



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2021 – 10:04 AM EDT

PDB ID : 7RK0
Title : Crystal structure of Thermovibrio ammonificans THI4
Authors : Li, Q.; Bruner, S.D.
Deposited on : 2021-07-21
Resolution : 2.28 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 : 2.23.1
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) : 2.23.1

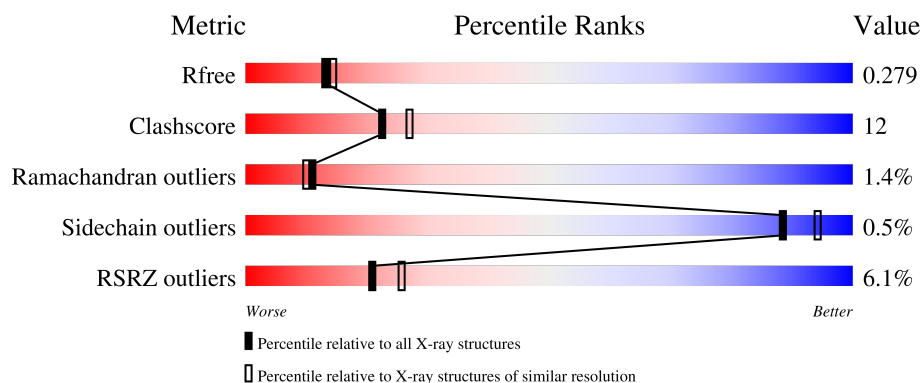
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	268	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	268	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	C	268	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>..</div> </div> </div>
1	D	268	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8029 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.

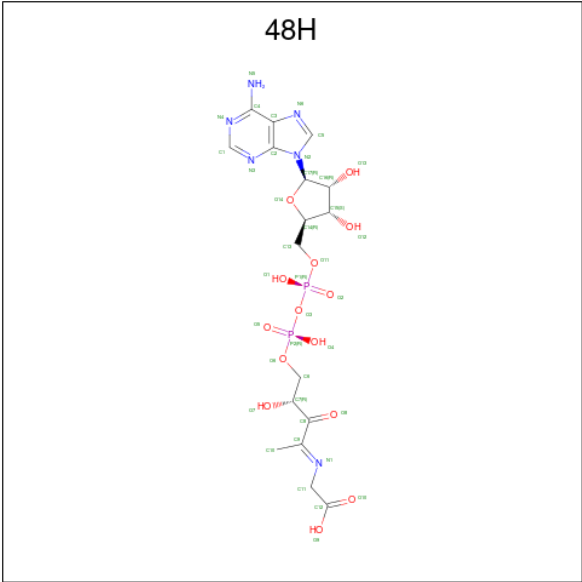
- Molecule 1 is a protein called Thiamine thiazole synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1958	1248	328	370	12			
1	B	262	Total	C	N	O	S	0	0	0
			1967	1253	330	372	12			
1	C	258	Total	C	N	O	S	0	0	0
			1943	1240	327	365	11			
1	D	262	Total	C	N	O	S	0	0	0
			1967	1253	330	372	12			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-[(E)-[(4R)-5-[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-4-oxidanyl-3-oxidanylidene-pentan-2-ylidene]amino]ethanoic acid (three-letter code: 48H) (formula: C₁₇H₂₄N₆O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
3	B	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
3	C	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
3	D	1	Total	C	N	O	P	0	0
			39	17	6	14	2		

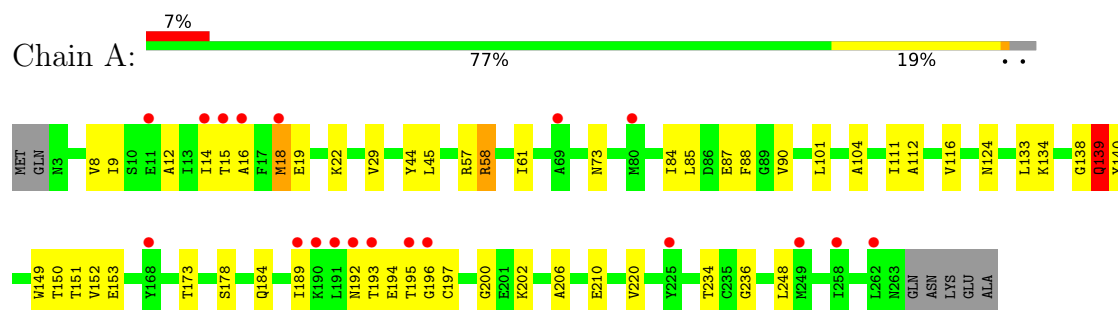
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	11	Total	O	0	0
			11	11		
4	C	9	Total	O	0	0
			9	9		
4	D	3	Total	O	0	0
			3	3		

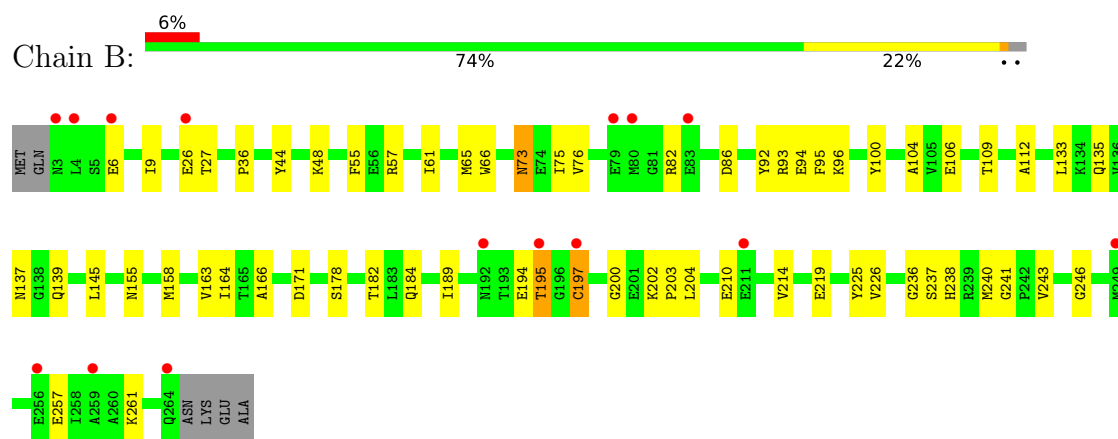
3 Residue-property plots [i](#)

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

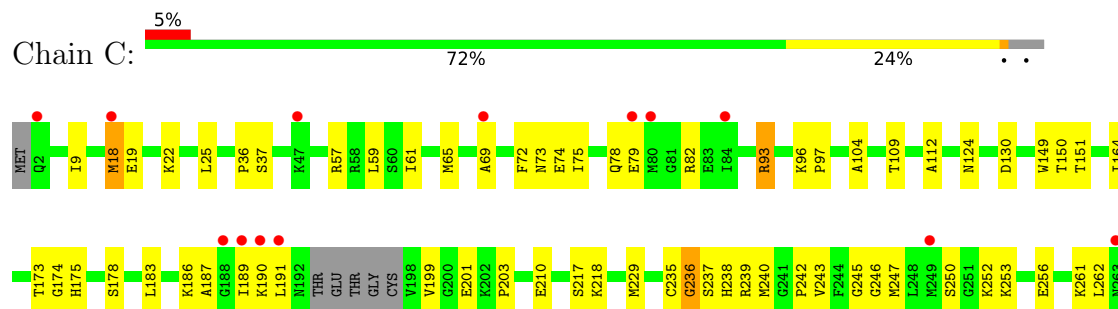
• Molecule 1: Thiamine thiazole synthase



• Molecule 1: Thiamine thiazole synthase



• Molecule 1: Thiamine thiazole synthase





● Molecule 1: Thiamine thiazole synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.89Å 89.69Å 131.81Å 90.00° 96.98° 90.00°	Depositor
Resolution (Å)	44.84 – 2.28 44.84 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.84-2.28) 99.5 (44.84-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.277 0.219 , 0.279	Depositor DCC
R_{free} test set	2514 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8029	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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: 48H, FE

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	0.48	1/1991 (0.1%)	0.78	7/2694 (0.3%)
1	B	0.46	0/2000	0.68	0/2706
1	C	0.52	1/1975 (0.1%)	0.74	3/2670 (0.1%)
1	D	0.48	0/2000	0.68	2/2706 (0.1%)
All	All	0.49	2/7966 (0.0%)	0.72	12/10776 (0.1%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	ARG	CZ-NH2	6.84	1.42	1.33
1	A	139	GLN	CD-NE2	6.03	1.48	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	MET	CB-CG-SD	8.79	138.77	112.40
1	C	93	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	4	LEU	CB-CG-CD1	-7.47	98.30	111.00
1	A	133	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	18	MET	CA-CB-CG	-6.53	102.20	113.30
1	A	139	GLN	N-CA-CB	6.46	122.23	110.60
1	A	139	GLN	CA-CB-CG	6.29	127.23	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	GLN	CB-CA-C	-6.23	97.95	110.40
1	C	18	MET	CA-CB-CG	-6.06	103.00	113.30
1	A	58	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	154	LEU	CA-CB-CG	5.06	126.93	115.30
1	C	93	ARG	CD-NE-CZ	-5.05	116.52	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLN	Sidechain

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	1958	0	1980	49	1
1	B	1967	0	1988	53	0
1	C	1943	0	1967	58	1
1	D	1967	0	1988	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	39	0	0	1	0
3	B	39	0	0	1	0
3	C	39	0	0	3	0
3	D	39	0	0	1	0
4	A	11	0	0	0	0
4	B	11	0	0	3	1
4	C	9	0	0	5	0
4	D	3	0	0	0	0
All	All	8029	0	7923	185	3

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 12.

All (185) 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)
3:C:302:48H:C17	3:C:302:48H:O14	1.65	1.26
3:B:302:48H:O14	3:B:302:48H:C17	1.64	1.19
3:A:302:48H:C17	3:A:302:48H:O14	1.65	1.16
1:A:58:ARG:NH2	1:B:158:MET:SD	2.22	1.12
3:D:302:48H:C17	3:D:302:48H:O14	1.66	1.12
1:B:6:GLU:HB2	1:D:163:VAL:HG11	1.56	0.85
1:A:193:THR:OG1	1:A:195:THR:O	2.00	0.80
1:A:12:ALA:HB1	1:D:101:LEU:HD11	1.63	0.79
1:C:173:THR:HG21	1:C:178:SER:HB2	1.65	0.79
1:A:139:GLN:HE21	1:A:139:GLN:HA	1.49	0.77
1:B:82:ARG:NH1	1:B:86:ASP:OD1	2.18	0.77
1:A:184:GLN:NE2	1:A:197:CYS:SG	2.63	0.72
1:D:227:SER:HB3	1:D:254:VAL:HG21	1.73	0.70
1:B:243:VAL:HB	1:C:9:ILE:HD13	1.74	0.68
1:B:86:ASP:CG	1:B:92:TYR:HH	1.97	0.68
1:B:106:GLU:OE1	4:B:401:HOH:O	2.12	0.68
1:C:173:THR:HG21	1:C:178:SER:CB	2.24	0.67
1:C:18:MET:HE3	1:C:19:GLU:HG2	1.78	0.66
1:A:61:ILE:HD12	1:A:112:ALA:HB1	1.77	0.66
1:C:183:LEU:O	4:C:401:HOH:O	2.14	0.65
1:B:194:GLU:O	1:B:195:THR:OG1	2.12	0.65
1:A:139:GLN:HA	1:A:139:GLN:NE2	2.12	0.64
1:D:190:LYS:HE3	1:D:196:GLY:HA3	1.78	0.64
1:A:210:GLU:OE1	1:D:4:LEU:HD11	1.98	0.63
1:C:201:GLU:OE2	1:D:186:LYS:NZ	2.30	0.62
1:A:14:ILE:HA	1:A:18:MET:HE3	1.82	0.62
1:A:195:THR:OG1	1:A:196:GLY:N	2.31	0.62
1:B:184:GLN:CB	1:B:197:CYS:HB3	2.30	0.61
1:C:252:LYS:O	1:C:256:GLU:HG3	2.03	0.58
1:B:9:ILE:HD13	1:C:243:VAL:HB	1.85	0.58
1:D:193:THR:HG21	1:D:197:CYS:O	2.02	0.58
1:D:57:ARG:NH2	1:D:58:ARG:HH12	2.02	0.58
1:B:237:SER:OG	1:B:238:HIS:N	2.37	0.57
1:B:210:GLU:OE1	1:B:246:GLY:HA3	2.04	0.57
1:A:16:ALA:HB3	1:D:74:GLU:HG3	1.86	0.57
1:B:109:THR:HG21	1:C:61:ILE:HD11	1.87	0.57
1:B:178:SER:O	1:B:182:THR:HG23	2.05	0.56
1:B:240:MET:HE3	1:B:240:MET:H	1.69	0.56
1:C:78:GLN:OE1	1:C:245:GLY:HA3	2.06	0.56
1:D:47:LYS:NZ	1:D:87:GLU:OE2	2.26	0.56
1:A:173:THR:HG21	1:A:178:SER:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:SER:N	4:C:403:HOH:O	2.35	0.56
1:C:69:ALA:HB2	1:C:242:PRO:HB3	1.88	0.56
1:A:14:ILE:HA	1:A:18:MET:CE	2.34	0.56
1:C:210:GLU:OE2	1:C:243:VAL:HG13	2.06	0.56
1:D:45:LEU:HG	1:D:255:ALA:HB1	1.88	0.55
1:C:217:SER:OG	1:C:250:SER:HB2	2.06	0.55
1:B:76:VAL:HG11	1:C:9:ILE:HG12	1.88	0.55
1:C:75:ILE:HD12	1:C:104:ALA:HA	1.88	0.55
1:C:187:ALA:N	4:C:401:HOH:O	2.39	0.55
1:B:137:ASN:O	1:B:139:GLN:HG2	2.06	0.55
1:A:194:GLU:N	1:A:195:THR:O	2.40	0.54
1:C:130:ASP:OD2	1:C:186:LYS:NZ	2.27	0.54
1:B:184:GLN:HB3	1:B:197:CYS:HB3	1.90	0.54
1:C:218:LYS:HE2	1:C:253:LYS:NZ	2.22	0.54
1:B:219:GLU:OE1	1:B:261:LYS:NZ	2.38	0.54
3:C:302:48H:O14	3:C:302:48H:N2	2.34	0.54
1:B:184:GLN:CG	1:B:197:CYS:HB3	2.38	0.53
1:A:29:VAL:HG21	1:A:45:LEU:HD13	1.91	0.53
1:A:61:ILE:CD1	1:A:112:ALA:HB1	2.39	0.53
1:A:61:ILE:HD11	1:D:109:THR:HG21	1.90	0.53
1:B:240:MET:H	1:B:240:MET:CE	2.22	0.52
1:B:204:LEU:HD11	1:B:241:GLY:HA2	1.90	0.52
1:A:16:ALA:HB2	1:D:101:LEU:HD23	1.92	0.52
1:C:65:MET:CG	1:C:75:ILE:HD11	2.38	0.52
1:C:149:TRP:HB3	1:C:151:THR:HG22	1.92	0.52
1:D:252:LYS:O	1:D:256:GLU:HG3	2.09	0.52
1:D:200:GLY:O	1:D:236:GLY:HA2	2.10	0.52
1:A:210:GLU:CD	1:D:4:LEU:HD11	2.30	0.52
1:B:171:ASP:HB3	1:B:226:VAL:HG12	1.92	0.52
1:B:26:GLU:O	1:B:26:GLU:HG2	2.11	0.51
1:A:193:THR:HG21	1:A:234:THR:HG22	1.92	0.51
1:A:9:ILE:HD13	1:D:243:VAL:HB	1.92	0.51
1:B:95:PHE:CD2	1:B:96:LYS:HG3	2.46	0.51
1:A:57:ARG:HH22	1:A:153:GLU:HG2	1.75	0.51
1:B:210:GLU:OE2	1:B:243:VAL:HG13	2.10	0.50
1:C:18:MET:CE	1:C:19:GLU:HG2	2.41	0.50
1:C:247:MET:HB3	4:C:403:HOH:O	2.10	0.50
1:D:264:GLN:OE1	1:D:264:GLN:N	2.36	0.50
1:B:94:GLU:HB3	1:B:100:TYR:CE1	2.47	0.50
1:B:55:PHE:CZ	1:B:164:ILE:HD13	2.47	0.50
1:C:59:LEU:O	1:C:124:ASN:ND2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HD11	1:C:109:THR:HG21	1.93	0.49
1:D:198:VAL:HG13	1:D:234:THR:HA	1.93	0.49
1:C:72:PHE:O	1:C:74:GLU:N	2.40	0.49
1:D:75:ILE:HG13	1:D:75:ILE:O	2.13	0.49
1:A:206:ALA:HB2	1:D:6:GLU:HG3	1.94	0.49
1:B:202:LYS:HB2	1:B:238:HIS:HA	1.94	0.49
1:A:14:ILE:O	1:A:18:MET:HE3	2.13	0.49
1:B:36:PRO:HG3	1:B:65:MET:HB2	1.93	0.49
1:A:88:PHE:CD2	1:A:111:ILE:HA	2.48	0.49
1:C:203:PRO:HB3	1:D:130:ASP:OD2	2.13	0.48
1:B:210:GLU:OE1	1:B:210:GLU:HA	2.12	0.48
1:D:84:ILE:HG21	1:D:248:LEU:HB3	1.95	0.48
1:C:96:LYS:HG3	1:C:97:PRO:HD2	1.94	0.48
1:B:155:ASN:HD22	1:D:151:THR:HG22	1.79	0.48
1:A:192:ASN:HB2	1:A:220:VAL:HA	1.95	0.48
1:B:145:LEU:HD12	1:B:164:ILE:HD11	1.94	0.48
1:D:77:VAL:HG21	1:D:85:LEU:HD11	1.96	0.47
1:C:238:HIS:HD2	4:C:402:HOH:O	1.97	0.47
1:C:183:LEU:HG	1:C:189:ILE:CD1	2.44	0.47
1:A:206:ALA:O	1:A:210:GLU:HG2	2.14	0.47
1:A:14:ILE:CA	1:A:18:MET:HE3	2.44	0.47
1:C:82:ARG:C	1:C:82:ARG:HD3	2.35	0.47
1:D:10:SER:O	1:D:14:ILE:HG13	2.14	0.47
1:C:61:ILE:CD1	1:C:112:ALA:HB1	2.45	0.47
1:B:184:GLN:HG3	1:B:197:CYS:HB3	1.97	0.47
1:C:25:LEU:HA	1:C:164:ILE:HD12	1.96	0.47
1:A:124:ASN:OD1	1:D:73:ASN:ND2	2.45	0.46
1:A:134:LYS:O	1:A:140:TYR:HA	2.14	0.46
1:A:149:TRP:HB2	1:A:152:VAL:HG23	1.96	0.46
1:C:187:ALA:CB	1:C:189:ILE:HG23	2.46	0.46
1:C:78:GLN:HG2	1:C:79:GLU:N	2.31	0.46
1:C:261:LYS:O	1:C:264:GLN:HG2	2.16	0.46
1:A:139:GLN:NE2	1:A:139:GLN:CA	2.79	0.46
1:D:61:ILE:CD1	1:D:112:ALA:HB1	2.46	0.45
1:B:204:LEU:HD11	1:B:241:GLY:CA	2.46	0.45
1:A:73:ASN:HB2	1:A:104:ALA:HB3	1.98	0.45
1:B:214:VAL:HG13	4:B:411:HOH:O	2.15	0.45
1:C:190:LYS:HG3	1:C:191:LEU:N	2.32	0.45
1:A:150:THR:O	1:A:153:GLU:HB3	2.17	0.45
1:A:202:LYS:HD3	1:A:236:GLY:O	2.16	0.44
1:B:61:ILE:O	1:B:66:TRP:NE1	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:HG11	1:D:6:GLU:HB3	1.99	0.44
1:C:190:LYS:HA	1:C:190:LYS:HD2	1.66	0.44
1:D:32:VAL:HG22	1:D:145:LEU:HD11	1.99	0.44
1:A:15:THR:O	1:A:19:GLU:HG3	2.18	0.44
1:C:22:LYS:HA	1:C:25:LEU:HG	2.00	0.44
1:A:8:VAL:HG13	1:D:96:LYS:HD3	2.00	0.44
1:C:36:PRO:HG3	1:C:65:MET:HB2	1.99	0.44
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.89	0.44
1:C:218:LYS:HE2	1:C:253:LYS:HZ3	1.83	0.44
1:A:116:VAL:HG11	1:D:106:GLU:HA	2.00	0.43
1:B:61:ILE:CD1	1:B:112:ALA:HB1	2.48	0.43
1:C:61:ILE:H	1:C:61:ILE:HG12	1.63	0.43
1:C:237:SER:OG	1:C:238:HIS:N	2.51	0.43
1:C:235:CYS:O	1:C:237:SER:N	2.52	0.43
1:D:27:THR:O	1:D:166:ALA:HA	2.18	0.43
1:B:137:ASN:O	1:B:137:ASN:OD1	2.37	0.43
1:C:175:HIS:ND1	1:C:201:GLU:OE1	2.42	0.43
1:B:73:ASN:ND2	1:C:124:ASN:OD1	2.31	0.43
1:A:61:ILE:HD12	1:A:112:ALA:CB	2.46	0.43
1:C:57:ARG:HH21	1:C:150:THR:HG23	1.84	0.43
1:C:173:THR:HG23	3:C:302:48H:C5	2.49	0.43
1:A:200:GLY:O	1:A:236:GLY:HA2	2.19	0.43
1:C:187:ALA:HB3	1:C:189:ILE:HG23	2.01	0.43
1:A:44:TYR:OH	1:A:87:GLU:OE2	2.33	0.42
1:B:225:TYR:OH	1:B:257:GLU:HG2	2.19	0.42
1:A:87:GLU:OE1	1:A:87:GLU:N	2.41	0.42
1:A:139:GLN:HB3	1:A:140:TYR:H	1.51	0.42
1:A:184:GLN:HE21	1:A:197:CYS:HA	1.85	0.42
1:B:75:ILE:HG23	1:B:104:ALA:HB2	2.02	0.42
1:D:21:LEU:HD12	1:D:21:LEU:HA	1.85	0.42
1:B:44:TYR:O	1:B:48:LYS:HG3	2.18	0.42
1:C:199:VAL:HB	1:C:236:GLY:H	1.85	0.42
1:C:183:LEU:HG	1:C:189:ILE:HD11	2.00	0.42
1:D:116:VAL:HG23	1:D:120:ALA:O	2.20	0.42
1:A:85:LEU:HD22	1:A:90:VAL:HB	2.02	0.42
1:B:200:GLY:O	1:B:236:GLY:HA2	2.20	0.42
1:C:173:THR:HG21	1:C:178:SER:H	1.84	0.42
1:C:173:THR:O	1:C:173:THR:CG2	2.67	0.42
1:B:86:ASP:OD1	1:B:92:TYR:OH	2.33	0.42
1:D:77:VAL:HG21	1:D:85:LEU:CD1	2.50	0.42
1:A:84:ILE:HG21	1:A:248:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.78	0.41
1:D:148:ASN:HB3	1:D:153:GLU:OE2	2.20	0.41
1:A:101:LEU:HD13	1:D:16:ALA:HB2	2.02	0.41
1:D:45:LEU:HG	1:D:255:ALA:CB	2.50	0.41
1:D:221:PHE:CG	1:D:222:PRO:HD2	2.55	0.41
1:B:135:GLN:HG3	4:B:406:HOH:O	2.19	0.41
1:B:6:GLU:HA	1:B:9:ILE:HD12	2.02	0.41
1:B:57:ARG:NH1	1:B:57:ARG:HG2	2.36	0.41
1:D:55:PHE:CZ	1:D:164:ILE:HD13	2.56	0.41
1:B:57:ARG:HG2	1:B:57:ARG:HH11	1.85	0.41
1:C:210:GLU:HA	1:C:210:GLU:OE1	2.21	0.41
1:B:27:THR:O	1:B:166:ALA:HA	2.21	0.41
1:C:65:MET:HG2	1:C:75:ILE:HD11	2.03	0.41
1:D:30:ALA:O	1:D:169:VAL:HA	2.20	0.41
1:D:44:TYR:O	1:D:48:LYS:HG3	2.21	0.41
1:D:181:SER:O	1:D:184:GLN:HG2	2.21	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.91	0.40
1:B:202:LYS:HE2	1:B:236:GLY:O	2.21	0.40
1:C:174:GLY:HA2	1:C:229:MET:HB3	2.04	0.40
1:C:210:GLU:OE1	1:C:246:GLY:HA3	2.21	0.40
1:A:138:GLY:O	1:A:139:GLN:NE2	2.55	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:THR:OG1	1:C:151:THR:OG1[2_656]	1.98	0.22
4:B:406:HOH:O	4:B:406:HOH:O[2_556]	2.06	0.14
1:A:15:THR:OG1	1:A:22:LYS:NZ[2_656]	2.13	0.07

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	259/268 (97%)	235 (91%)	23 (9%)	1 (0%)	34	40
1	B	260/268 (97%)	244 (94%)	11 (4%)	5 (2%)	8	6
1	C	254/268 (95%)	239 (94%)	11 (4%)	4 (2%)	9	8
1	D	260/268 (97%)	245 (94%)	11 (4%)	4 (2%)	10	9
All	All	1033/1072 (96%)	963 (93%)	56 (5%)	14 (1%)	11	10

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	THR
1	C	73	ASN
1	C	236	GLY
1	D	73	ASN
1	D	137	ASN
1	B	73	ASN
1	B	197	CYS
1	D	68	GLY
1	D	203	PRO
1	A	189	ILE
1	C	239	ARG
1	C	240	MET
1	B	203	PRO
1	B	189	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/211 (97%)	204 (100%)	1 (0%)	88	94
1	B	206/211 (98%)	205 (100%)	1 (0%)	88	94
1	C	203/211 (96%)	202 (100%)	1 (0%)	88	94
1	D	206/211 (98%)	205 (100%)	1 (0%)	88	94
All	All	820/844 (97%)	816 (100%)	4 (0%)	88	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	THR
1	B	93	ARG
1	C	93	ARG
1	D	240	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	184	GLN
1	B	137	ASN
1	B	216	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	48H	C	302	2	30,41,41	4.74	13 (43%)	32,61,61	2.97	7 (21%)
3	48H	B	302	2	30,41,41	4.65	13 (43%)	32,61,61	2.88	5 (15%)
3	48H	D	302	2	30,41,41	4.74	11 (36%)	32,61,61	2.88	5 (15%)
3	48H	A	302	2	30,41,41	4.81	11 (36%)	32,61,61	2.94	7 (21%)

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	48H	C	302	2	-	4/28/51/51	0/3/3/3
3	48H	B	302	2	-	5/28/51/51	0/3/3/3
3	48H	D	302	2	-	4/28/51/51	0/3/3/3
3	48H	A	302	2	-	6/28/51/51	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	48H	O14-C17	17.91	1.66	1.41
3	A	302	48H	O14-C17	17.34	1.65	1.41
3	C	302	48H	O14-C17	17.31	1.65	1.41
3	B	302	48H	O14-C17	16.90	1.64	1.41
3	A	302	48H	C16-C17	-15.75	1.29	1.53
3	C	302	48H	C16-C17	-15.15	1.30	1.53
3	D	302	48H	C16-C17	-14.89	1.31	1.53
3	B	302	48H	C16-C17	-14.57	1.31	1.53
3	A	302	48H	O14-C14	-7.02	1.29	1.45
3	B	302	48H	O14-C14	-6.97	1.29	1.45
3	C	302	48H	O14-C14	-6.39	1.30	1.45
3	D	302	48H	O14-C14	-6.32	1.30	1.45
3	D	302	48H	O12-C15	-4.83	1.31	1.43
3	B	302	48H	O12-C15	-4.72	1.31	1.43
3	C	302	48H	O12-C15	-4.51	1.32	1.43
3	A	302	48H	O12-C15	-4.31	1.32	1.43
3	B	302	48H	O13-C16	3.23	1.50	1.43
3	A	302	48H	C1-N4	3.15	1.39	1.33
3	C	302	48H	C1-N4	3.11	1.39	1.33
3	B	302	48H	C1-N4	2.95	1.39	1.33
3	C	302	48H	O13-C16	2.88	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	48H	O13-C16	2.85	1.49	1.43
3	A	302	48H	C3-C2	-2.84	1.33	1.40
3	D	302	48H	C10-C9	2.83	1.55	1.49
3	C	302	48H	O8-C8	-2.82	1.17	1.22
3	B	302	48H	C10-C9	2.79	1.55	1.49
3	A	302	48H	P2-O6	2.74	1.70	1.59
3	A	302	48H	C10-C9	2.73	1.55	1.49
3	C	302	48H	C10-C9	2.71	1.55	1.49
3	C	302	48H	C3-C2	-2.66	1.33	1.40
3	D	302	48H	C3-C2	-2.65	1.33	1.40
3	B	302	48H	C4-N5	2.60	1.43	1.34
3	D	302	48H	C1-N4	2.55	1.38	1.33
3	B	302	48H	C15-C14	2.49	1.59	1.53
3	D	302	48H	P2-O6	2.38	1.68	1.59
3	D	302	48H	O8-C8	-2.34	1.18	1.22
3	A	302	48H	C4-N5	2.32	1.42	1.34
3	B	302	48H	C3-C2	-2.31	1.34	1.40
3	D	302	48H	O13-C16	2.28	1.48	1.43
3	B	302	48H	O8-C8	-2.26	1.18	1.22
3	C	302	48H	O7-C7	-2.22	1.38	1.42
3	D	302	48H	C4-N5	2.20	1.42	1.34
3	C	302	48H	P2-O6	2.19	1.68	1.59
3	A	302	48H	O8-C8	-2.19	1.18	1.22
3	B	302	48H	C1-N3	2.10	1.35	1.32
3	C	302	48H	C4-N5	2.09	1.41	1.34
3	B	302	48H	O7-C7	-2.04	1.38	1.42
3	C	302	48H	C15-C14	2.02	1.58	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	48H	C3-C4-N5	11.65	138.05	120.35
3	C	302	48H	C3-C4-N5	11.51	137.85	120.35
3	B	302	48H	C3-C4-N5	11.15	137.29	120.35
3	D	302	48H	C3-C4-N5	11.04	137.13	120.35
3	C	302	48H	N5-C4-N4	-8.18	101.59	118.57
3	A	302	48H	N5-C4-N4	-8.06	101.85	118.57
3	B	302	48H	N5-C4-N4	-7.75	102.49	118.57
3	D	302	48H	N5-C4-N4	-7.59	102.81	118.57
3	C	302	48H	N3-C1-N4	-5.97	119.34	128.68
3	D	302	48H	N3-C1-N4	-5.87	119.50	128.68
3	B	302	48H	N3-C1-N4	-5.68	119.80	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	48H	N3-C1-N4	-5.33	120.34	128.68
3	B	302	48H	O8-C8-C9	4.45	121.76	118.77
3	D	302	48H	O8-C8-C9	4.10	121.52	118.77
3	C	302	48H	C10-C9-C8	3.01	121.61	118.93
3	A	302	48H	C15-C16-C17	2.90	105.34	100.98
3	C	302	48H	O14-C17-C16	-2.75	102.91	106.93
3	A	302	48H	C17-N2-C2	-2.67	121.95	126.64
3	A	302	48H	C13-C14-C15	-2.61	105.39	115.18
3	D	302	48H	P2-O3-P1	-2.47	124.37	132.83
3	C	302	48H	C13-C14-C15	-2.30	106.58	115.18
3	B	302	48H	C15-C16-C17	2.21	104.31	100.98
3	A	302	48H	C10-C9-C8	2.20	120.89	118.93
3	C	302	48H	C17-N2-C2	-2.04	123.06	126.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

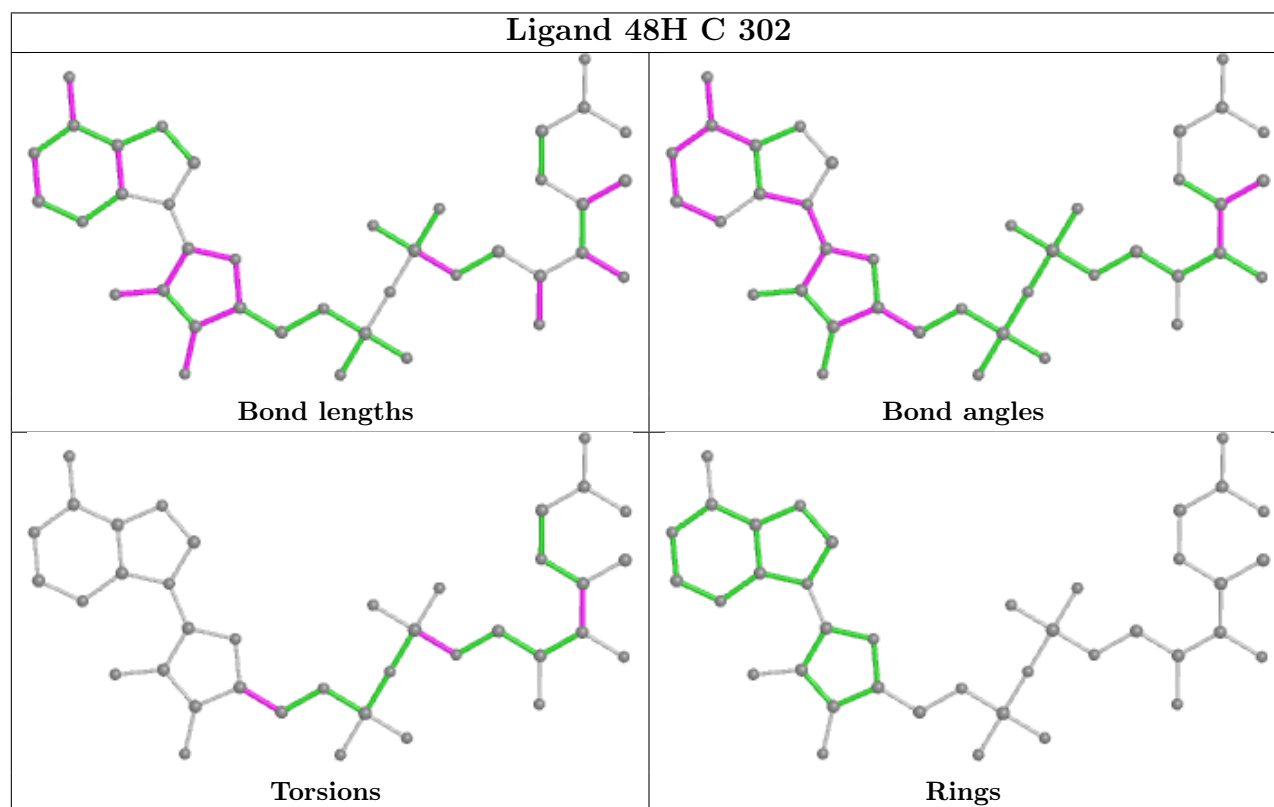
Mol	Chain	Res	Type	Atoms
3	A	302	48H	P1-O3-P2-O6
3	A	302	48H	O8-C8-C9-C10
3	A	302	48H	O8-C8-C9-N1
3	B	302	48H	O8-C8-C9-C10
3	B	302	48H	O8-C8-C9-N1
3	C	302	48H	O8-C8-C9-N1
3	D	302	48H	P1-O3-P2-O6
3	D	302	48H	O8-C8-C9-C10
3	D	302	48H	O8-C8-C9-N1
3	B	302	48H	P1-O3-P2-O6
3	A	302	48H	O11-C13-C14-O14
3	B	302	48H	O11-C13-C14-O14
3	D	302	48H	O11-C13-C14-O14
3	C	302	48H	C6-O6-P2-O3
3	A	302	48H	P2-O3-P1-O2
3	B	302	48H	P2-O3-P1-O1
3	A	302	48H	O11-C13-C14-C15
3	C	302	48H	O11-C13-C14-O14
3	C	302	48H	O8-C8-C9-C10

There are no ring outliers.

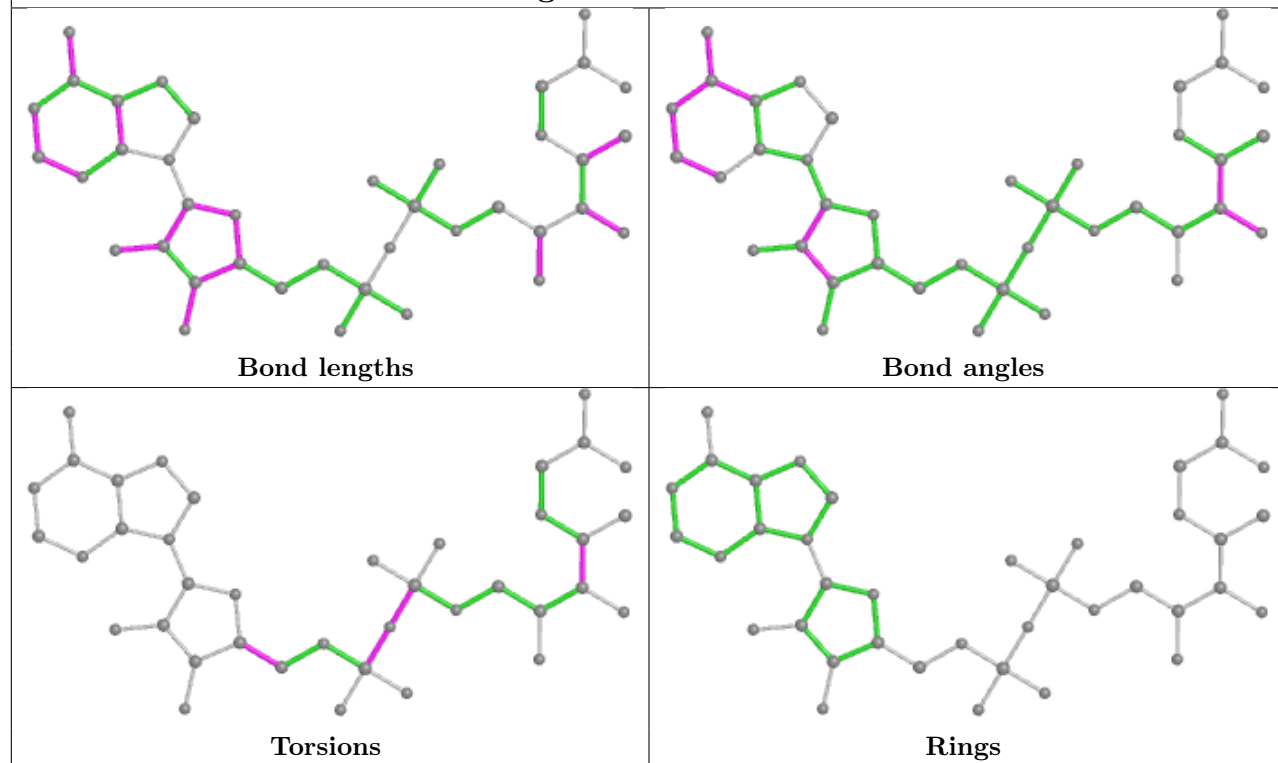
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	48H	3	0
3	B	302	48H	1	0
3	D	302	48H	1	0
3	A	302	48H	1	0

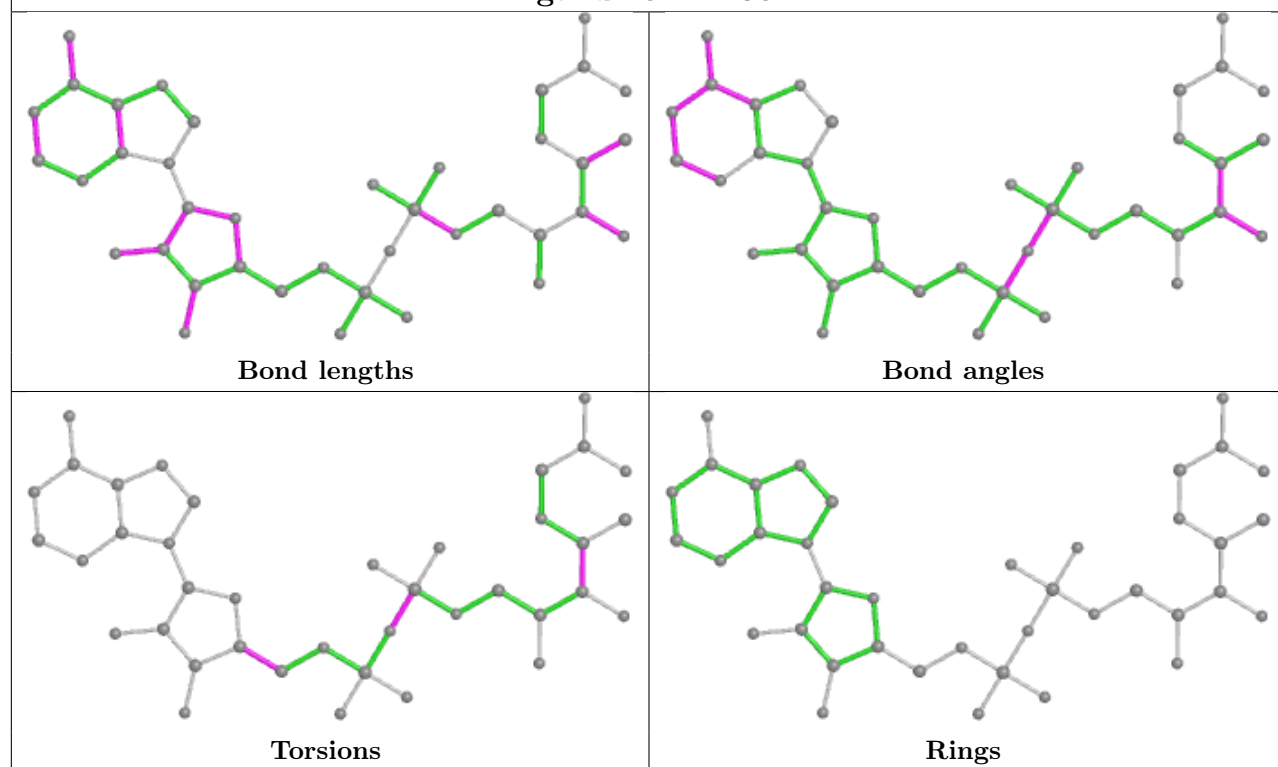
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

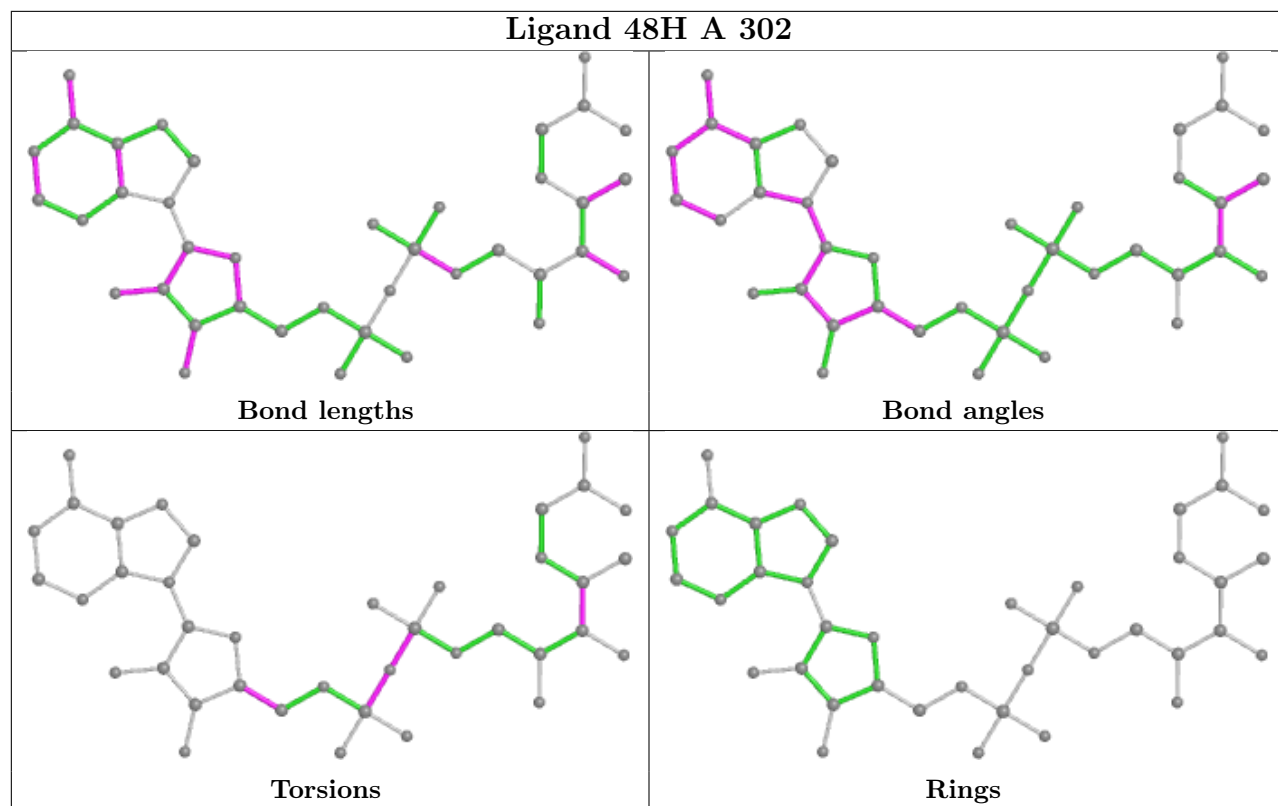


Ligand 48H B 302



Ligand 48H D 302





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	261/268 (97%)	0.49	19 (7%)	15 18	36, 51, 67, 77	0
1	B	262/268 (97%)	0.39	15 (5%)	23 28	29, 46, 64, 81	0
1	C	258/268 (96%)	0.39	14 (5%)	25 31	27, 44, 66, 78	0
1	D	262/268 (97%)	0.45	16 (6%)	21 26	33, 48, 67, 77	0
All	All	1043/1072 (97%)	0.43	64 (6%)	21 26	27, 48, 67, 81	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	MET	5.2
1	B	3	ASN	4.8
1	C	79	GLU	4.2
1	C	191	LEU	4.2
1	A	195	THR	4.1
1	B	197	CYS	4.0
1	A	258	ILE	4.0
1	D	82	ARG	3.9
1	D	80	MET	3.9
1	C	2	GLN	3.8
1	C	264	GLN	3.7
1	D	264	GLN	3.7
1	A	190	LYS	3.7
1	C	47	LYS	3.6
1	D	210	GLU	3.5
1	D	81	GLY	3.5
1	A	192	ASN	3.4
1	B	4	LEU	3.4
1	D	79	GLU	3.4
1	D	103	ASP	3.4
1	C	188	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	259	ALA	3.4
1	D	85	LEU	3.3
1	C	189	ILE	3.3
1	D	259	ALA	3.2
1	A	191	LEU	3.1
1	D	137	ASN	3.1
1	A	262	LEU	3.1
1	B	264	GLN	3.0
1	C	249	MET	2.9
1	B	83	GLU	2.9
1	A	80	MET	2.8
1	D	92	TYR	2.8
1	A	189	ILE	2.7
1	D	86	ASP	2.6
1	A	69	ALA	2.6
1	A	15	THR	2.6
1	B	26	GLU	2.6
1	C	190	LYS	2.6
1	A	196	GLY	2.5
1	B	249	MET	2.5
1	C	80	MET	2.5
1	B	192	ASN	2.5
1	D	93	ARG	2.5
1	D	263	ASN	2.5
1	C	69	ALA	2.4
1	A	14	ILE	2.3
1	A	225	TYR	2.3
1	B	6	GLU	2.3
1	D	97	PRO	2.2
1	D	248	LEU	2.2
1	B	79	GLU	2.2
1	A	193	THR	2.2
1	C	84	ILE	2.2
1	C	263	ASN	2.1
1	A	11	GLU	2.1
1	A	168	TYR	2.1
1	B	256	GLU	2.1
1	B	195	THR	2.1
1	A	16	ALA	2.1
1	A	249	MET	2.1
1	B	211	GLU	2.1
1	C	18	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	80	MET	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

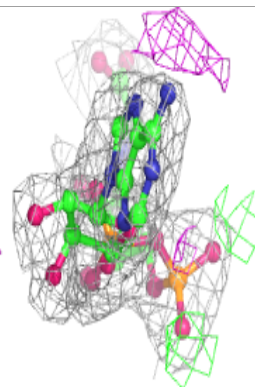
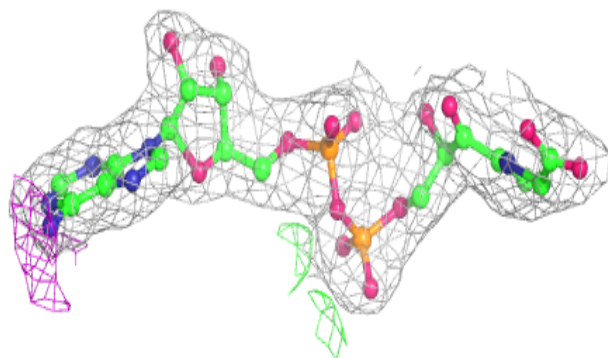
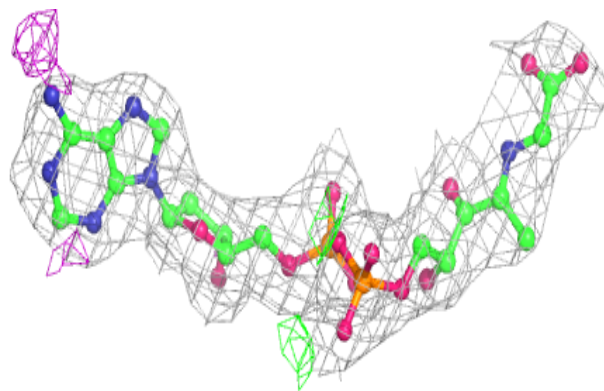
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE	C	301	1/1	0.95	0.11	60,60,60,60	0
3	48H	D	302	39/39	0.96	0.14	32,38,57,57	0
3	48H	B	302	39/39	0.97	0.14	22,31,54,55	0
3	48H	C	302	39/39	0.97	0.14	21,32,59,63	0
3	48H	A	302	39/39	0.97	0.12	31,38,58,63	0
2	FE	A	301	1/1	0.98	0.07	55,55,55,55	0
2	FE	D	301	1/1	0.98	0.06	56,56,56,56	0
2	FE	B	301	1/1	0.98	0.05	51,51,51,51	0

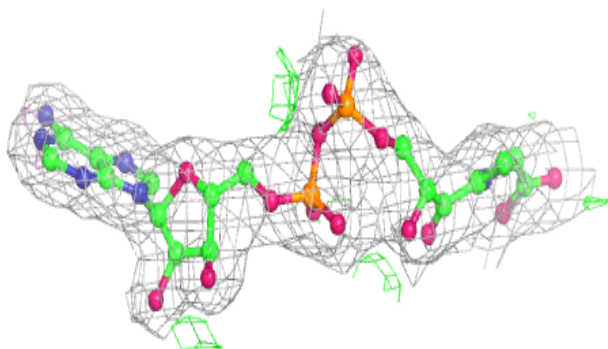
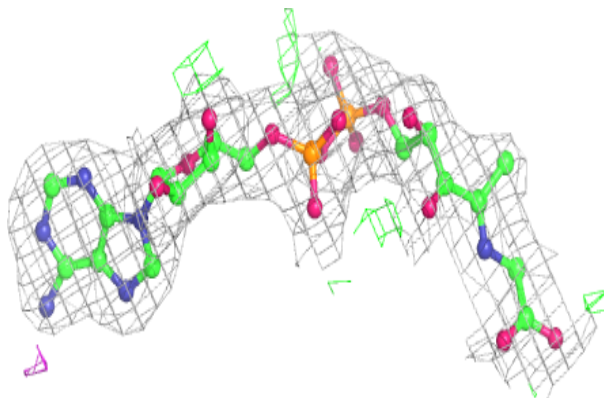
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 48H D 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

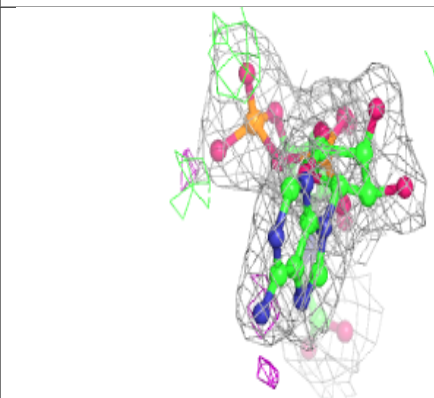
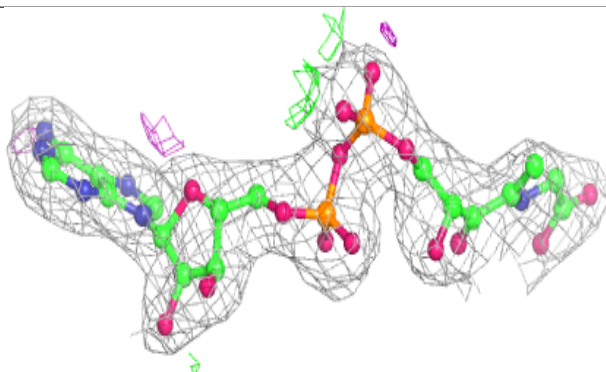
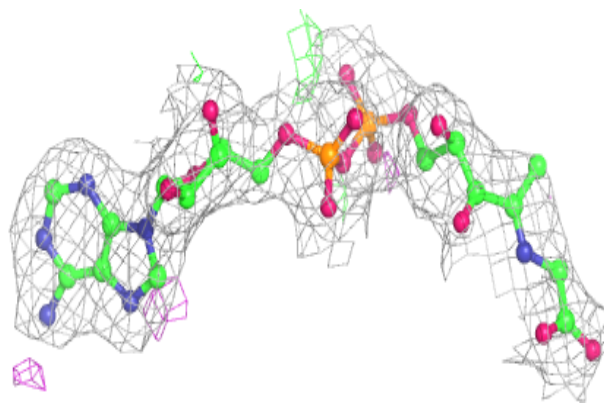
**Electron density around 48H B 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

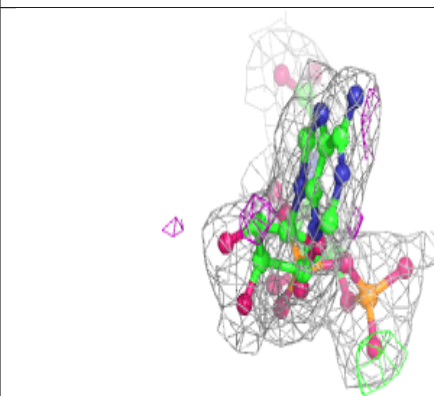
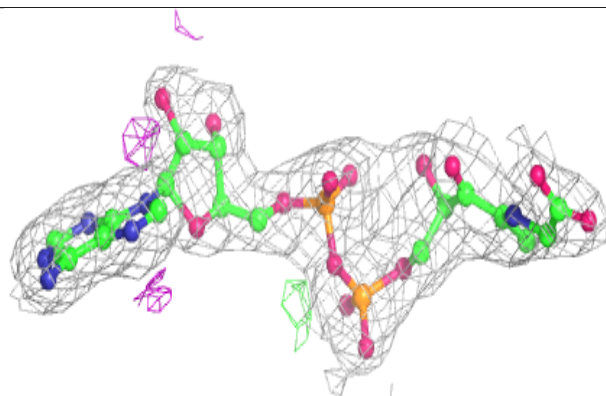
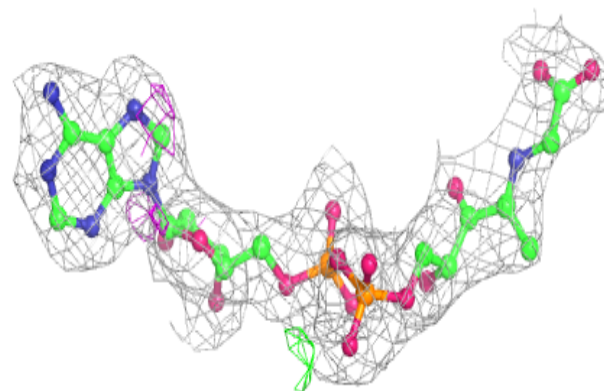


Electron density around 48H C 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 48H A 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.