



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:19 pm BST

PDB ID : 5V68
Title : Crystal structure of cell division protein FtsZ from Mycobacterium tuberculosis bounded via the T9 loop
Authors : Lazo, E.O.; Ojima, I.; Chowdhury, S.R.; Awasthi, D.; Jakoncic, J.
Deposited on : 2017-03-16
Resolution : 3.46 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

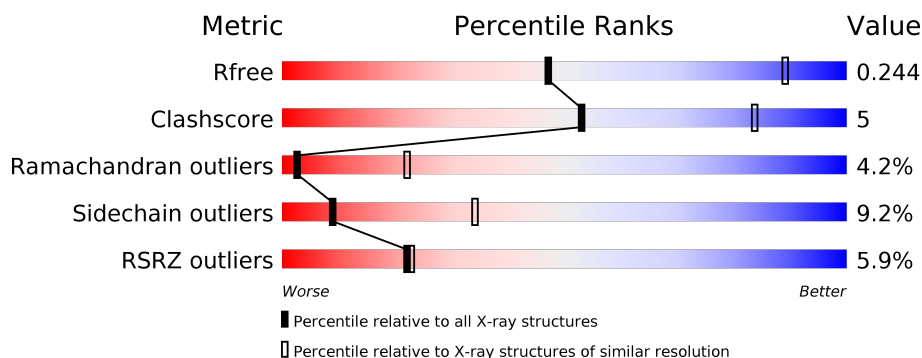
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 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	379	<div> <div>5%</div> <div> <div>55%</div> <div>12%</div> <div>•</div> <div>31%</div> </div> </div>
1	B	379	<div> <div>57%</div> <div>20%</div> <div>•</div> <div>21%</div> </div>
1	C	379	<div> <div>2%</div> <div> <div>63%</div> <div>14%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	379	<div> <div>8%</div> <div> <div>48%</div> <div>7%</div> <div>44%</div> </div> </div>
1	E	379	<div> <div>6%</div> <div> <div>61%</div> <div>16%</div> <div>•</div> <div>21%</div> </div> </div>
1	F	379	<div> <div>5%</div> <div> <div>63%</div> <div>15%</div> <div>•</div> <div>21%</div> </div> </div>

2 Entry composition [i](#)

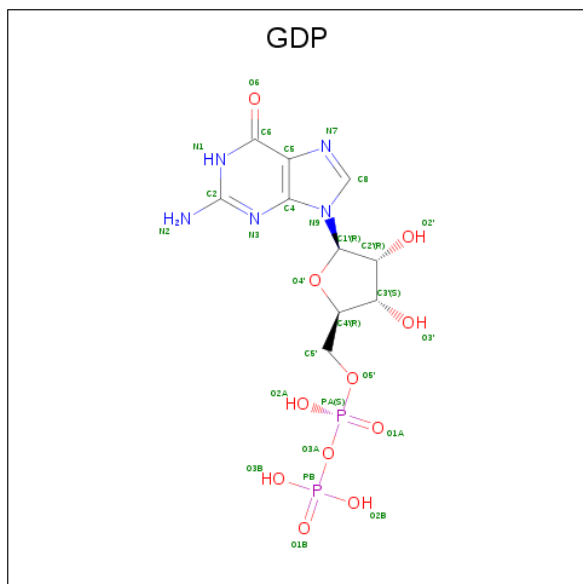
There are 3 unique types of molecules in this entry. The entry contains 11940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cell division protein FtsZ.

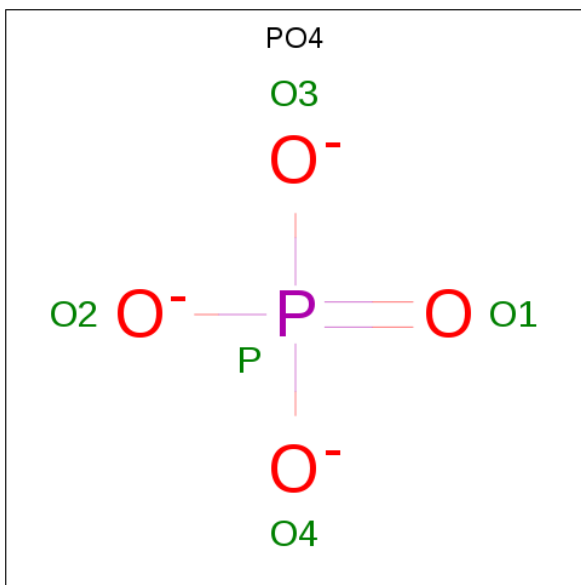
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1862	1143	325	385	9			
1	B	301	Total	C	N	O	S	0	0	0
			2142	1326	372	434	10			
1	C	297	Total	C	N	O	S	0	0	0
			2126	1320	371	426	9			
1	D	212	Total	C	N	O	S	0	0	0
			1485	912	262	303	8			
1	E	298	Total	C	N	O	S	0	0	0
			2121	1315	369	427	10			
1	F	300	Total	C	N	O	S	0	0	0
			2138	1324	373	432	9			

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

These plots are drawn for all protein, RNA and DNA 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.

- Chain A:
-
- | Amino Acid | Category |
|------------|----------|
| ASP | Red |
| VAL | Green |
| ASP | Green |
| VAL | Green |
| PRO | Green |
| PRO | Green |
| PHE | Green |
| MET | Green |
| ARG | Green |
| ARG | Green |
| VAL | Green |
| GLY | Green |
| ARG | Green |
| LYS | Green |
| PRO | Green |
| VAL | Green |
| MET | Green |
| GLY | Green |
| GLU | Green |
| THR | Green |
| GLY | Green |
| ALA | Green |
| HIS | Green |
| ARG | Green |
| ILE | Green |
| GLU | Green |
| SER | Green |
| ALA | Green |
| LYS | Green |
| ALA | Green |
| GLY | Green |
| LYS | Green |
| GLY | Green |
| VAL | Green |
| LEU | Green |
| THR | Green |
| SER | Green |
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| LEU | Green |
| PHE | Green |
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| PRO | Green |
| VAL | Green |
| ASP | Green |
| ALA | Green |
| VAL | Green |
| SER | Green |
| VAL | Green |
| PRO | Green |
| LEU | Green |
| LEU | Green |
| HIS | Green |
| THR | Green |
| ASN | Green |
| GLY | Green |
| ALA | Green |
| THR | Green |
| LEU | Green |
| ASP | Green |
| VAL | Green |
| G59 | Green |
| R60 | Green |
| D61 | Green |
| S62 | Green |
| THR | Green |
| ARG | Green |
| GLY | Green |
| LEU | Green |
| GLY | Green |
| ALA | Green |
| VAL | Green |
| LEU | Green |
| LYS | Green |
| ASP | Green |
| VAL | Green |
| D51 | Yellow |
| A52 | Yellow |
| D53 | Yellow |
| VAL | Yellow |
| LYS | Yellow |
| LEU | Yellow |
| ASP | Yellow |
| VAL | Yellow |
| G15 | Yellow |
| D156 | Yellow |
| T157 | Yellow |
| L158 | Yellow |
| I159 | Yellow |
| M163 | Yellow |
| Q168 | Yellow |
| M169 | Yellow |
| G170 | Yellow |
| D171 | Yellow |
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- Chain B:
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- 57% 20% 21%
- | Label | Value |
|-------|-------|
| MET | 1 |
| THR | 2 |
| PRO | 3 |
| PRO | 4 |
| HIS | 5 |
| ASN | 6 |
| TYR | 7 |
| L8 | 8 |
| I11 | 9 |
| K12 | 10 |
| V13 | 11 |
| V14 | 12 |
| G15 | 13 |
| I16 | 14 |
| G17 | 15 |
| V21 | 16 |
| R26 | 17 |
| Q30 | 18 |
| G31 | 19 |
| L32 | 20 |
| V35 | 21 |
| I38 | 22 |
| A39 | 23 |
| I40 | 24 |
| N41 | 25 |
| T42 | 26 |
| L47 | 27 |
| I48 | 28 |
| N49 | 29 |
| L56 | 30 |
| D57 | 31 |
| V58 | 32 |
| T63 | 33 |
| ARG | 34 |
| GLY | 35 |
| LEU | 36 |
| GLY | 37 |
| A68 | 38 |
| G69 | 39 |
| A70 | 40 |
| K83 | 41 |
| D84 | 42 |
| E85 | 43 |
| I86 | 44 |
| R91 | 45 |
| G92 | 46 |
| V93 | 47 |
| G105 | 48 |
| T106 | 49 |
| G107 | 50 |
| A111 | 51 |
| F112 | 52 |
| V113 | 53 |
| V114 | 54 |
| R119 | 55 |
| A123 | 56 |
| L124 | 57 |
| F135 | 58 |
| E136 | 59 |
| R140 | 60 |
| S141 | 61 |
| N142 | 62 |
| L151 | 63 |
| R152 | 64 |
| D156 | 65 |
| N163 | 66 |
| D164 | 67 |
| R165 | 68 |
| L166 | 69 |
| D171 | 70 |
| A172 | 71 |
| A173 | 72 |
| V174 | 73 |
| V186 | 74 |
| L187 | 75 |
| L188 | 76 |
| V191 | 77 |
| Q192 | 78 |
| G193 | 79 |
| I194 | 80 |
| L197 | 81 |
| I198 | 82 |
| T199 | 83 |
| T200 | 84 |
| G217 | 85 |
| L225 | 86 |
| A228 | 87 |
| R229 | 88 |
| G230 | 89 |
| E231 | 90 |
| G232 | 91 |
| R232 | 92 |
| A237 | 93 |
| ALA | 94 |
| GLY | 95 |
| LYS | 96 |
| LEU | 97 |
| P245 | 98 |
| E252 | 99 |
| S260 | 100 |
| T261 | 101 |
| G268 | 102 |
| L269 | 103 |
| I272 | 104 |
| S277 | 105 |
| L278 | 106 |
| V279 | 107 |
| Q280 | 108 |
| D281 | 109 |
| L289 | 110 |
| T290 | 111 |
| G291 | 112 |
| F292 | 113 |
| T293 | 114 |
| S298 | 115 |
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| G300 | 117 |
| V303 | 118 |
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THR	GLY	GLY	ALA	HIS	ARG	ILE	GLU	SER	ALA	LYS	LEU	THR	THR	LEU	PHE	GLU	PRO	VAL	ASP	ALA	VAL	SER	VAL	PRO	LEU	HIS	THR	ASN	GLY	ALA	THR	LEU	SER	ILE	GLY	GLY	ASP	ASP	ASP	VAL	VAL	PRO	PHE	MET	ARG
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● Molecule 1: Cell division protein FtsZ



ALA	LYS	ALA	GLY	LYS	LEU	THR	SER	THR	LEU	PHE	GLU	PRO	VAL	ASP	ALA	VAL	SER	VAL	PRO	LEU	HIS	THR	ASN	GLY	ALA	THR	LEU	SER	ILE	GLY	GLY	ASP	ASP	ASP	ASP	VAL	PRO	PRO	PHE	MET	ARG	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A228	E231	E237	A238	E248	A249	S250	M251	E252	G253	A254	V257	L258	M259	S260	T261	G264	S265	A275	L278	V279	F291	E302	V303	R304	V305	A309	D313	VAL	SER	GLY	PRO	GLY	ARG	LYS	PRO	VAL	MET	ARG	ILE	GLU	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.11Å 180.85Å 220.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.05 – 3.46 55.05 – 3.46	Depositor EDS
% Data completeness (in resolution range)	95.5 (55.05-3.46) 95.5 (55.05-3.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0151, PHENIX	Depositor
R, R_{free}	0.243 , 0.309 0.244 , 0.244	Depositor DCC
R_{free} test set	3704 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	110.7	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11940	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4669e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GDP, PO4

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	0.54	0/1872	0.70	0/2524
1	B	0.58	0/2157	0.81	2/2914 (0.1%)
1	C	0.53	0/2141	0.74	1/2891 (0.0%)
1	D	0.48	0/1491	0.64	0/2013
1	E	0.52	0/2136	0.75	0/2885
1	F	0.53	0/2153	0.74	0/2908
All	All	0.53	0/11950	0.74	3/16135 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	304	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	304	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	176	LEU	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	1862	0	1841	17	0
1	B	2142	0	2161	39	0
1	C	2126	0	2147	18	0
1	D	1485	0	1492	9	0
1	E	2121	0	2145	28	0
1	F	2138	0	2161	26	0
2	B	28	0	12	0	0
2	E	28	0	12	0	0
3	C	5	0	0	0	0
3	F	5	0	0	0	0
All	All	11940	0	11971	129	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 5.

All (129) 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:B:42:THR:HG23	1:B:106:THR:HG23	1.64	0.78
1:F:63:THR:HG21	1:F:66:LEU:HD12	1.69	0.73
1:E:14:VAL:HG22	1:E:38:ILE:HD11	1.70	0.71
1:F:131:ARG:NH1	1:F:145:GLU:OE2	2.25	0.69
1:F:38:ILE:HG22	1:F:54:VAL:HB	1.76	0.67
1:F:161:ILE:HG21	1:F:186:VAL:HG11	1.76	0.66
1:A:261:ILE:HD13	1:A:305:VAL:HG22	1.78	0.66
1:B:86:ILE:HD13	1:B:114:VAL:HG12	1.76	0.65
1:C:67:GLY:O	1:C:69:GLY:N	2.27	0.64
1:D:129:VAL:HG22	1:D:158:LEU:HD11	1.79	0.64
1:E:202:GLY:HA2	1:E:295:ILE:HD12	1.79	0.63
1:B:41:ASN:HB3	1:B:47:LEU:HD11	1.80	0.63
1:C:16:ILE:HG23	1:C:40:ILE:HB	1.82	0.62
1:F:54:VAL:HG11	1:F:89:LEU:HD21	1.82	0.62
1:A:269:LEU:HD21	1:B:135:PHE:CE2	2.34	0.62
1:C:47:LEU:HD22	1:C:55:LYS:HB2	1.81	0.61
1:C:14:VAL:HG21	1:C:114:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:HD13	1:C:96:VAL:HG11	1.83	0.59
1:F:129:VAL:HG21	1:F:148:ILE:HD11	1.84	0.58
1:B:42:THR:HG23	1:B:106:THR:CG2	2.34	0.57
1:E:11:ILE:HB	1:E:35:VAL:HG12	1.86	0.57
1:D:176:LEU:HD12	1:D:179:ALA:HB2	1.86	0.57
1:E:167:LEU:HD11	1:E:174:VAL:HG21	1.88	0.56
1:E:126:VAL:HG13	1:E:157:THR:HG23	1.87	0.56
1:A:174:VAL:HB	1:A:178:ASP:HB2	1.88	0.56
1:D:111:ALA:HB3	1:D:112:PRO:HD3	1.87	0.55
1:C:133:PHE:CE1	1:C:163:ASN:HB3	2.42	0.55
1:E:240:ILE:HG22	1:F:176:LEU:HG	1.86	0.55
1:F:214:ILE:HD11	1:F:257:VAL:N	2.22	0.55
1:A:128:VAL:HG21	1:A:191:VAL:HG22	1.89	0.55
1:A:129:VAL:HG11	1:A:158:LEU:HD21	1.89	0.53
1:C:202:GLY:HA2	1:C:295:ILE:HG13	1.89	0.53
1:E:32:LEU:HD11	1:E:195:THR:HG21	1.91	0.53
1:B:197:LEU:HD21	1:B:260:SER:CB	2.39	0.53
1:B:268:GLY:O	1:B:272:ILE:HG12	2.08	0.52
1:C:133:PHE:HB2	1:C:136:GLU:HG3	1.90	0.52
1:C:29:GLU:OE1	1:C:30:GLN:NE2	2.43	0.52
1:C:63:THR:OG1	1:C:66:LEU:HD13	2.10	0.52
1:B:21:VAL:HG23	1:B:39:ALA:HB1	1.91	0.51
1:F:163:ASN:HA	1:F:166:LEU:HD23	1.93	0.51
1:E:126:VAL:HA	1:E:157:THR:O	2.10	0.51
1:E:41:ASN:HB3	1:E:47:LEU:HD11	1.93	0.51
1:E:225:ILE:HG22	1:E:306:THR:HG23	1.90	0.51
1:E:197:LEU:HD11	1:E:260:SER:HB3	1.93	0.51
1:F:42:THR:HG22	1:F:58:VAL:HG23	1.93	0.51
1:E:198:ILE:HD11	1:E:211:VAL:HG11	1.92	0.50
1:C:86:ILE:HD13	1:C:114:VAL:HG22	1.93	0.50
1:E:231:GLU:OE1	1:F:136:GLU:OE1	2.29	0.49
1:B:163:ASN:O	1:B:164:ASP:C	2.50	0.49
1:B:56:LEU:HD21	1:B:85:GLU:HB3	1.94	0.49
1:E:257:VAL:HB	1:E:289:ILE:HG22	1.94	0.49
1:A:76:ARG:O	1:A:80:GLU:HB3	2.12	0.49
1:B:31:GLY:O	1:B:32:LEU:C	2.51	0.49
1:E:202:GLY:CA	1:E:295:ILE:HD12	2.42	0.49
1:F:161:ILE:HG21	1:F:186:VAL:CG1	2.43	0.49
1:E:42:THR:HG23	1:E:106:THR:HG23	1.94	0.48
1:A:47:LEU:HD12	1:A:48:LEU:N	2.28	0.48
1:B:194:ILE:HD11	1:B:308:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:GLN:HA	1:D:195:THR:HG22	1.96	0.48
1:A:214:ILE:HG23	1:A:258:LEU:HD11	1.96	0.48
1:A:279:VAL:HA	1:A:282:ALA:HB3	1.96	0.47
1:B:86:ILE:HD13	1:B:114:VAL:CG1	2.42	0.47
1:E:236:LYS:O	1:E:240:ILE:HG23	2.14	0.47
1:C:192:GLN:HA	1:C:195:THR:HB	1.96	0.47
1:B:269:LEU:HD13	1:C:65:GLY:O	2.15	0.47
1:F:104:GLY:N	1:F:108:THR:OG1	2.43	0.47
1:D:247:LEU:HD21	1:D:251:MET:HB2	1.96	0.46
1:E:259:MET:SD	1:E:276:ALA:HA	2.55	0.46
1:E:227:SER:O	1:E:240:ILE:HD11	2.15	0.46
1:F:158:LEU:HD23	1:F:159:ILE:N	2.30	0.46
1:B:156:ASP:N	1:B:156:ASP:OD2	2.49	0.46
1:B:26:ARG:NH2	1:B:30:GLN:OE1	2.48	0.46
1:F:98:VAL:HG21	1:F:115:ALA:HB2	1.98	0.46
1:B:191:VAL:O	1:B:192:GLN:C	2.54	0.46
1:F:14:VAL:O	1:F:99:THR:HG22	2.16	0.46
1:B:228:ALA:HB3	1:B:237:ALA:HB2	1.97	0.45
1:F:117:ILE:HG23	1:F:120:LYS:HE2	1.97	0.45
1:C:87:GLU:HG3	1:C:121:LEU:HD21	1.99	0.45
1:B:11:ILE:HD12	1:B:199:THR:CG2	2.47	0.45
1:B:277:SER:O	1:B:281:ASP:OD1	2.34	0.45
1:D:273:ASN:OD1	1:E:135:PHE:N	2.48	0.45
1:B:245:PRO:CG	1:C:174:VAL:HG13	2.47	0.44
1:B:13:VAL:HG23	1:B:35:VAL:HB	1.99	0.44
1:B:42:THR:HG22	1:B:58:VAL:O	2.17	0.44
1:B:68:ALA:O	1:B:70:ALA:N	2.51	0.44
1:A:124:LEU:HD11	1:A:216:SER:CB	2.48	0.44
1:B:197:LEU:HD21	1:B:260:SER:HB3	2.00	0.44
1:F:218:ALA:O	1:F:219:GLY:C	2.56	0.44
1:C:261:ILE:O	1:C:294:VAL:N	2.51	0.43
1:E:159:ILE:HG21	1:E:223:MET:HB3	2.00	0.43
1:A:128:VAL:HG21	1:A:191:VAL:CG2	2.48	0.43
1:E:23:ALA:O	1:E:26:ARG:N	2.50	0.43
1:D:269:LEU:HD23	1:E:135:PHE:CZ	2.54	0.43
1:B:113:VAL:O	1:B:114:VAL:C	2.57	0.43
1:B:98:VAL:HG11	1:B:114:VAL:HG23	2.00	0.43
1:F:70:ALA:O	1:F:72:PRO:HD3	2.19	0.43
1:A:198:ILE:HD11	1:A:211:VAL:HG21	1.99	0.43
1:A:200:THR:HB	1:E:48:LEU:HD13	2.01	0.43
1:B:14:VAL:HG22	1:B:38:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ALA:O	1:B:124:LEU:C	2.57	0.42
1:C:194:ILE:HD11	1:C:308:ILE:HG13	2.00	0.42
1:B:151:LEU:O	1:B:152:ARG:C	2.58	0.42
1:B:16:ILE:HG23	1:B:107:GLY:HA2	2.01	0.42
1:E:263:GLY:HA2	1:E:299:LEU:HD22	2.00	0.42
1:B:111:ALA:HB3	1:B:151:LEU:HD21	2.02	0.42
1:A:155:CYS:SG	1:A:156:ASP:N	2.93	0.41
1:B:194:ILE:CD1	1:B:308:ILE:HG13	2.50	0.41
1:F:128:VAL:HG22	1:F:159:ILE:HD12	2.02	0.41
1:B:21:VAL:HG23	1:B:39:ALA:CB	2.50	0.41
1:F:16:ILE:HG21	1:F:111:ALA:HA	2.03	0.41
1:E:264:GLY:HA2	1:E:297:ASP:HA	2.01	0.41
1:F:54:VAL:HG11	1:F:89:LEU:CD2	2.48	0.41
1:F:98:VAL:HG23	1:F:127:GLY:HA2	2.03	0.41
1:E:261:ILE:HD11	1:E:267:LEU:HD21	2.03	0.41
1:E:28:ILE:HD11	1:E:37:PHE:HB2	2.02	0.41
1:F:85:GLU:N	1:F:85:GLU:OE2	2.53	0.41
1:A:16:ILE:HG23	1:A:111:ALA:HA	2.03	0.41
1:A:241:ALA:HB1	1:A:307:VAL:HG23	2.01	0.41
1:B:197:LEU:HD21	1:B:260:SER:HB2	2.01	0.41
1:B:229:ARG:HA	1:B:233:ARG:HB2	2.02	0.41
1:A:251:MET:CE	1:A:307:VAL:HG11	2.51	0.41
1:B:21:VAL:CG2	1:B:39:ALA:HB1	2.50	0.41
1:D:155:CYS:SG	1:D:156:ASP:N	2.94	0.41
1:B:17:GLY:O	1:B:21:VAL:HG12	2.21	0.40
1:B:279:VAL:O	1:B:281:ASP:N	2.54	0.40
1:C:27:MET:HG2	1:C:188:LEU:HD13	2.03	0.40
1:F:128:VAL:HG21	1:F:191:VAL:HG22	2.03	0.40
1:D:198:ILE:HD11	1:D:211:VAL:HG21	2.03	0.40
1:F:166:LEU:HD12	1:F:182:SER:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/379 (66%)	185 (74%)	51 (20%)	15 (6%)	1	14
1	B	297/379 (78%)	231 (78%)	50 (17%)	16 (5%)	2	16
1	C	289/379 (76%)	234 (81%)	46 (16%)	9 (3%)	4	29
1	D	202/379 (53%)	170 (84%)	23 (11%)	9 (4%)	2	20
1	E	294/379 (78%)	242 (82%)	43 (15%)	9 (3%)	4	29
1	F	296/379 (78%)	241 (81%)	44 (15%)	11 (4%)	3	25
All	All	1629/2274 (72%)	1303 (80%)	257 (16%)	69 (4%)	3	22

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	VAL
1	C	68	ALA
1	E	267	LEU
1	F	52	ALA
1	A	16	ILE
1	A	105	GLY
1	A	108	THR
1	A	201	PRO
1	A	246	LEU
1	A	300	GLY
1	B	32	LEU
1	B	69	GLY
1	B	136	GLU
1	B	172	ALA
1	B	232	GLY
1	B	298	SER
1	B	300	GLY
1	C	278	LEU
1	C	287	ALA
1	D	23	ALA
1	D	144	ALA
1	E	282	ALA
1	F	31	GLY
1	F	64	ARG
1	F	219	GLY
1	F	249	ALA
1	A	23	ALA

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Mol	Chain	Res	Type
1	A	46	ALA
1	A	286	ASP
1	B	291	PHE
1	B	292	GLY
1	C	105	GLY
1	D	111	ALA
1	D	249	ALA
1	E	292	GLY
1	F	251	MET
1	B	252	GLU
1	C	282	ALA
1	D	19	GLY
1	D	143	GLN
1	E	260	SER
1	F	278	LEU
1	A	174	VAL
1	A	245	PRO
1	A	267	LEU
1	B	105	GLY
1	B	192	GLN
1	D	173	ALA
1	D	174	VAL
1	E	216	SER
1	E	264	GLY
1	F	202	GLY
1	F	309	ALA
1	A	136	GLU
1	A	233	ARG
1	B	92	GLY
1	B	217	GLY
1	E	162	PRO
1	F	62	SER
1	B	174	VAL
1	C	279	VAL
1	C	300	GLY
1	F	200	THR
1	C	311	GLY
1	C	253	GLY
1	E	245	PRO
1	D	103	GLY
1	E	31	GLY
1	B	98	VAL

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	190/281 (68%)	172 (90%)	18 (10%)	8	33
1	B	219/281 (78%)	192 (88%)	27 (12%)	4	22
1	C	218/281 (78%)	197 (90%)	21 (10%)	8	32
1	D	152/281 (54%)	147 (97%)	5 (3%)	38	68
1	E	216/281 (77%)	192 (89%)	24 (11%)	6	26
1	F	219/281 (78%)	202 (92%)	17 (8%)	12	41
All	All	1214/1686 (72%)	1102 (91%)	112 (9%)	9	34

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	51	ASP
1	A	61	ASP
1	A	62	SER
1	A	94	ASP
1	A	119	ARG
1	A	152	ARG
1	A	168	GLN
1	A	178	ASP
1	A	181	ARG
1	A	187	LEU
1	A	200	THR
1	A	208	PHE
1	A	231	GLU
1	A	246	LEU
1	A	247	LEU
1	A	260	SER
1	A	279	VAL
1	B	49	MET
1	B	58	VAL
1	B	83	LYS
1	B	84	ASP

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Mol	Chain	Res	Type
1	B	85	GLU
1	B	91	ARG
1	B	98	VAL
1	B	106	THR
1	B	119	ARG
1	B	136	GLU
1	B	140	ARG
1	B	142	ASN
1	B	152	ARG
1	B	156	ASP
1	B	166	LEU
1	B	171	ASP
1	B	186	VAL
1	B	188	LEU
1	B	200	THR
1	B	225	ILE
1	B	229	ARG
1	B	231	GLU
1	B	252	GLU
1	B	261	ILE
1	B	289	ILE
1	B	293	THR
1	B	303	VAL
1	C	16	ILE
1	C	29	GLU
1	C	30	GLN
1	C	35	VAL
1	C	55	LYS
1	C	60	ARG
1	C	77	LYS
1	C	94	ASP
1	C	102	GLU
1	C	176	LEU
1	C	180	PHE
1	C	182	SER
1	C	184	ASP
1	C	206	VAL
1	C	236	LYS
1	C	239	GLU
1	C	246	LEU
1	C	281	ASP
1	C	297	ASP

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Mol	Chain	Res	Type
1	C	299	LEU
1	C	301	ASP
1	D	25	ASN
1	D	167	LEU
1	D	191	VAL
1	D	252	GLU
1	D	286	ASP
1	E	22	ASN
1	E	43	ASP
1	E	45	GLN
1	E	49	MET
1	E	73	GLU
1	E	76	ARG
1	E	98	VAL
1	E	135	PHE
1	E	138	LYS
1	E	145	GLU
1	E	151	LEU
1	E	163	ASN
1	E	171	ASP
1	E	203	LEU
1	E	223	MET
1	E	231	GLU
1	E	233	ARG
1	E	244	SER
1	E	260	SER
1	E	261	ILE
1	E	266	ASP
1	E	270	PHE
1	E	290	ILE
1	E	295	ILE
1	F	74	VAL
1	F	76	ARG
1	F	81	ASP
1	F	95	MET
1	F	98	VAL
1	F	136	GLU
1	F	148	ILE
1	F	153	GLU
1	F	157	THR
1	F	200	THR
1	F	204	ILE

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Mol	Chain	Res	Type
1	F	231	GLU
1	F	248	GLU
1	F	252	GLU
1	F	260	SER
1	F	261	ILE
1	F	302	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	GLN
1	C	243	ASN
1	D	189	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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
3	PO4	F	401	-	4,4,4	0.50	0	6,6,6	0.99	0
2	GDP	B	401	-	24,30,30	1.10	2 (8%)	31,47,47	2.11	10 (32%)
2	GDP	E	401	-	24,30,30	1.10	2 (8%)	31,47,47	2.03	10 (32%)
3	PO4	C	401	-	4,4,4	0.49	0	6,6,6	0.98	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	GDP	B	401	-	-	5/12/32/32	0/3/3/3
2	GDP	E	401	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	GDP	C6-C5	3.72	1.47	1.41
2	E	401	GDP	C6-C5	3.38	1.47	1.41
2	E	401	GDP	C5-C4	2.32	1.47	1.40
2	B	401	GDP	C5-C4	2.26	1.46	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	GDP	C2-N3-C4	4.91	120.97	115.36
2	E	401	GDP	C2-N3-C4	4.69	120.71	115.36
2	B	401	GDP	C6-N1-C2	4.53	123.12	115.93
2	B	401	GDP	C5-C6-N1	-4.07	117.86	123.43
2	B	401	GDP	C6-C5-C4	-4.06	116.92	120.80
2	B	401	GDP	N3-C2-N1	-4.04	121.84	127.22
2	E	401	GDP	C6-N1-C2	3.92	122.15	115.93
2	E	401	GDP	C5-C6-N1	-3.80	118.24	123.43
2	E	401	GDP	C6-C5-C4	-3.77	117.19	120.80
2	E	401	GDP	N3-C2-N1	-3.68	122.32	127.22
2	B	401	GDP	PA-O3A-PB	-3.55	120.64	132.83
2	E	401	GDP	C3'-C2'-C1'	3.26	105.89	100.98
2	E	401	GDP	C1'-N9-C4	-2.73	121.84	126.64
2	B	401	GDP	C3'-C2'-C1'	2.45	104.67	100.98
2	B	401	GDP	O5'-C5'-C4'	2.39	117.22	108.99
2	B	401	GDP	C4-C5-N7	-2.39	106.91	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	GDP	C4-C5-N7	-2.36	106.94	109.40
2	E	401	GDP	N2-C2-N1	2.05	120.44	117.25
2	E	401	GDP	PA-O3A-PB	-2.03	125.84	132.83
2	B	401	GDP	C1'-N9-C4	-2.00	123.12	126.64

There are no chirality outliers.

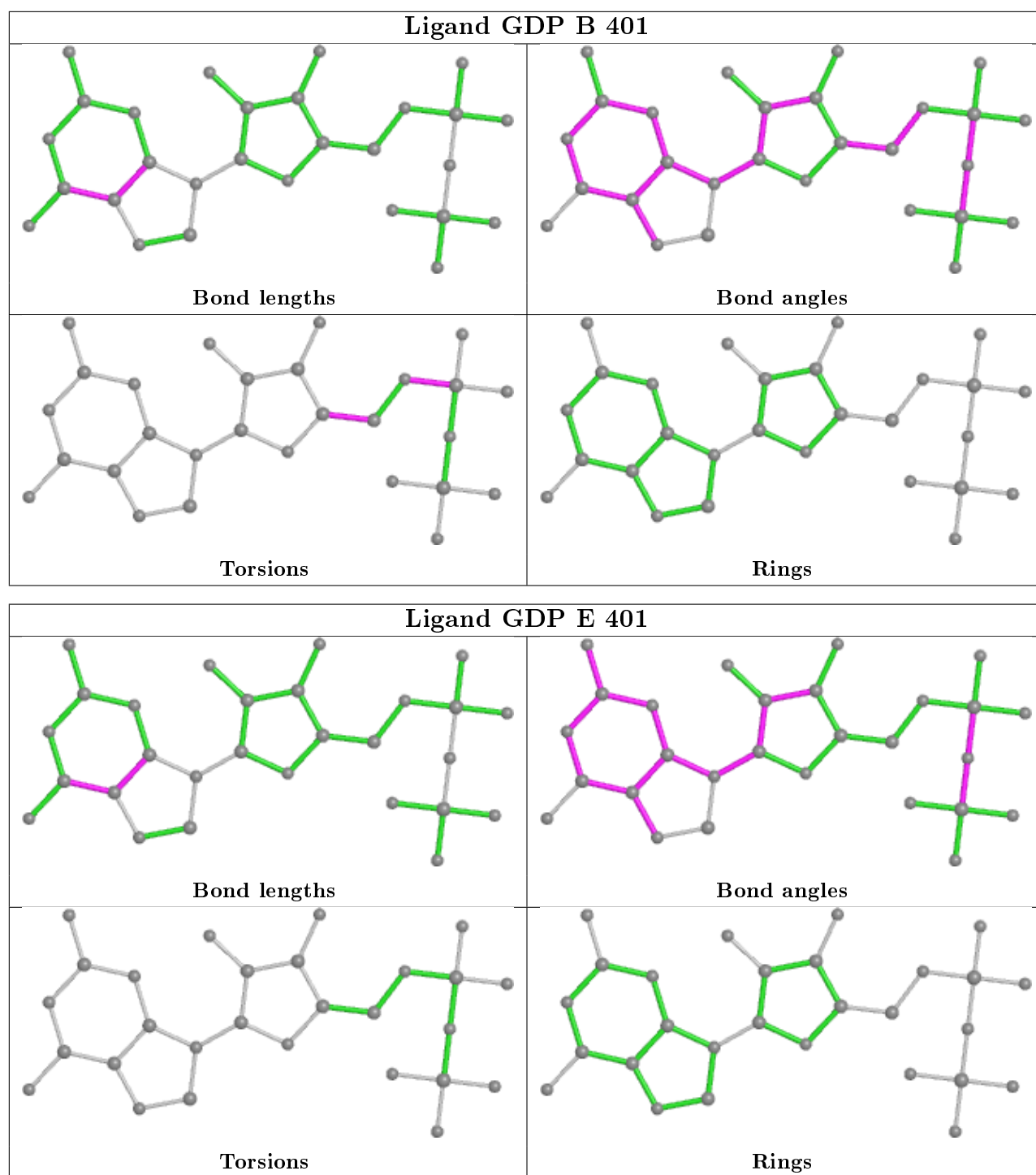
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GDP	C5'-O5'-PA-O1A
2	B	401	GDP	O4'-C4'-C5'-O5'
2	B	401	GDP	C5'-O5'-PA-O2A
2	B	401	GDP	C3'-C4'-C5'-O5'
2	B	401	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	263/379 (69%)	0.50	19 (7%) 15 17	82, 148, 202, 225	0
1	B	301/379 (79%)	-0.04	1 (0%) 94 92	49, 83, 131, 196	0
1	C	297/379 (78%)	0.07	8 (2%) 54 52	52, 109, 175, 215	0
1	D	212/379 (55%)	0.71	29 (13%) 3 4	98, 161, 201, 245	0
1	E	298/379 (78%)	0.40	22 (7%) 14 17	52, 112, 156, 234	0
1	F	300/379 (79%)	0.31	19 (6%) 20 20	56, 106, 176, 211	0
All	All	1671/2274 (73%)	0.30	98 (5%) 22 23	49, 116, 188, 245	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	PHE	6.4
1	D	220	THR	6.2
1	A	97	PHE	5.7
1	E	41	ASN	5.2
1	A	171	ASP	5.0
1	D	223	MET	4.8
1	E	98	VAL	4.7
1	C	227	SER	4.6
1	A	126	VAL	4.4
1	D	251	MET	4.3
1	D	257	VAL	4.2
1	E	40	ILE	4.0
1	E	75	GLY	3.8
1	E	90	LEU	3.7
1	D	221	ALA	3.7
1	E	93	ALA	3.6
1	A	133	PHE	3.5
1	A	100	ALA	3.5
1	F	226	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	203	LEU	3.4
1	D	234	SER	3.3
1	A	155	CYS	3.3
1	D	168	GLN	3.2
1	E	92	GLY	3.2
1	F	264	GLY	3.2
1	D	159	ILE	3.1
1	A	99	THR	3.1
1	D	171	ASP	3.1
1	F	227	SER	3.1
1	F	275	ALA	3.1
1	F	208	PHE	3.0
1	D	224	GLY	3.0
1	F	206	VAL	3.0
1	D	170	GLY	3.0
1	D	132	PRO	3.0
1	E	103	GLY	2.9
1	D	208	PHE	2.9
1	D	169	MET	2.9
1	E	121	LEU	2.9
1	E	68	ALA	2.9
1	E	86	ILE	2.8
1	E	39	ALA	2.8
1	D	127	GLY	2.7
1	F	279	VAL	2.7
1	C	295	ILE	2.7
1	F	305	VAL	2.7
1	D	289	ILE	2.7
1	A	78	ALA	2.7
1	E	56	LEU	2.6
1	D	215	MET	2.6
1	F	254	ALA	2.6
1	F	291	PHE	2.6
1	B	114	VAL	2.6
1	D	256	GLY	2.5
1	A	234	SER	2.5
1	F	228	ALA	2.4
1	E	194	ILE	2.4
1	E	54	VAL	2.4
1	E	122	GLY	2.4
1	E	79	ALA	2.3
1	A	51	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	238	ALA	2.3
1	D	190	GLY	2.3
1	D	193	GLY	2.3
1	D	309	ALA	2.3
1	E	218	ALA	2.3
1	A	223	MET	2.3
1	A	159	ILE	2.3
1	A	163	ASN	2.3
1	E	99	THR	2.3
1	E	38	ILE	2.3
1	F	67	GLY	2.2
1	A	291	PHE	2.2
1	C	297	ASP	2.2
1	D	263	GLY	2.2
1	F	265	SER	2.2
1	C	296	ASP	2.2
1	A	170	GLY	2.2
1	F	203	LEU	2.2
1	C	6	ASN	2.2
1	D	300	GLY	2.2
1	F	237	ALA	2.1
1	D	225	ILE	2.1
1	D	259	MET	2.1
1	A	259	MET	2.1
1	F	259	MET	2.1
1	F	251	MET	2.1
1	E	124	LEU	2.1
1	A	190	GLY	2.1
1	D	105	GLY	2.1
1	D	299	LEU	2.1
1	E	102	GLU	2.1
1	D	177	MET	2.1
1	D	298	SER	2.1
1	C	195	THR	2.0
1	F	304	ARG	2.0
1	A	53	ASP	2.0
1	C	303	VAL	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](#)

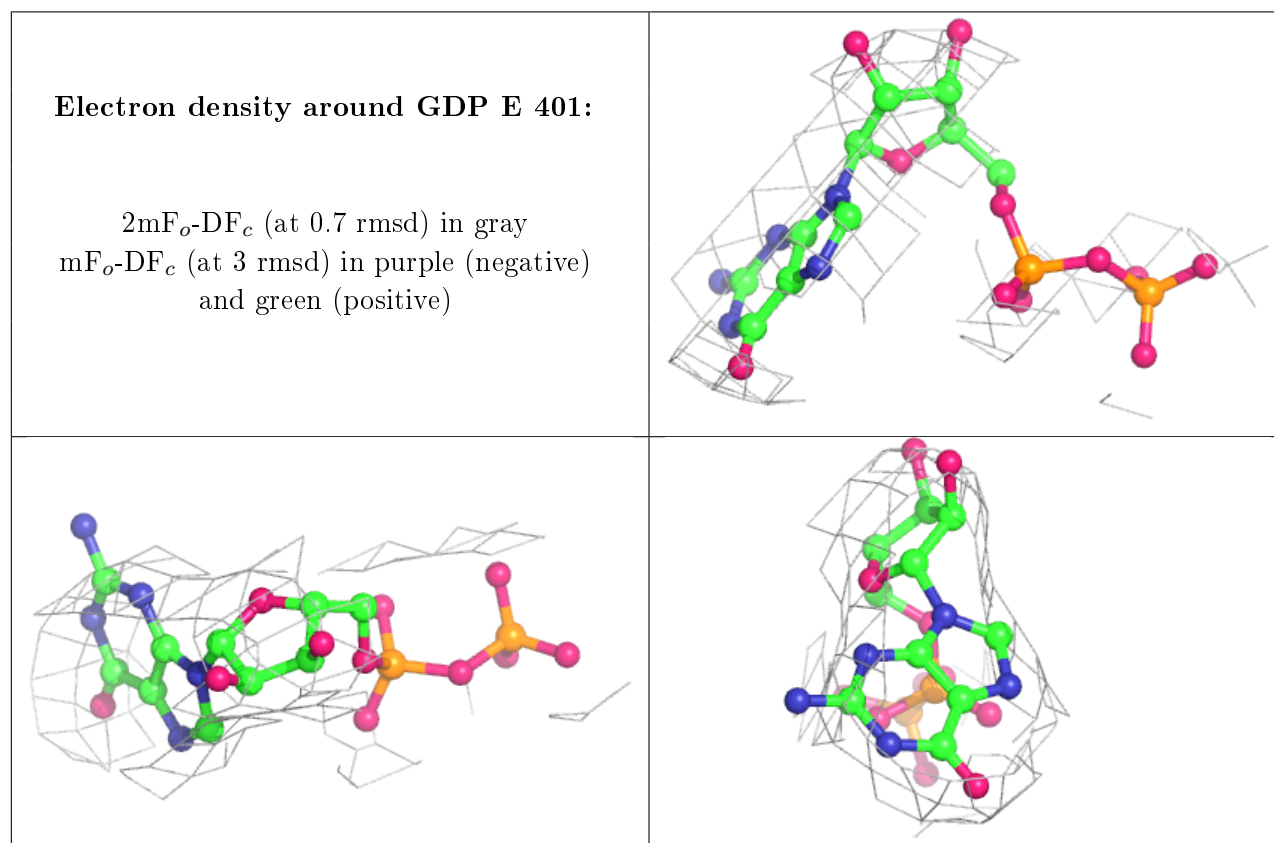
There are no carbohydrates in this entry.

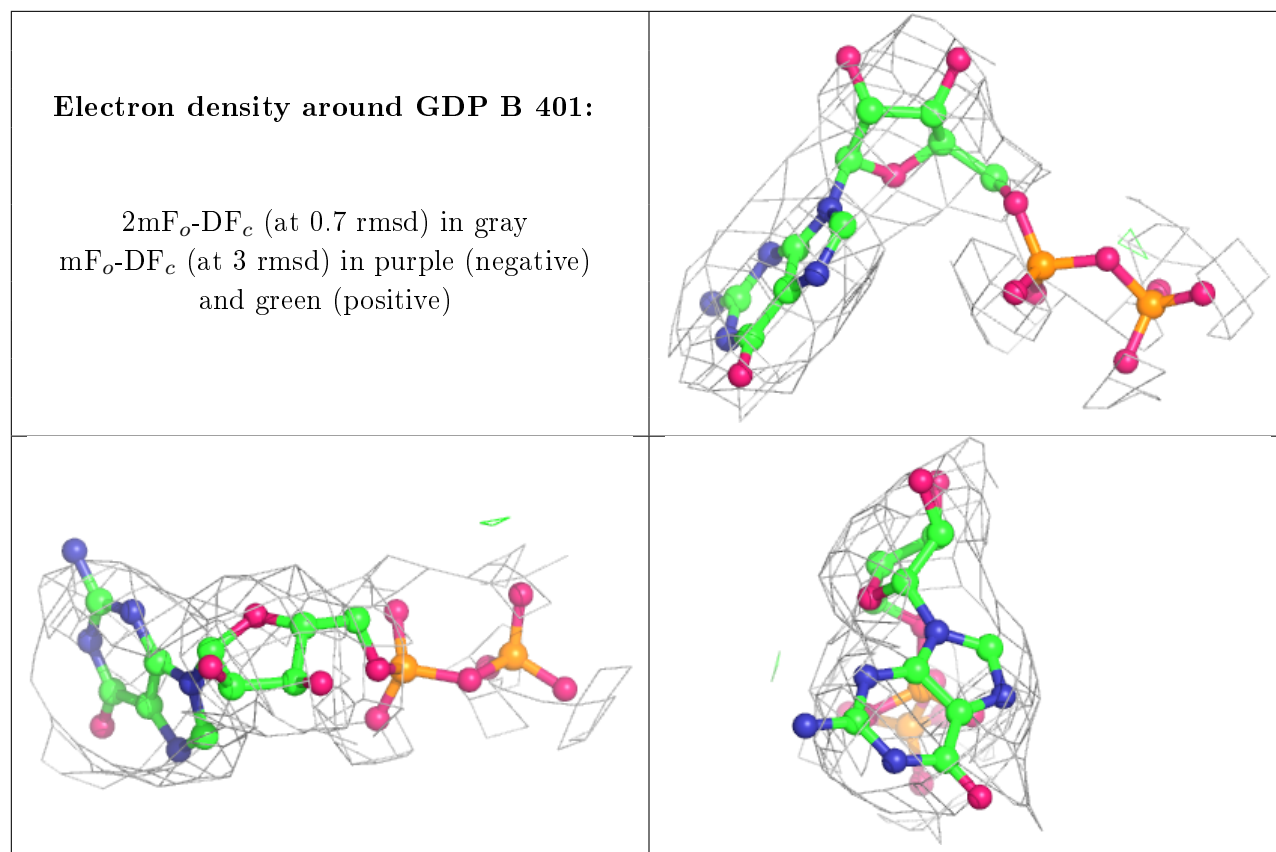
6.4 Ligands [i](#)

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. 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
3	PO4	F	401	5/5	0.90	0.43	88,96,105,106	0
3	PO4	C	401	5/5	0.91	0.42	98,99,112,119	0
2	GDP	E	401	28/28	0.92	0.18	103,142,159,166	0
2	GDP	B	401	28/28	0.94	0.20	79,101,108,112	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.