:395:TRP:CE2	2.46	0.50
1:A:29:ARG:HH11	1:A:29:ARG:CG	2.24	0.50
1:A:213:VAL:HA	1:B:249:ARG:NH2	2.25	0.50
1:B:135:LEU:HD12	1:B:173:PHE:CB	2.39	0.50
1:B:187:PHE:CD2	1:B:210:ASP:HB2	2.46	0.50
1:D:289:ILE:HD12	1:D:388:CYS:SG	2.52	0.50
1:C:277:ASP:OD1	1:C:278:PHE:N	2.44	0.50
1:D:21:GLU:O	1:D:24:GLU:HG3	2.11	0.50
1:D:184:GLU:HG3	1:F:189:THR:HG23	1.92	0.50
1:A:345:LEU:HD22	1:A:410:ALA:HB1	1.94	0.50
1:C:271:ILE:CD1	1:C:409:LYS:HG3	2.42	0.50
1:D:294:ASN:C	1:D:296:GLY:H	2.14	0.50
1:A:184:GLU:HG2	1:B:189:THR:HG22	1.93	0.50
1:D:85:PRO:HB2	1:D:95:THR:HG21	1.94	0.50
1:A:303:THR:HG21	1:A:317:GLU:HB2	1.93	0.49
1:D:44:HIS:HA	1:D:47:TRP:CD1	2.46	0.49
1:D:99:VAL:HG12	1:D:125:VAL:CG1	2.39	0.49
1:D:335:ARG:CA	1:D:335:ARG:HE	2.25	0.49
1:D:375:LEU:HD11	1:D:377:ASN:OD1	2.12	0.49
1:E:68:VAL:HG22	1:E:209:THR:HG23	1.94	0.49
1:A:181:GLU:OE2	1:B:36:SER:OG	2.29	0.49
1:E:93:ILE:HG12	1:E:94:PRO:HD2	1.95	0.49
1:F:271:ILE:HD13	1:F:409:LYS:HG3	1.95	0.49
1:F:99:VAL:CG1	2:F:525:ACP:C5'	2.73	0.49
1:F:331:TYR:CD1	1:F:331:TYR:C	2.86	0.49
1:C:134:ARG:O	1:C:174:TRP:HE3	1.96	0.49
1:D:134:ARG:NH1	1:F:299:GLU:O	2.36	0.49
1:F:129:ASN:OD1	1:F:153:SER:HA	2.12	0.49
1:B:85:PRO:HB2	1:B:95:THR:HG21	1.95	0.49
1:C:34:ILE:HG12	1:C:35:GLY:N	2.28	0.49
1:D:181:GLU:OE2	1:F:36:SER:OG	2.28	0.49
1:A:276:VAL:HG22	1:A:395:TRP:CE2	2.48	0.49
1:D:84:ILE:HG21	1:D:96:VAL:HG13	1.95	0.49
1:A:388:CYS:O	1:A:392:LEU:HB2	2.13	0.49
1:A:97:ASP:OD1	1:A:148:GLN:NE2	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ASP:HB3	1:D:335:ARG:HH21	1.76	0.48
1:F:146:TRP:CH2	1:F:160:GLN:HG3	2.47	0.48
1:E:40:ARG:NH1	1:F:180:PHE:O	2.45	0.48
1:B:347:GLY:HA2	1:B:350:ILE:CD1	2.35	0.48
1:D:99:VAL:CG1	1:D:125:VAL:CG1	2.91	0.48
1:A:68:VAL:HG22	1:A:209:THR:HG23	1.95	0.48
1:A:84:ILE:CD1	1:A:169:SER:CB	2.91	0.48
1:D:337:LEU:HD13	1:D:407:VAL:CG1	2.44	0.48
1:F:138:GLU:HG3	1:F:138:GLU:O	2.14	0.48
1:F:276:VAL:O	1:F:290:ALA:HA	2.14	0.48
1:B:207:ASN:OD1	1:B:250:THR:HG23	2.14	0.47
1:C:194:LEU:HD12	1:C:208:LEU:HG	1.96	0.47
1:C:173:PHE:HD1	1:C:173:PHE:N	2.12	0.47
1:F:89:HIS:CG	1:F:90:ALA:N	2.83	0.47
1:D:271:ILE:HD13	1:D:409:LYS:HG3	1.96	0.47
1:A:184:GLU:CG	1:B:189:THR:HG22	2.45	0.47
1:F:56:GLU:OE2	2:F:525:ACP:C2	2.62	0.47
1:F:194:LEU:HD12	1:F:208:LEU:HG	1.97	0.47
1:A:337:LEU:CD1	1:A:407:VAL:HG11	2.44	0.47
1:A:368:GLU:O	1:A:374:LYS:HB3	2.14	0.47
1:C:388:CYS:O	1:C:392:LEU:HB2	2.15	0.47
1:A:294:ASN:C	1:A:296:GLY:H	2.17	0.47
2:E:525:ACP:HO3'	2:E:525:ACP:PB	2.38	0.47
1:D:34:ILE:O	1:D:34:ILE:CG2	2.60	0.47
1:D:310:THR:HB	1:D:373:THR:O	2.15	0.47
1:A:123:VAL:HB	1:A:124:GLY:H	1.34	0.47
1:A:40:ARG:NH2	1:C:180:PHE:O	2.45	0.47
1:F:131:LEU:HD22	1:F:179:VAL:HG11	1.95	0.47
1:B:345:LEU:HD22	1:B:349:ASP:HB2	1.96	0.47
1:E:137:VAL:HG12	1:E:139:ILE:HG13	1.96	0.47
1:F:93:ILE:HG12	1:F:94:PRO:HD2	1.96	0.47
1:B:325:THR:HG23	1:B:347:GLY:HA2	1.95	0.47
1:D:246:VAL:HG12	1:D:247:LYS:N	2.29	0.47
1:F:47:TRP:HH2	1:F:190:VAL:HA	1.80	0.47
1:F:125:VAL:O	1:F:128:VAL:N	2.47	0.46
1:B:346:THR:O	1:B:350:ILE:HD12	2.14	0.46
1:E:276:VAL:HG22	1:E:395:TRP:CE2	2.49	0.46
1:B:85:PRO:HB2	1:B:95:THR:CG2	2.45	0.46
1:E:388:CYS:O	1:E:392:LEU:HB2	2.16	0.46
1:D:194:LEU:HD22	1:D:206:ILE:HG21	1.97	0.46
1:F:124:GLY:HA2	2:F:525:ACP:O2A	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ASP:O	1:D:278:PHE:HB3	2.16	0.46
1:B:294:ASN:C	1:B:296:GLY:H	2.18	0.46
1:B:331:TYR:CD2	1:B:396:PHE:HB3	2.51	0.46
1:C:194:LEU:HB3	1:C:206:ILE:HG21	1.96	0.46
1:E:331:TYR:CD1	1:E:331:TYR:C	2.88	0.46
1:A:258:VAL:HG12	1:A:262:LYS:HE3	1.98	0.46
1:C:44:HIS:CE1	1:C:48:GLU:HG2	2.50	0.46
2:D:525:ACP:H5'1	2:D:525:ACP:PB	2.56	0.46
1:C:277:ASP:O	1:C:278:PHE:HB3	2.15	0.46
1:C:85:PRO:HB2	1:C:95:THR:HG21	1.98	0.46
1:A:257:LEU:O	1:A:261:VAL:HG23	2.15	0.46
1:A:337:LEU:HD13	1:A:407:VAL:HG11	1.97	0.45
1:D:308:ILE:CD1	1:D:308:ILE:N	2.79	0.45
1:D:346:THR:HG22	1:D:348:ASP:H	1.81	0.45
1:E:335:ARG:HD3	1:E:335:ARG:HA	1.78	0.45
1:C:44:HIS:HE1	1:C:48:GLU:HG2	1.80	0.45
1:F:297:TYR:O	1:F:352:GLU:HG2	2.16	0.45
1:D:408:ASN:CA	1:D:411:VAL:HG22	2.43	0.45
1:A:182:THR:HG23	1:A:184:GLU:H	1.81	0.45
1:D:367:PHE:N	1:D:367:PHE:CD1	2.84	0.45
1:C:331:TYR:CD1	1:C:331:TYR:C	2.89	0.45
1:F:294:ASN:OD1	1:F:353:GLY:C	2.54	0.45
1:A:210:ASP:HB3	1:A:247:LYS:HG2	1.99	0.45
1:A:82:ARG:O	1:A:141:ARG:HD2	2.17	0.45
1:C:68:VAL:HG22	1:C:209:THR:HG23	1.98	0.45
1:B:184:GLU:HG3	1:C:189:THR:CG2	2.46	0.45
1:D:28:LYS:C	1:D:30:PRO:HD3	2.36	0.45
1:D:375:LEU:HD12	1:D:376:GLY:N	2.32	0.45
1:D:352:GLU:HG2	1:D:409:LYS:HE3	1.99	0.45
1:A:327:VAL:HG12	1:A:396:PHE:CD2	2.52	0.45
1:C:266:ARG:NH2	1:C:267:THR:HG23	2.32	0.45
1:B:324:LEU:CD1	1:B:328:VAL:HG23	2.47	0.44
1:B:184:GLU:CG	1:C:189:THR:HG22	2.48	0.44
1:A:352:GLU:OE1	1:A:413:SER:CB	2.65	0.44
1:B:103:LEU:HD23	1:B:126:SER:OG	2.17	0.44
1:C:315:THR:HB	1:C:381:LYS:HB2	2.00	0.44
1:E:44:HIS:O	1:E:44:HIS:CD2	2.70	0.44
1:F:85:PRO:HB2	1:F:95:THR:HG21	2.00	0.44
1:D:192:ARG:NH1	1:E:184:GLU:OE2	2.50	0.44
1:C:85:PRO:O	1:C:95:THR:HB	2.17	0.44
1:D:187:PHE:CZ	1:D:208:LEU:HD13	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:525:ACP:H5'1	2:F:525:ACP:H8	2.00	0.44
1:C:79:ASP:N	1:C:79:ASP:OD1	2.51	0.44
1:F:291:MET:HB2	1:F:354:LEU:HD11	1.99	0.43
1:D:47:TRP:HH2	1:D:190:VAL:HA	1.82	0.43
1:D:297:TYR:CD2	1:E:147:SER:HB3	2.53	0.43
1:E:352:GLU:HG2	1:E:409:LYS:HE3	2.00	0.43
1:B:187:PHE:CZ	1:B:208:LEU:HD13	2.53	0.43
1:F:312:GLU:OE1	1:F:371:THR:HB	2.18	0.43
1:F:368:GLU:N	1:F:374:LYS:O	2.40	0.43
1:E:85:PRO:O	1:E:95:THR:HB	2.18	0.43
1:B:388:CYS:O	1:B:392:LEU:HB2	2.18	0.43
1:E:312:GLU:CB	1:E:373:THR:O	2.62	0.43
1:D:137:VAL:HG12	1:D:139:ILE:HG13	1.99	0.43
1:D:184:GLU:OE1	1:D:212:ARG:NH1	2.52	0.43
1:D:345:LEU:HD13	1:D:410:ALA:HB1	2.00	0.43
1:C:386:LYS:HD2	1:C:386:LYS:HA	1.85	0.43
1:D:344:ASN:HA	1:D:344:ASN:HD22	1.58	0.43
1:F:145:GLU:HG3	1:F:162:ALA:O	2.18	0.43
1:F:257:LEU:HD13	1:F:357:VAL:HB	2.00	0.43
1:A:86:VAL:HG12	1:A:158:LEU:CD2	2.46	0.43
1:D:34:ILE:HD11	1:D:127:VAL:HG11	1.99	0.43
1:A:200:LEU:HD13	1:A:307:THR:HA	2.01	0.43
1:E:297:TYR:C	1:E:297:TYR:CD1	2.92	0.43
1:A:47:TRP:CE3	1:A:47:TRP:HA	2.53	0.42
1:A:47:TRP:HA	1:A:47:TRP:HE3	1.83	0.42
1:F:84:ILE:CG1	2:F:525:ACP:C5	2.97	0.42
1:A:141:ARG:HH11	1:A:141:ARG:HD2	1.73	0.42
1:C:246:VAL:HA	1:C:247:LYS:HA	1.67	0.42
1:E:138:GLU:HB3	1:E:170:THR:HB	2.01	0.42
1:A:352:GLU:CD	1:A:413:SER:HB2	2.40	0.42
1:D:187:PHE:CE1	1:D:208:LEU:HD13	2.55	0.42
1:D:75:VAL:O	1:D:172:ARG:HA	2.19	0.42
1:C:47:TRP:CH2	1:C:190:VAL:HA	2.52	0.42
1:A:265:ASN:OD1	1:A:294:ASN:ND2	2.53	0.42
1:D:134:ARG:NE	1:D:151:GLU:OE1	2.50	0.42
1:A:26:VAL:HG11	1:A:127:VAL:HG13	2.01	0.42
1:E:84:ILE:HD11	2:E:525:ACP:N7	2.35	0.42
1:A:303:THR:HB	1:A:316:HIS:CD2	2.54	0.42
1:F:315:THR:HB	1:F:381:LYS:HB2	2.02	0.42
1:E:271:ILE:CD1	1:E:409:LYS:HG3	2.49	0.42
1:C:276:VAL:O	1:C:290:ALA:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:O	1:A:410:ALA:HB3	2.20	0.42
1:A:45:LEU:HD22	1:A:128:VAL:HA	2.01	0.42
1:E:303:THR:HG21	1:E:317:GLU:HB2	2.01	0.41
1:E:320:PHE:CD2	1:E:358:ILE:HD11	2.55	0.41
1:F:187:PHE:CD2	1:F:210:ASP:HB2	2.55	0.41
1:F:42:LEU:HG	1:F:185:TYR:CE1	2.55	0.41
1:D:315:THR:HB	1:D:381:LYS:HB2	2.02	0.41
1:F:310:THR:HB	1:F:373:THR:O	2.21	0.41
1:C:328:VAL:HG11	1:C:350:ILE:HG12	2.02	0.41
1:C:200:LEU:HD23	1:C:257:LEU:HD21	2.02	0.41
1:C:247:LYS:O	1:C:247:LYS:HG3	2.20	0.41
1:B:246:VAL:HG22	1:B:247:LYS:N	2.36	0.41
1:D:46:ILE:CD1	1:D:185:TYR:CD1	3.03	0.41
1:C:49:VAL:HA	1:C:52:ASN:ND2	2.32	0.41
1:A:187:PHE:CD2	1:A:210:ASP:HB2	2.56	0.41
1:B:36:SER:O	1:B:41:GLY:HA3	2.20	0.41
1:F:89:HIS:CG	1:F:90:ALA:H	2.39	0.41
1:A:194:LEU:HD12	1:A:208:LEU:HG	2.02	0.41
1:A:86:VAL:CG1	1:A:158:LEU:HD21	2.45	0.41
1:F:81:GLY:C	1:F:83:GLY:H	2.24	0.41
1:F:271:ILE:CD1	1:F:409:LYS:HG3	2.50	0.41
1:F:141:ARG:HG2	1:F:142:ASP:N	2.36	0.41
1:A:85:PRO:HB2	1:A:95:THR:HG21	2.03	0.41
1:F:58:MET:CE	1:F:307:THR:OG1	2.69	0.41
1:A:140:LYS:O	1:A:167:THR:HA	2.20	0.41
1:F:187:PHE:CZ	1:F:208:LEU:HD13	2.56	0.41
1:B:276:VAL:HG22	1:B:395:TRP:CD2	2.55	0.41
1:E:44:HIS:HA	1:E:47:TRP:CD1	2.55	0.41
1:F:44:HIS:HA	1:F:47:TRP:CD1	2.56	0.41
1:A:58:MET:HG2	1:A:361:LYS:HE2	2.02	0.41
1:D:408:ASN:HA	1:D:411:VAL:CG2	2.42	0.41
1:A:149:VAL:HG21	1:B:298:SER:HB3	2.02	0.41
1:C:30:PRO:O	1:C:34:ILE:HG22	2.21	0.40
1:F:137:VAL:HG13	1:F:171:VAL:HG22	2.03	0.40
1:D:36:SER:CB	1:E:181:GLU:HG2	2.50	0.40
1:C:85:PRO:HB2	1:C:95:THR:CG2	2.51	0.40
1:C:335:ARG:HD3	1:C:335:ARG:HA	1.73	0.40
1:F:84:ILE:HG13	2:F:525:ACP:C5	2.51	0.40
1:A:303:THR:HG22	1:A:358:ILE:HD12	2.03	0.40
1:B:276:VAL:O	1:B:290:ALA:HA	2.21	0.40
1:D:345:LEU:HA	1:D:345:LEU:HD23	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:OE1	2:A:525:ACP:C2	2.69	0.40
1:C:127:VAL:HG23	1:C:128:VAL:N	2.36	0.40
1:B:158:LEU:HD12	1:B:159:LYS:H	1.85	0.40
1:A:339:LYS:O	1:A:342:ASP:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	353/442 (80%)	339 (96%)	12 (3%)	2 (1%)	30	68
1	B	346/442 (78%)	331 (96%)	13 (4%)	2 (1%)	30	68
1	C	336/442 (76%)	319 (95%)	16 (5%)	1 (0%)	46	81
1	D	349/442 (79%)	336 (96%)	11 (3%)	2 (1%)	30	68
1	E	332/442 (75%)	318 (96%)	13 (4%)	1 (0%)	46	81
1	F	347/442 (78%)	329 (95%)	15 (4%)	3 (1%)	21	60
All	All	2063/2652 (78%)	1972 (96%)	80 (4%)	11 (0%)	34	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	343	PRO
1	D	295	ALA
1	F	82	ARG
1	F	123	VAL
1	A	295	ALA
1	B	295	ALA
1	D	343	PRO
1	E	295	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	352	GLU
1	B	83	GLY
1	A	365	PRO

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	283/361 (78%)	265 (94%)	18 (6%)	22	60
1	B	278/361 (77%)	260 (94%)	18 (6%)	21	59
1	C	273/361 (76%)	252 (92%)	21 (8%)	16	51
1	D	278/361 (77%)	255 (92%)	23 (8%)	14	47
1	E	275/361 (76%)	255 (93%)	20 (7%)	17	53
1	F	282/361 (78%)	264 (94%)	18 (6%)	22	60
All	All	1669/2166 (77%)	1551 (93%)	118 (7%)	18	55

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	39	GLU
1	A	56	GLU
1	A	86	VAL
1	A	123	VAL
1	A	125	VAL
1	A	144	TYR
1	A	147	SER
1	A	169	SER
1	A	182	THR
1	A	208	LEU
1	A	209	THR
1	A	248	SER
1	A	260	PHE
1	A	344	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	371	THR
1	A	392	LEU
1	A	412	SER
1	B	82	ARG
1	B	86	VAL
1	B	147	SER
1	B	169	SER
1	B	208	LEU
1	B	260	PHE
1	B	266	ARG
1	B	271	ILE
1	B	279	SER
1	B	288	GLU
1	B	316	HIS
1	B	324	LEU
1	B	325	THR
1	B	334	ASP
1	B	346	THR
1	B	349	ASP
1	B	373	THR
1	B	412	SER
1	C	34	ILE
1	C	56	GLU
1	C	70	LEU
1	C	103	LEU
1	C	126	SER
1	C	132	SER
1	C	134	ARG
1	C	147	SER
1	C	153	SER
1	C	169	SER
1	C	173	PHE
1	C	208	LEU
1	C	209	THR
1	C	260	PHE
1	C	266	ARG
1	C	268	LYS
1	C	288	GLU
1	C	316	HIS
1	C	335	ARG
1	C	373	THR
1	C	406	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	16	SER
1	D	23	LEU
1	D	24	GLU
1	D	39	GLU
1	D	88	THR
1	D	126	SER
1	D	138	GLU
1	D	147	SER
1	D	153	SER
1	D	169	SER
1	D	208	LEU
1	D	209	THR
1	D	212	ARG
1	D	260	PHE
1	D	279	SER
1	D	312	GLU
1	D	316	HIS
1	D	335	ARG
1	D	337	LEU
1	D	344	ASN
1	D	348	ASP
1	D	352	GLU
1	D	412	SER
1	E	88	THR
1	E	125	VAL
1	E	153	SER
1	E	169	SER
1	E	192	ARG
1	E	208	LEU
1	E	209	THR
1	E	257	LEU
1	E	260	PHE
1	E	279	SER
1	E	316	HIS
1	E	335	ARG
1	E	345	LEU
1	E	346	THR
1	E	372	LYS
1	E	373	THR
1	E	402	ASP
1	E	406	VAL
1	E	412	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	417	ARG
1	F	136	GLU
1	F	137	VAL
1	F	138	GLU
1	F	153	SER
1	F	169	SER
1	F	208	LEU
1	F	209	THR
1	F	257	LEU
1	F	260	PHE
1	F	316	HIS
1	F	334	ASP
1	F	345	LEU
1	F	348	ASP
1	F	349	ASP
1	F	373	THR
1	F	378	THR
1	F	402	ASP
1	F	412	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	344	ASN

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

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	ACP	A	525	3	25,33,33	0.71	0	31,52,52	1.12	2 (6%)
2	ACP	B	525	3	25,33,33	1.50	2 (8%)	31,52,52	1.22	2 (6%)
2	ACP	C	525	3	25,33,33	1.02	1 (4%)	31,52,52	0.73	0
2	ACP	D	525	3	25,33,33	1.30	2 (8%)	31,52,52	0.97	1 (3%)
2	ACP	E	525	3	25,33,33	1.47	2 (8%)	31,52,52	1.57	3 (9%)
2	ACP	F	525	3	25,33,33	1.99	3 (12%)	31,52,52	1.06	2 (6%)

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	ACP	A	525	3	-	0/15/38/38	0/3/3/3
2	ACP	B	525	3	-	0/15/38/38	0/3/3/3
2	ACP	C	525	3	-	0/15/38/38	0/3/3/3
2	ACP	D	525	3	-	0/15/38/38	0/3/3/3
2	ACP	E	525	3	-	0/15/38/38	0/3/3/3
2	ACP	F	525	3	-	0/15/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	525	ACP	PB-O3A	-7.43	1.50	1.58
2	B	525	ACP	PB-O3A	-5.73	1.51	1.58
2	E	525	ACP	PB-O3A	-5.02	1.52	1.58
2	D	525	ACP	PB-O3A	-4.75	1.53	1.58
2	C	525	ACP	PB-O3A	-3.14	1.54	1.58
2	D	525	ACP	PG-O2G	2.57	1.61	1.54
2	B	525	ACP	PB-O1B	2.71	1.58	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	525	ACP	PG-O2G	3.53	1.63	1.54
2	E	525	ACP	PB-O1B	3.82	1.61	1.51
2	F	525	ACP	PB-O1B	4.28	1.62	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	525	ACP	O1G-PG-C3B	-4.58	100.70	111.13
2	D	525	ACP	O1G-PG-C3B	-3.31	103.58	111.13
2	A	525	ACP	O1G-PG-C3B	-2.96	104.37	111.13
2	E	525	ACP	O1G-PG-C3B	-2.94	104.43	111.13
2	B	525	ACP	O2B-PB-O1B	2.54	118.09	110.12
2	F	525	ACP	O1B-PB-C3B	2.60	115.56	109.02
2	E	525	ACP	O2B-PB-O1B	2.72	118.67	110.12
2	A	525	ACP	O2B-PB-O1B	3.17	120.09	110.12
2	F	525	ACP	O2B-PB-O1B	3.29	120.47	110.12
2	E	525	ACP	PA-O3A-PB	6.84	151.94	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	525	ACP	1	0
2	B	525	ACP	1	0
2	C	525	ACP	3	0
2	D	525	ACP	2	0
2	E	525	ACP	8	0
2	F	525	ACP	16	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	359/442 (81%)	0.10	4 (1%) 82 78	66, 106, 153, 185	0
1	B	356/442 (80%)	0.11	4 (1%) 82 78	69, 110, 149, 203	0
1	C	346/442 (78%)	0.10	3 (0%) 85 82	80, 116, 151, 214	0
1	D	357/442 (80%)	0.09	5 (1%) 78 73	77, 110, 146, 170	0
1	E	342/442 (77%)	0.25	7 (2%) 68 62	84, 121, 170, 205	0
1	F	357/442 (80%)	0.15	0 100 100	71, 105, 159, 216	0
All	All	2117/2652 (79%)	0.13	23 (1%) 82 78	66, 112, 154, 216	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	ASN	4.1
1	E	33	TYR	3.6
1	D	86	VAL	3.3
1	E	338	LEU	3.1
1	E	247	LYS	3.1
1	C	338	LEU	2.9
1	B	280	GLY	2.7
1	B	345	LEU	2.7
1	A	21	GLU	2.7
1	D	396	PHE	2.6
1	E	86	VAL	2.5
1	A	137	VAL	2.4
1	E	137	VAL	2.4
1	D	331	TYR	2.3
1	D	406	VAL	2.3
1	A	406	VAL	2.2
1	B	420	ALA	2.2
1	D	362	VAL	2.2
1	A	19	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	204	LEU	2.2
1	C	179	VAL	2.1
1	E	32	MET	2.1
1	C	162	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	ACP	C	525	31/31	0.95	0.20	-0.23	109,115,121,123	0
2	ACP	B	525	31/31	0.96	0.19	-0.35	100,113,120,121	0
2	ACP	A	525	31/31	0.93	0.20	-0.40	104,115,124,126	0
2	ACP	D	525	31/31	0.94	0.20	-0.52	96,110,118,118	0
2	ACP	E	525	31/31	0.92	0.20	-0.52	125,129,132,133	0
2	ACP	F	525	31/31	0.94	0.21	-0.62	88,95,106,108	0
3	MG	F	526	1/1	0.95	0.18	-	81,81,81,81	0
3	MG	A	526	1/1	0.92	0.16	-	106,106,106,106	0
3	MG	B	526	1/1	1.00	0.14	-	90,90,90,90	0
3	MG	D	526	1/1	0.99	0.15	-	100,100,100,100	0
3	MG	C	526	1/1	0.98	0.13	-	102,102,102,102	0
3	MG	E	526	1/1	0.99	0.12	-	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.