



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:37 AM UTC

PDB ID : 3U2Q / pdb_00003u2q
Title : EF-Tu (Escherichia coli) in complex with NVP-LFF571
Authors : Palestrant, D.J.
Deposited on : 2011-10-04
Resolution : 2.70 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

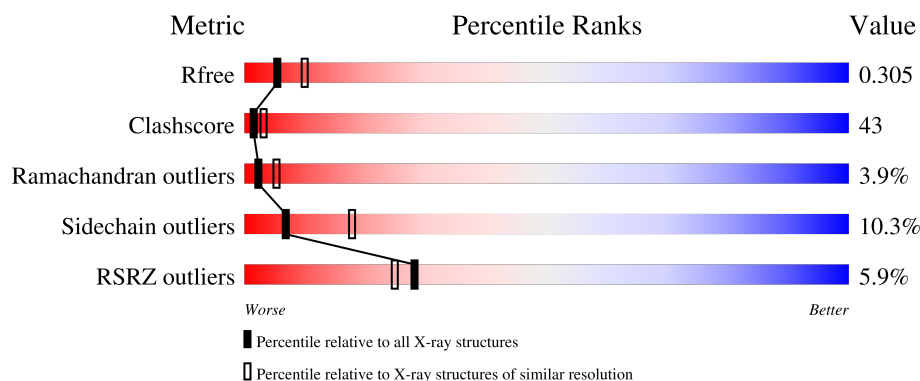
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

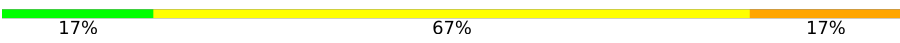
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	394	
2	B	12	

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	BB9	B	10	-	X	-	-
2	MH6	B	11	-	X	-	-
2	BB8	B	8	-	X	-	-
2	BB9	B	9	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3176 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 Elongation factor Tu 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2966	1874	510	569	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P0CE47
A	1	ALA	-	expression tag	UNP P0CE47

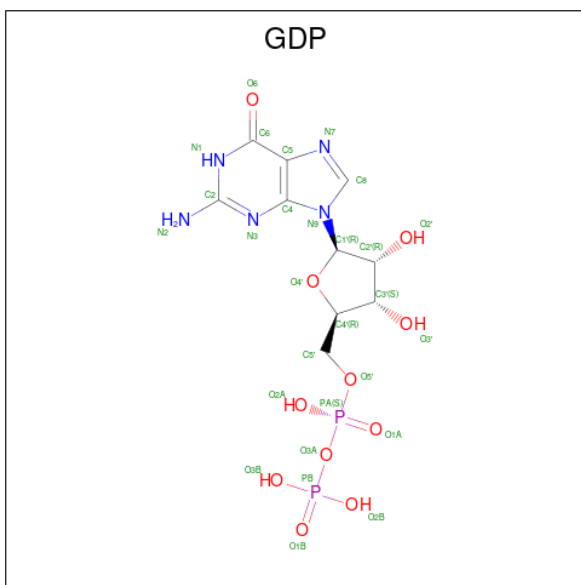
- Molecule 2 is a protein called Thiocillin GE2270 analogue NVP-LFF571.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	S	0	0	0
			92	60	13	13	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	7BB	CYS	SEE REMARK 999	UNP Q7M0J8

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

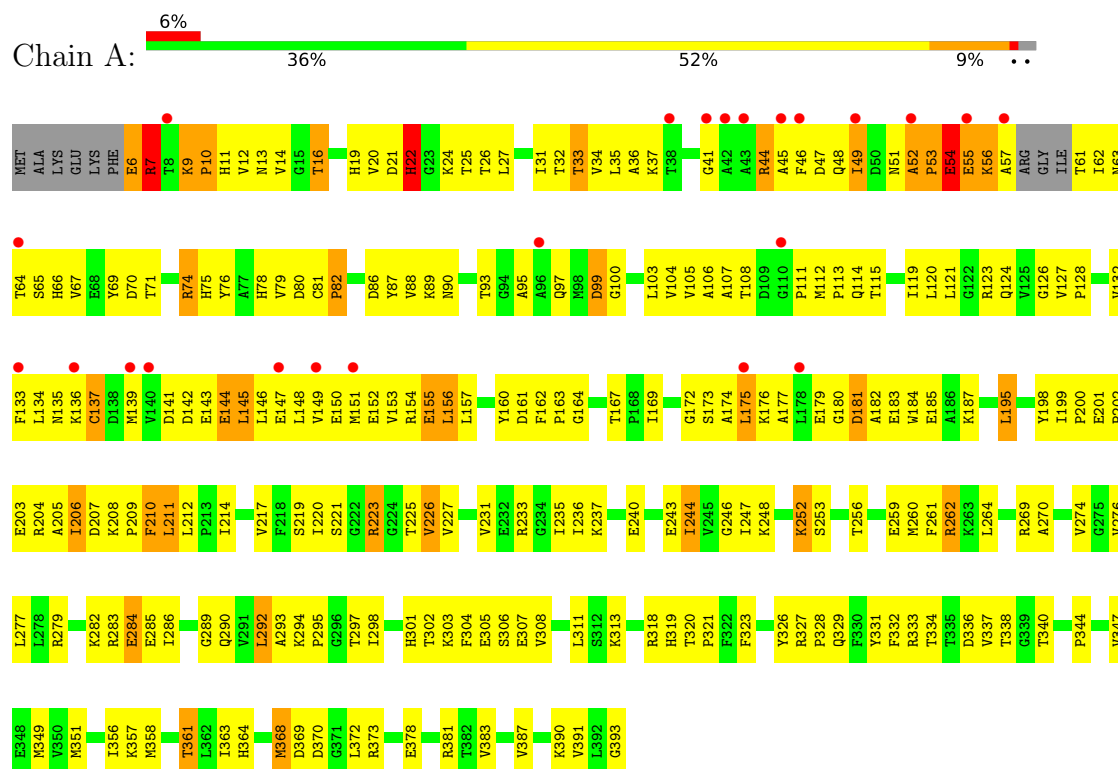
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	82	Total O 82 82	0	0
5	B	7	Total O 7 7	0	0

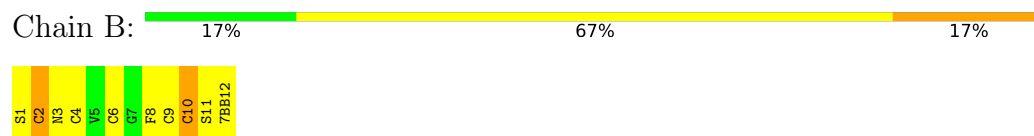
3 Residue-property plots

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

• Molecule 1: Elongation factor Tu 1



• Molecule 2: Thiocillin GE2270 analogue NVP-LFF571



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.30Å 132.47Å 37.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.02 – 2.70 39.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.02-2.70) 93.7 (39.02-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.69Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.233 , 0.315 0.229 , 0.305	Depositor DCC
R_{free} test set	584 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3176	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: BB7, BB8, MG, GDP, BB6, MH6, 7BB, MEN, BB9

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	0.47	0/3020	1.03	17/4089 (0.4%)
2	B	1.84	0/10	2.38	1/9 (11.1%)
All	All	0.48	0/3030	1.03	18/4098 (0.4%)

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
2	B	1	0

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ASP	N-CA-C	-7.08	104.12	112.89
1	A	49	ILE	N-CA-C	-6.79	106.62	113.47
1	A	210	PHE	N-CA-C	6.40	119.00	109.59
1	A	292	LEU	N-CA-C	-6.17	99.66	109.59
1	A	54	GLU	N-CA-C	5.73	123.01	110.80
1	A	274	VAL	N-CA-C	5.50	115.25	108.53
1	A	52	ALA	CA-C-N	5.44	126.64	119.84
1	A	52	ALA	C-N-CA	5.44	126.64	119.84
1	A	74	ARG	N-CA-C	5.43	117.44	109.24
1	A	269	ARG	N-CA-C	5.41	118.38	109.72
1	A	356	ILE	N-CA-C	5.32	116.69	108.44
1	A	71	THR	N-CA-C	-5.26	99.93	109.09
1	A	219	SER	N-CA-C	5.24	118.27	110.52
1	A	368	MET	N-CA-C	5.23	116.09	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ILE	N-CA-C	5.17	115.77	109.30
2	B	1	SER	CB-CA-C	5.16	119.91	110.10
1	A	22	HIS	N-CA-C	-5.10	107.06	113.28
1	A	195	LEU	N-CA-C	-5.06	105.66	111.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	SER	CA

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	2966	0	2973	264	0
2	B	92	0	62	1	0
3	A	28	0	12	6	0
4	A	1	0	0	0	0
5	A	82	0	0	11	0
5	B	7	0	0	0	0
All	All	3176	0	3047	265	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 43.

All (265) 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:55:GLU:HG2	1:A:61:THR:HA	1.24	1.11
1:A:52:ALA:HB1	1:A:63:ASN:HB3	1.23	1.10
1:A:119:ILE:HD12	1:A:156:LEU:HD12	1.41	0.99
1:A:44:ARG:HB3	1:A:49:ILE:HD11	1.51	0.93
1:A:202:PRO:HD3	5:A:446:HOH:O	1.69	0.92
1:A:208:LYS:HB2	1:A:233:ARG:HD2	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:HIS:CD2	1:A:106:ALA:H	1.89	0.90
1:A:112:MET:HB3	1:A:113:PRO:HD2	1.55	0.88
1:A:327:ARG:CD	1:A:340:THR:HG22	2.03	0.88
1:A:52:ALA:HB2	1:A:82:PRO:HG2	1.56	0.86
1:A:55:GLU:HG2	1:A:61:THR:CA	2.08	0.84
1:A:308:VAL:HG11	1:A:358:MET:HE2	1.59	0.83
1:A:112:MET:HE2	1:A:112:MET:HA	1.62	0.82
1:A:318:ARG:HD3	1:A:320:THR:O	1.83	0.79
1:A:55:GLU:CG	1:A:56:LYS:H	1.97	0.77
1:A:52:ALA:CB	1:A:63:ASN:HB3	2.12	0.77
1:A:327:ARG:HD2	1:A:340:THR:HG22	1.64	0.76
1:A:370:ASP:OD1	1:A:390:LYS:HA	1.86	0.74
1:A:303:LYS:HG2	1:A:361:THR:HG22	1.69	0.73
1:A:55:GLU:CD	1:A:56:LYS:H	1.97	0.72
1:A:243:GLU:HG2	1:A:252:LYS:HE3	1.71	0.72
1:A:62:ILE:HG21	1:A:90:ASN:ND2	2.03	0.72
1:A:88:VAL:HG22	1:A:121:LEU:HD11	1.72	0.71
1:A:22:HIS:HD2	1:A:105:VAL:HA	1.56	0.70
1:A:331:TYR:HA	1:A:336:ASP:HA	1.73	0.70
1:A:55:GLU:HG3	1:A:56:LYS:H	1.57	0.69
1:A:208:LYS:CB	1:A:233:ARG:HD2	2.22	0.69
1:A:303:LYS:HG2	1:A:361:THR:CG2	2.21	0.69
1:A:244:ILE:HD12	1:A:244:ILE:N	2.07	0.69
1:A:204:ARG:HD2	5:A:457:HOH:O	1.93	0.69
1:A:331:TYR:HD1	1:A:336:ASP:HB3	1.57	0.69
1:A:55:GLU:HG3	1:A:56:LYS:N	2.08	0.68
1:A:55:GLU:CG	1:A:56:LYS:N	2.58	0.67
1:A:151:MET:HE3	1:A:155:GLU:OE1	1.95	0.67
1:A:20:VAL:HG23	1:A:114:GLN:HE22	1.60	0.65
1:A:145:LEU:C	1:A:147:GLU:H	2.03	0.65
1:A:7:ARG:CB	1:A:7:ARG:HH11	2.09	0.65
1:A:135:ASN:CG	1:A:136:LYS:H	2.05	0.64
1:A:25:THR:HA	1:A:80:ASP:OD1	1.97	0.64
1:A:243:GLU:CG	1:A:252:LYS:HE3	2.27	0.64
1:A:327:ARG:HD3	1:A:340:THR:HG22	1.79	0.64
1:A:181:ASP:OD1	1:A:183:GLU:HB3	1.98	0.64
1:A:119:ILE:HD13	1:A:157:LEU:HD23	1.80	0.63
1:A:283:ARG:HD3	1:A:283:ARG:O	1.99	0.63
1:A:44:ARG:HD2	1:A:49:ILE:HG13	1.82	0.62
1:A:100:GLY:HA3	1:A:199:ILE:HD12	1.80	0.62
1:A:302:THR:HG23	1:A:303:LYS:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:O	1:A:154:ARG:HG2	2.00	0.62
1:A:201:GLU:HA	5:A:446:HOH:O	1.99	0.61
1:A:20:VAL:HG23	1:A:114:GLN:NE2	2.15	0.61
1:A:212:LEU:HB3	1:A:292:LEU:HB2	1.83	0.61
1:A:252:LYS:HE2	1:A:295:PRO:HB3	1.82	0.61
1:A:259:GLU:OE2	1:A:262:ARG:HA	2.00	0.61
1:A:52:ALA:HB2	1:A:82:PRO:CG	2.30	0.60
1:A:55:GLU:OE2	1:A:62:ILE:HB	2.01	0.60
1:A:203:GLU:HG2	1:A:207:ASP:HB2	1.84	0.60
1:A:31:ILE:O	1:A:35:LEU:HB2	2.01	0.60
1:A:107:ALA:HB1	1:A:146:LEU:CD2	2.31	0.60
1:A:112:MET:HB3	1:A:113:PRO:CD	2.30	0.59
1:A:261:PHE:O	1:A:262:ARG:HB2	2.01	0.59
1:A:373:ARG:HD2	1:A:387:VAL:HG23	1.84	0.59
1:A:44:ARG:HD3	1:A:45:ALA:H	1.66	0.59
1:A:99:ASP:O	1:A:128:PRO:HG2	2.02	0.59
1:A:52:ALA:CB	1:A:82:PRO:HG2	2.30	0.59
1:A:260:MET:HE3	1:A:261:PHE:CE2	2.37	0.59
1:A:150:GLU:HG2	1:A:169:ILE:HG21	1.85	0.59
1:A:111:PRO:HG2	1:A:152:GLU:HB3	1.85	0.59
1:A:137:CYS:HB2	1:A:172:GLY:O	2.02	0.59
1:A:145:LEU:C	1:A:145:LEU:HD13	2.29	0.58
1:A:160:TYR:O	1:A:161:ASP:HB2	2.04	0.58
1:A:226:VAL:HA	1:A:276:VAL:O	2.04	0.58
1:A:51:ASN:C	1:A:53:PRO:HD3	2.28	0.58
1:A:142:ASP:OD1	1:A:143:GLU:N	2.37	0.58
1:A:119:ILE:CD1	1:A:156:LEU:HD12	2.24	0.57
1:A:7:ARG:HD2	1:A:7:ARG:N	2.18	0.57
1:A:6:GLU:O	1:A:7:ARG:CB	2.53	0.57
1:A:136:LYS:HA	3:A:501:GDP:O6	2.05	0.57
1:A:107:ALA:HB1	1:A:146:LEU:HD21	1.86	0.57
1:A:198:TYR:O	1:A:200:PRO:HD3	2.04	0.57
1:A:67:VAL:HG23	1:A:78:HIS:HB3	1.87	0.56
1:A:136:LYS:HZ3	1:A:139:MET:HG3	1.69	0.56
1:A:225:THR:HG21	1:A:286:ILE:HD12	1.87	0.56
1:A:244:ILE:HG22	1:A:290:GLN:NE2	2.21	0.56
1:A:6:GLU:O	1:A:7:ARG:HB2	2.06	0.56
1:A:33:THR:HG22	1:A:34:VAL:N	2.20	0.56
1:A:329:GLN:HB3	1:A:336:ASP:HB2	1.87	0.56
1:A:243:GLU:CD	1:A:295:PRO:HA	2.31	0.55
1:A:51:ASN:O	1:A:53:PRO:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:HB1	1:A:63:ASN:CB	2.15	0.55
1:A:332:PHE:O	1:A:334:THR:N	2.39	0.55
1:A:7:ARG:HA	5:A:464:HOH:O	2.06	0.55
1:A:19:HIS:ND1	1:A:20:VAL:N	2.54	0.54
1:A:210:PHE:O	1:A:293:ALA:HA	2.08	0.54
1:A:119:ILE:HD12	1:A:156:LEU:CD1	2.26	0.54
1:A:145:LEU:C	1:A:147:GLU:N	2.63	0.54
1:A:64:THR:HG22	1:A:65:SER:N	2.23	0.54
1:A:227:VAL:CG1	1:A:286:ILE:HD13	2.38	0.54
1:A:26:THR:HG22	1:A:174:ALA:O	2.07	0.53
1:A:331:TYR:HE2	5:A:465:HOH:O	1.90	0.53
1:A:180:GLY:O	1:A:182:ALA:N	2.42	0.53
1:A:195:LEU:O	1:A:199:ILE:HB	2.08	0.53
1:A:344:PRO:HB2	1:A:347:VAL:HG21	1.89	0.53
1:A:173:SER:C	1:A:175:LEU:H	2.17	0.53
1:A:304:PHE:HE1	1:A:306:SER:HB3	1.74	0.53
1:A:323:PHE:O	1:A:326:TYR:HB2	2.09	0.53
1:A:74:ARG:HD2	1:A:76:TYR:OH	2.09	0.52
1:A:243:GLU:C	1:A:244:ILE:HD12	2.34	0.52
1:A:244:ILE:N	1:A:244:ILE:CD1	2.72	0.52
1:A:11:HIS:ND1	1:A:75:HIS:HD2	2.08	0.52
1:A:19:HIS:CD2	1:A:113:PRO:HG2	2.45	0.52
1:A:176:LYS:HE2	1:A:179:GLU:OE1	2.10	0.52
1:A:252:LYS:CE	1:A:295:PRO:HB3	2.38	0.52
1:A:176:LYS:HE2	1:A:176:LYS:HA	1.92	0.52
1:A:19:HIS:CD2	1:A:112:MET:HB3	2.44	0.52
1:A:162:PHE:O	1:A:164:GLY:N	2.42	0.52
1:A:19:HIS:HA	1:A:114:GLN:HB2	1.91	0.52
1:A:252:LYS:HE2	1:A:295:PRO:CG	2.39	0.52
1:A:237:LYS:HE3	5:A:467:HOH:O	2.10	0.51
1:A:63:ASN:O	1:A:82:PRO:HD2	2.10	0.51
1:A:135:ASN:CG	1:A:136:LYS:N	2.67	0.51
1:A:20:VAL:CG2	1:A:114:GLN:HE22	2.23	0.51
1:A:247:ILE:HD12	1:A:247:ILE:N	2.26	0.51
1:A:304:PHE:CE1	1:A:306:SER:HB3	2.44	0.51
1:A:259:GLU:HB2	1:A:264:LEU:HD23	1.92	0.51
1:A:55:GLU:CG	1:A:62:ILE:H	2.24	0.51
1:A:90:ASN:OD1	1:A:95:ALA:HB3	2.11	0.51
1:A:135:ASN:OD1	1:A:173:SER:HA	2.10	0.51
1:A:154:ARG:NH2	1:A:169:ILE:HG12	2.26	0.51
1:A:56:LYS:HG3	1:A:57:ALA:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:TYR:HB2	5:A:466:HOH:O	2.10	0.51
1:A:137:CYS:SG	1:A:146:LEU:HD13	2.51	0.51
1:A:332:PHE:HD2	1:A:372:LEU:HD21	1.76	0.51
1:A:157:LEU:HB3	1:A:162:PHE:HB2	1.92	0.50
1:A:320:THR:OG1	1:A:321:PRO:HD2	2.12	0.50
1:A:7:ARG:HH11	1:A:7:ARG:HA	1.77	0.50
1:A:231:VAL:HB	1:A:270:ALA:HA	1.94	0.50
1:A:203:GLU:HG2	1:A:207:ASP:CB	2.41	0.50
1:A:21:ASP:HA	3:A:501:GDP:PB	2.52	0.50
1:A:148:LEU:C	1:A:150:GLU:N	2.69	0.50
1:A:151:MET:O	1:A:151:MET:HG2	2.11	0.49
1:A:282:LYS:HD2	1:A:285:GLU:OE2	2.12	0.49
1:A:338:THR:O	1:A:363:ILE:HG23	2.12	0.49
1:A:126:GLY:O	1:A:127:VAL:C	2.55	0.49
1:A:331:TYR:CD1	1:A:336:ASP:HB3	2.41	0.49
1:A:27:LEU:O	1:A:31:ILE:HG13	2.13	0.49
1:A:21:ASP:HA	3:A:501:GDP:O3A	2.12	0.48
1:A:175:LEU:HD12	3:A:501:GDP:N3	2.28	0.48
1:A:123:ARG:HH21	1:A:160:TYR:HA	1.79	0.48
1:A:236:ILE:HG23	1:A:236:ILE:O	2.12	0.48
1:A:53:PRO:HD2	1:A:64:THR:O	2.13	0.48
1:A:252:LYS:HE2	1:A:295:PRO:CB	2.43	0.48
1:A:283:ARG:HD3	1:A:283:ARG:C	2.39	0.48
1:A:27:LEU:HD13	1:A:133:PHE:CE2	2.48	0.48
1:A:145:LEU:HD13	1:A:146:LEU:N	2.28	0.48
1:A:148:LEU:O	1:A:151:MET:N	2.46	0.48
1:A:7:ARG:HH11	1:A:7:ARG:CA	2.27	0.48
1:A:19:HIS:NE2	1:A:113:PRO:HG2	2.29	0.48
1:A:103:LEU:HD11	1:A:115:THR:HG23	1.96	0.48
1:A:284:GLU:HG2	1:A:284:GLU:O	2.14	0.48
1:A:344:PRO:HB2	1:A:347:VAL:CG2	2.44	0.48
1:A:64:THR:HG23	1:A:81:CYS:SG	2.53	0.47
1:A:177:ALA:HB1	1:A:185:GLU:HA	1.96	0.47
1:A:173:SER:OG	1:A:176:LYS:HG2	2.15	0.47
1:A:20:VAL:HG12	1:A:21:ASP:N	2.30	0.47
1:A:19:HIS:CD2	1:A:114:GLN:H	2.32	0.47
1:A:308:VAL:HG11	1:A:358:MET:CE	2.38	0.47
1:A:49:ILE:HG22	1:A:49:ILE:O	2.15	0.47
1:A:54:GLU:O	1:A:55:GLU:HB2	2.14	0.47
1:A:124:GLN:HE21	1:A:307:GLU:HG2	1.80	0.47
1:A:211:LEU:CD1	1:A:211:LEU:C	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:OE1	1:A:295:PRO:HA	2.16	0.46
1:A:259:GLU:OE2	1:A:262:ARG:HD2	2.15	0.46
1:A:16:THR:OG1	1:A:78:HIS:HE1	1.98	0.46
1:A:206:ILE:HG13	1:A:235:ILE:HD11	1.96	0.46
1:A:237:LYS:HB2	1:A:240:GLU:CD	2.41	0.46
1:A:124:GLN:HE21	1:A:307:GLU:CG	2.29	0.46
1:A:82:PRO:HA	5:A:405:HOH:O	2.14	0.46
1:A:176:LYS:CB	1:A:184:TRP:CD1	2.99	0.46
1:A:210:PHE:CZ	1:A:236:ILE:HB	2.51	0.46
1:A:187:LYS:HA	1:A:187:LYS:HD3	1.60	0.45
1:A:19:HIS:HE2	1:A:113:PRO:HG2	1.80	0.45
1:A:24:LYS:HB2	3:A:501:GDP:O2B	2.16	0.45
1:A:62:ILE:HD13	1:A:90:ASN:CG	2.42	0.45
1:A:100:GLY:HA3	1:A:199:ILE:CD1	2.45	0.45
1:A:332:PHE:CD2	1:A:372:LEU:HD21	2.52	0.45
1:A:12:VAL:HG22	5:A:446:HOH:O	2.17	0.45
1:A:22:HIS:N	3:A:501:GDP:O3B	2.48	0.45
1:A:44:ARG:HD2	1:A:49:ILE:CG1	2.46	0.45
1:A:112:MET:CB	1:A:113:PRO:HD2	2.37	0.45
2:B:2:BB9:N	2:B:10:BB9:N	2.65	0.45
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.81	0.45
1:A:67:VAL:CG2	1:A:78:HIS:HB3	2.47	0.45
1:A:256:THR:HG23	1:A:279:ARG:HB2	1.99	0.45
1:A:305:GLU:CD	1:A:357:LYS:HE3	2.42	0.45
1:A:173:SER:C	1:A:175:LEU:N	2.74	0.45
1:A:6:GLU:HB3	1:A:7:ARG:H	1.60	0.44
1:A:20:VAL:HG23	1:A:114:GLN:CD	2.43	0.44
1:A:53:PRO:O	1:A:54:GLU:O	2.35	0.44
1:A:47:ASP:OD1	1:A:48:GLN:HG2	2.17	0.44
1:A:134:LEU:HD22	1:A:150:GLU:HG3	1.99	0.44
1:A:33:THR:O	1:A:36:ALA:N	2.50	0.44
1:A:45:ALA:O	1:A:49:ILE:HG13	2.18	0.44
1:A:211:LEU:HD13	1:A:212:LEU:N	2.32	0.44
1:A:331:TYR:CE2	5:A:465:HOH:O	2.56	0.44
1:A:64:THR:HG22	1:A:65:SER:H	1.80	0.44
1:A:111:PRO:HG2	1:A:152:GLU:CB	2.46	0.44
1:A:149:VAL:O	1:A:153:VAL:HG23	2.18	0.44
1:A:311:LEU:HG	1:A:383:VAL:O	2.17	0.44
1:A:132:VAL:HG23	1:A:167:THR:CG2	2.48	0.44
1:A:246:GLY:O	1:A:248:LYS:N	2.48	0.44
1:A:108:THR:OG1	1:A:136:LYS:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD22	1:A:133:PHE:CD2	2.54	0.43
1:A:112:MET:HA	1:A:112:MET:CE	2.40	0.43
1:A:142:ASP:OD1	1:A:144:GLU:N	2.51	0.43
1:A:208:LYS:HB3	1:A:209:PRO:HD2	1.99	0.43
1:A:24:LYS:HG2	1:A:104:VAL:HB	2.01	0.43
1:A:176:LYS:HA	1:A:179:GLU:OE1	2.18	0.43
1:A:260:MET:HG2	1:A:261:PHE:CD2	2.54	0.43
1:A:294:LYS:HD2	1:A:297:THR:HG21	2.01	0.43
1:A:7:ARG:HH11	1:A:7:ARG:HB3	1.83	0.43
1:A:154:ARG:HD3	1:A:164:GLY:O	2.18	0.43
1:A:20:VAL:HG23	1:A:114:GLN:OE1	2.18	0.43
1:A:63:ASN:HB2	1:A:86:ASP:OD2	2.19	0.42
1:A:36:ALA:HB1	1:A:41:GLY:O	2.20	0.42
1:A:301:HIS:HD2	1:A:393:GLY:HA2	1.84	0.42
1:A:311:LEU:HG	1:A:383:VAL:C	2.45	0.42
1:A:108:THR:CG2	1:A:136:LYS:HD3	2.50	0.42
1:A:144:GLU:O	1:A:147:GLU:HB3	2.20	0.42
1:A:147:GLU:OE2	1:A:147:GLU:HA	2.19	0.42
1:A:206:ILE:CD1	1:A:235:ILE:HD11	2.49	0.42
1:A:363:ILE:HG13	1:A:364:HIS:CD2	2.54	0.42
1:A:6:GLU:O	1:A:7:ARG:CG	2.67	0.42
1:A:33:THR:O	1:A:34:VAL:C	2.63	0.42
1:A:89:LYS:O	1:A:93:THR:HG23	2.20	0.42
1:A:289:GLY:HA2	5:A:445:HOH:O	2.20	0.42
1:A:136:LYS:HG2	1:A:139:MET:HG3	2.02	0.42
1:A:321:PRO:HB3	1:A:351:MET:SD	2.60	0.41
1:A:337:VAL:HG12	1:A:338:THR:N	2.35	0.41
1:A:378:GLU:O	1:A:381:ARG:HB3	2.20	0.41
1:A:14:VAL:HG21	1:A:69:TYR:OH	2.20	0.41
1:A:20:VAL:CG1	1:A:21:ASP:N	2.83	0.41
1:A:32:THR:O	1:A:36:ALA:HB2	2.20	0.41
1:A:148:LEU:O	1:A:150:GLU:N	2.53	0.41
1:A:69:TYR:OH	1:A:78:HIS:HD2	2.04	0.41
1:A:69:TYR:CE1	1:A:76:TYR:HB2	2.56	0.41
1:A:252:LYS:O	1:A:253:SER:HB2	2.21	0.41
1:A:13:ASN:HB3	1:A:97:GLN:O	2.19	0.41
1:A:62:ILE:HG22	1:A:64:THR:OG1	2.21	0.41
1:A:176:LYS:HB2	1:A:184:TRP:CD1	2.55	0.41
1:A:206:ILE:HD11	1:A:235:ILE:HD11	2.02	0.41
1:A:220:ILE:HG22	1:A:223:ARG:HG2	2.02	0.41
1:A:262:ARG:HA	1:A:262:ARG:HD2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:HD11	1:A:368:MET:N	2.35	0.41
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.33	0.41
1:A:261:PHE:O	1:A:262:ARG:CB	2.68	0.41
1:A:313:LYS:HG2	1:A:319:HIS:HA	2.03	0.41
1:A:69:TYR:CD1	1:A:76:TYR:HB2	2.56	0.40
1:A:97:GLN:CA	1:A:97:GLN:HE21	2.35	0.40
1:A:124:GLN:NE2	1:A:307:GLU:HG2	2.37	0.40
1:A:294:LYS:HG2	1:A:297:THR:HG23	2.03	0.40
1:A:9:LYS:CB	1:A:10:PRO:CD	2.99	0.40
1:A:156:LEU:C	1:A:156:LEU:HD13	2.46	0.40
1:A:323:PHE:CD1	1:A:323:PHE:N	2.88	0.40
1:A:24:LYS:HE3	1:A:87:TYR:CE1	2.57	0.40
1:A:210:PHE:CE1	1:A:236:ILE:HB	2.56	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	381/394 (97%)	331 (87%)	35 (9%)	15 (4%)	2	5
2	B	2/12 (17%)	1 (50%)	1 (50%)	0	100	100
All	All	383/406 (94%)	332 (87%)	36 (9%)	15 (4%)	2	5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	54	GLU
1	A	56	LYS
1	A	53	PRO
1	A	55	GLU

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Mol	Chain	Res	Type
1	A	205	ALA
1	A	221	SER
1	A	333	ARG
1	A	33	THR
1	A	181	ASP
1	A	37	LYS
1	A	46	PHE
1	A	163	PRO
1	A	328	PRO
1	A	82	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	318/325 (98%)	285 (90%)	33 (10%)	7	17
2	B	1/2 (50%)	1 (100%)	0	100	100
All	All	319/327 (98%)	286 (90%)	33 (10%)	7	18

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	ARG
1	A	9	LYS
1	A	10	PRO
1	A	16	THR
1	A	22	HIS
1	A	44	ARG
1	A	54	GLU
1	A	66	HIS
1	A	70	ASP
1	A	79	VAL
1	A	120	LEU
1	A	137	CYS

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Mol	Chain	Res	Type
1	A	141	ASP
1	A	144	GLU
1	A	145	LEU
1	A	155	GLU
1	A	156	LEU
1	A	175	LEU
1	A	206	ILE
1	A	211	LEU
1	A	217	VAL
1	A	223	ARG
1	A	226	VAL
1	A	244	ILE
1	A	252	LYS
1	A	262	ARG
1	A	277	LEU
1	A	284	GLU
1	A	349	MET
1	A	361	THR
1	A	369	ASP
1	A	391	VAL

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	22	HIS
1	A	51	ASN
1	A	63	ASN
1	A	75	HIS
1	A	78	HIS
1	A	97	GLN
1	A	124	GLN
1	A	301	HIS
1	A	329	GLN
1	A	355	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	MEN	B	3	2	7,7,9	0.89	0	8,8,11	1.83	2 (25%)
2	7BB	B	12	2	22,24,24	2.04	9 (40%)	23,31,31	1.96	7 (30%)
2	MH6	B	11	2	3,3,6	2.83	3 (100%)	1,3,7	1.33	0
2	BB7	B	6	2	6,8,9	1.26	1 (16%)	4,9,11	1.72	1 (25%)
2	BB9	B	2	2	2,5,6	0.86	0	1,5,7	2.01	1 (100%)
2	BB9	B	9	2	2,4,6	2.66	2 (100%)	3,4,7	2.49	2 (66%)
2	BB6	B	4	2	4,6,7	3.03	2 (50%)	3,7,9	0.70	0
2	BB8	B	8	2	11,11,13	2.32	7 (63%)	12,14,17	0.90	0
2	BB9	B	10	2	2,4,6	1.47	1 (50%)	3,4,7	3.58	3 (100%)

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	MEN	B	3	2	-	0/6/6/10	-
2	7BB	B	12	2	-	3/19/35/35	0/1/1/1
2	BB7	B	6	2	-	0/1/9/11	-
2	BB9	B	2	2	-	0/0/4/6	-
2	BB9	B	9	2	-	0/0/2/6	-
2	BB6	B	4	2	-	0/0/6/8	-
2	BB8	B	8	2	-	7/8/8/12	0/1/1/1
2	BB9	B	10	2	-	0/0/2/6	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	BB6	C-CA	5.49	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	BB8	CD2-CG	3.99	1.45	1.39
2	B	12	7BB	O13-C60	3.87	1.34	1.22
2	B	12	7BB	C-N13	3.80	1.46	1.39
2	B	8	BB8	CD1-CG	3.67	1.44	1.39
2	B	11	MH6	CA-N	3.36	1.35	1.27
2	B	12	7BB	C52-C57	2.96	1.60	1.53
2	B	12	7BB	OXT-C	2.91	1.40	1.34
2	B	11	MH6	CB-CA	-2.78	1.45	1.49
2	B	9	BB9	C-CA	-2.77	1.41	1.49
2	B	12	7BB	O12-C60	-2.59	1.22	1.30
2	B	9	BB9	CA-N	2.54	1.39	1.33
2	B	12	7BB	C49-N13	2.52	1.53	1.47
2	B	8	BB8	CE2-CZ	2.46	1.43	1.38
2	B	4	BB6	CA-N	2.32	1.41	1.36
2	B	8	BB8	CB-CA	2.31	1.56	1.54
2	B	8	BB8	CE1-CD1	2.30	1.42	1.38
2	B	8	BB8	CZ-CE1	2.29	1.43	1.38
2	B	12	7BB	O-C	2.28	1.24	1.21
2	B	11	MH6	C-CA	-2.25	1.46	1.49
2	B	12	7BB	C56-C57	2.11	1.58	1.53
2	B	10	BB9	CA-N	2.05	1.38	1.33
2	B	6	BB7	C-CA	2.05	1.48	1.45
2	B	8	BB8	CE2-CD2	2.04	1.42	1.38
2	B	12	7BB	C53-C54	2.04	1.56	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	7BB	C54-OXT-C	4.72	127.18	117.12
2	B	10	BB9	C-CA-N	4.50	121.36	116.44
2	B	12	7BB	C53-C52-C57	3.83	117.92	111.18
2	B	3	MEN	C-CA-CB	-3.74	107.17	111.72
2	B	12	7BB	O12-C60-C59	3.68	125.63	114.00
2	B	12	7BB	O13-C60-C59	-3.48	112.05	123.09
2	B	10	BB9	CB-CA-N	-3.33	112.28	122.53
2	B	12	7BB	OXT-C54-C53	3.29	116.15	108.37
2	B	9	BB9	C-CA-CB	3.05	127.06	121.45
2	B	6	BB7	C-CA-N	3.00	123.03	116.15
2	B	10	BB9	C-CA-CB	2.65	126.34	121.45
2	B	9	BB9	CB-CA-N	-2.55	114.68	122.53
2	B	12	7BB	O-C-N13	2.53	129.25	123.76
2	B	3	MEN	CB-CG-ND2	2.49	118.78	115.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	7BB	C55-C56-C57	2.18	115.02	111.18
2	B	2	BB9	O-C-CA	-2.01	122.88	125.39

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	8	BB8	N-CA-CB-OB
2	B	8	BB8	C-CA-CB-CG
2	B	12	7BB	C53-C54-OXT-C
2	B	8	BB8	OB-CB-CG-CD2
2	B	8	BB8	OB-CB-CG-CD1
2	B	8	BB8	CA-CB-CG-CD2
2	B	8	BB8	CA-CB-CG-CD1
2	B	8	BB8	C-CA-CB-OB
2	B	12	7BB	C51-C59-C60-O12
2	B	12	7BB	C51-C59-C60-O13

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	BB9	1	0
2	B	10	BB9	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	GDP	A	501	4	29,30,30	1.82	4 (13%)	45,47,47	1.89	10 (22%)

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
3	GDP	A	501	4	-	6/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GDP	C4-N3	6.41	1.48	1.34
3	A	501	GDP	C5-N7	4.16	1.47	1.39
3	A	501	GDP	C4-N9	3.38	1.46	1.38
3	A	501	GDP	C8-N9	2.52	1.43	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GDP	C1'-N9-C4	-5.37	110.64	126.49
3	A	501	GDP	C5-C4-N3	-4.48	121.26	128.39
3	A	501	GDP	O4'-C1'-N9	3.93	117.27	108.36
3	A	501	GDP	C2-N3-C4	3.77	118.80	112.30
3	A	501	GDP	C2'-C1'-N9	-3.57	103.31	113.25
3	A	501	GDP	C8-N9-C4	-3.38	99.69	106.03
3	A	501	GDP	C5-C4-N9	3.30	111.56	105.66
3	A	501	GDP	O6-C6-C5	-2.75	119.28	126.53
3	A	501	GDP	O3B-PB-O3A	2.72	113.75	104.64
3	A	501	GDP	N1-C2-N3	-2.13	119.43	123.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GDP	PA-O3A-PB-O2B
3	A	501	GDP	C5'-O5'-PA-O1A
3	A	501	GDP	O4'-C4'-C5'-O5'
3	A	501	GDP	C3'-C4'-C5'-O5'
3	A	501	GDP	PA-O3A-PB-O3B

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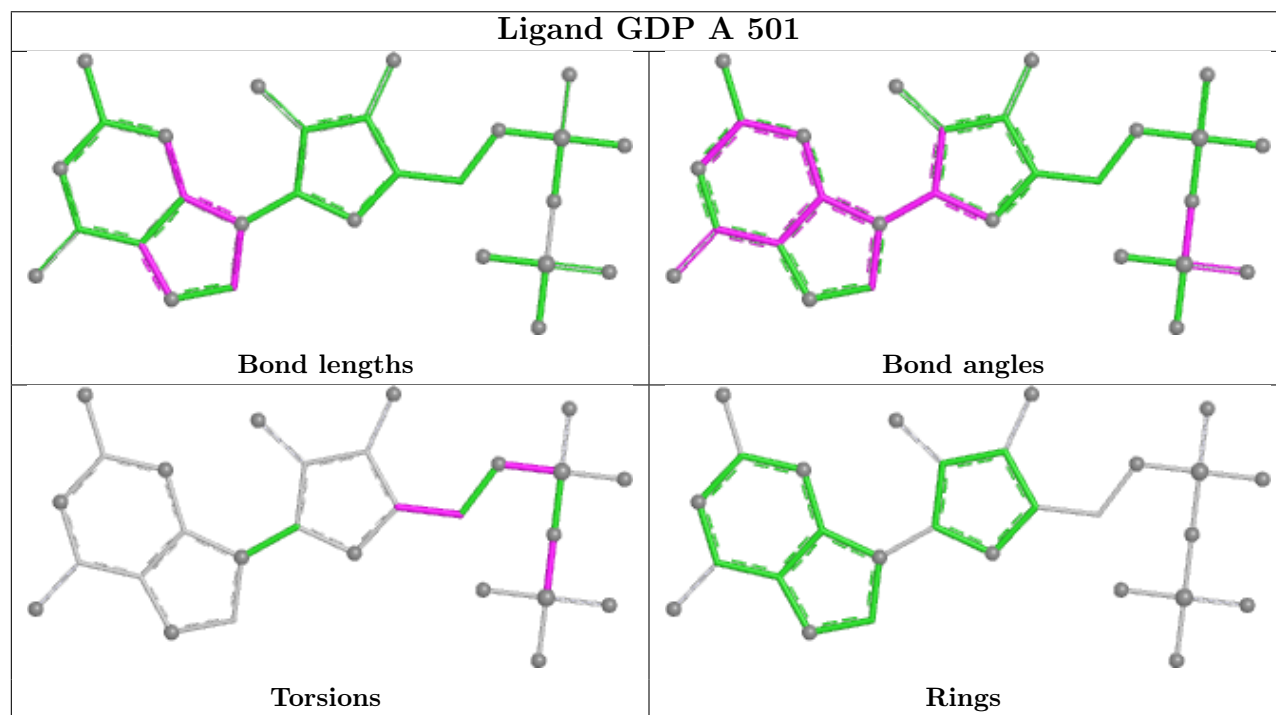
Mol	Chain	Res	Type	Atoms
3	A	501	GDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GDP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	385/394 (97%)	0.38	23 (5%) 27 24	11, 41, 85, 103	0
2	B	3/12 (25%)	0.09	0 100 100	27, 27, 34, 42	0
All	All	388/406 (95%)	0.38	23 (5%) 28 25	11, 41, 85, 103	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ALA	3.8
1	A	49	ILE	3.2
1	A	178	LEU	3.2
1	A	57	ALA	2.9
1	A	151	MET	2.8
1	A	43	ALA	2.8
1	A	55	GLU	2.8
1	A	38	THR	2.7
1	A	52	ALA	2.7
1	A	136	LYS	2.6
1	A	46	PHE	2.6
1	A	149	VAL	2.6
1	A	8	THR	2.5
1	A	147	GLU	2.4
1	A	139	MET	2.3
1	A	133	PHE	2.3
1	A	140	VAL	2.3
1	A	64	THR	2.2
1	A	110	GLY	2.2
1	A	175	LEU	2.2
1	A	41	GLY	2.2
1	A	45	ALA	2.1
1	A	96	ALA	2.0

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

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(Å ²)	Q<0.9
2	BB7	B	6	9/10	0.89	0.15	34,41,48,50	0
2	7BB	B	12	24/24	0.91	0.14	35,54,73,75	0
2	BB8	B	8	11/13	0.95	0.06	20,24,28,28	0
2	BB9	B	9	5/7	0.96	0.07	28,28,29,31	0
2	BB6	B	4	7/8	0.96	0.09	31,34,37,40	0
2	MH6	B	11	4/7	0.97	0.06	27,27,31,34	0
2	MEN	B	3	8/10	0.97	0.05	21,26,30,31	0
2	BB9	B	2	6/7	0.98	0.05	29,30,30,32	0
2	BB9	B	10	5/7	0.98	0.07	26,26,26,27	0

6.3 Carbohydrates ⓘ

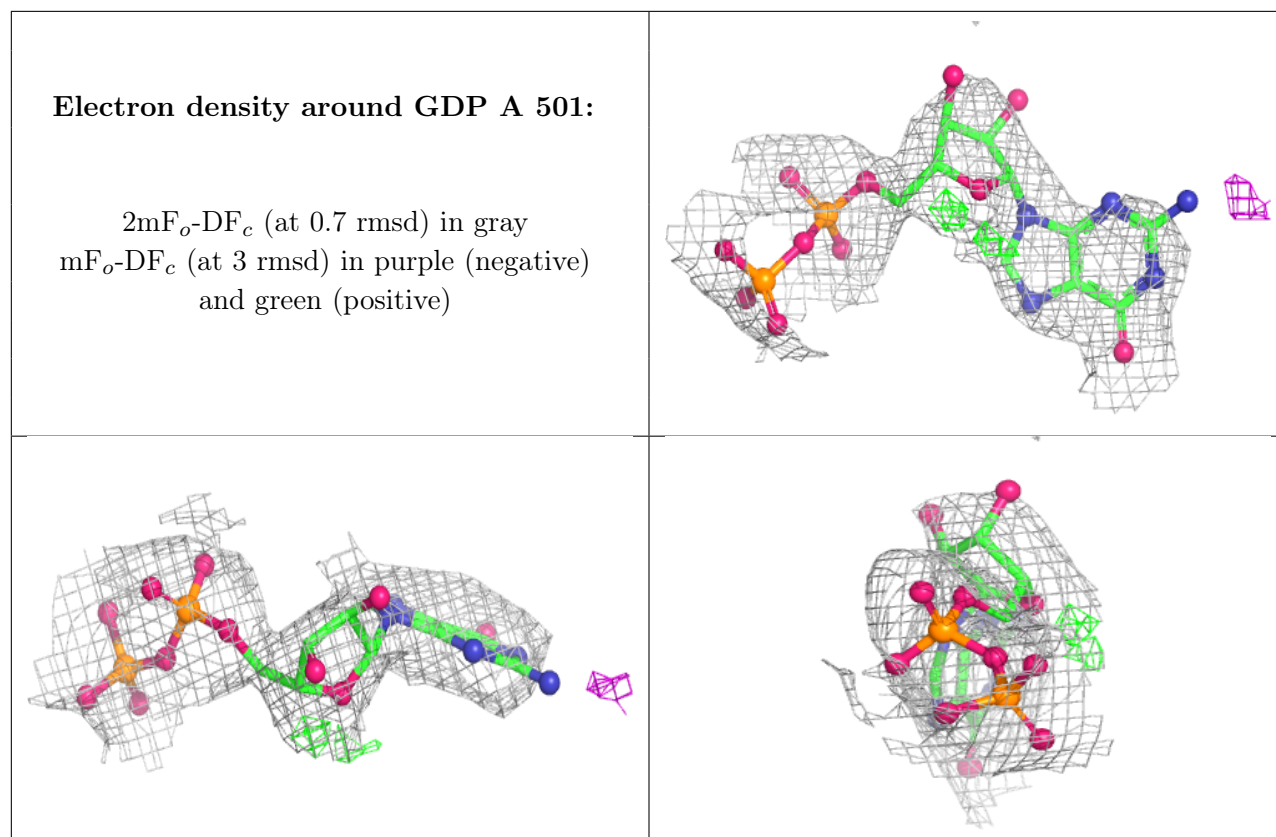
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
3	GDP	A	501	28/28	0.84	0.14	88,92,93,94	0
4	MG	A	503	1/1	0.95	0.13	42,42,42,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.