



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:15 AM UTC

PDB ID : 9DRS / pdb_00009drs
Title : Crystal structure of M. tuberculosis PheRS-tRNA complex bound to inhibitor D-116
Authors : Gade, P.; Chang, C.; Forte, B.; Wower, J.; Gilbert, I.H.; Baragana, B.; Michalska, K.; Joachimiak, A.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2024-09-26
Resolution : 2.35 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](#) ①) were used in the production of this report:

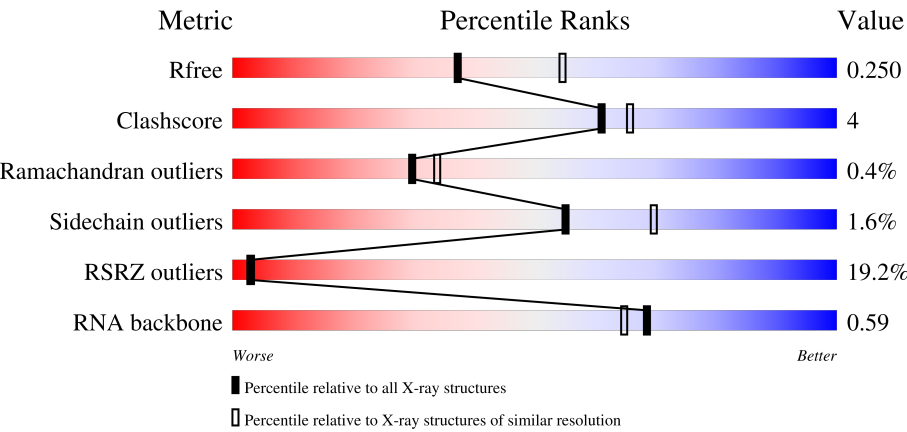
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)
RNA backbone	3983	1027 (2.66-2.06)

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	341	27% 82% 15% ..
1	D	341	23% 85% 13% .
2	B	835	4% 91% 9%
2	E	835	27% 85% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	77	
3	F	77	

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
4	AX7	A	401	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21276 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 Phenylalanine–tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2531	1595	455	472	9			
1	D	338	Total	C	N	O	S	0	1	0
			2598	1637	471	481	9			

- Molecule 2 is a protein called Phenylalanine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	834	Total	C	N	O	S	0	2	0
			6247	3924	1135	1167	21			
2	E	805	Total	C	N	O	S	0	0	0
			5963	3754	1072	1117	20			

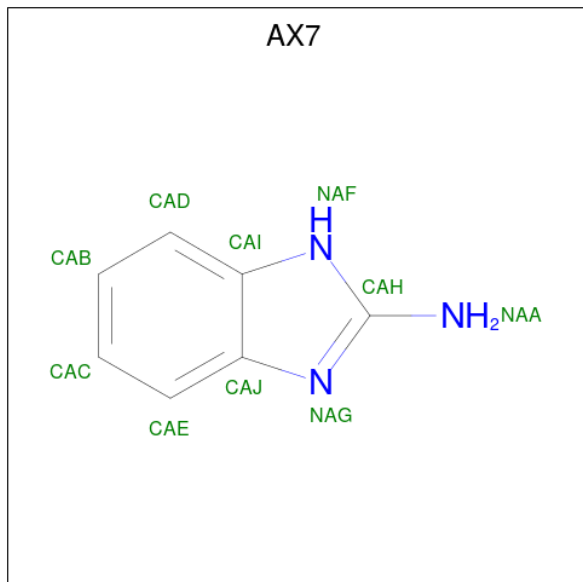
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLN	-	expression tag	UNP P9WFU1
B	-2	SER	-	expression tag	UNP P9WFU1
B	-1	ASN	-	expression tag	UNP P9WFU1
B	0	ALA	-	expression tag	UNP P9WFU1
E	-3	GLN	-	expression tag	UNP P9WFU1
E	-2	SER	-	expression tag	UNP P9WFU1
E	-1	ASN	-	expression tag	UNP P9WFU1
E	0	ALA	-	expression tag	UNP P9WFU1

- Molecule 3 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	71	Total	C	N	O	P	0	0	0
			1523	677	277	498	71			
3	F	71	Total	C	N	O	P	0	0	0
			1522	677	277	497	71			

- Molecule 4 is 1H-benzimidazol-2-amine (CCD ID: AX7) (formula: $C_7H_7N_3$) (labeled as "Ligand of Interest" by depositor).

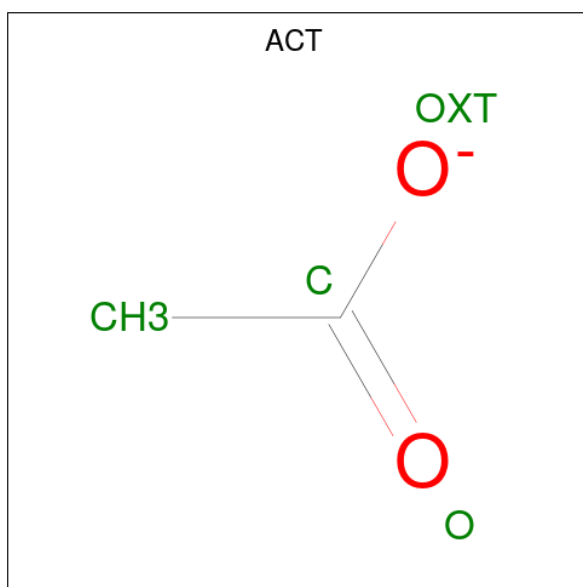


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	7	3		
4	D	1	Total	C	N	0	0
			10	7	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	4	Total	Mg	0	0
			4	4		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



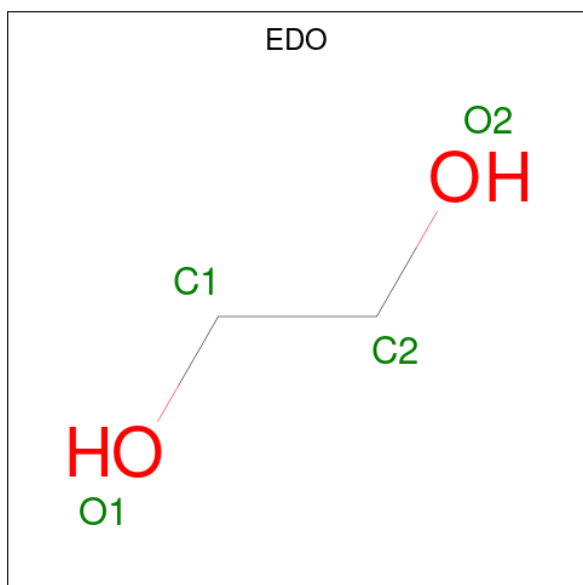
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

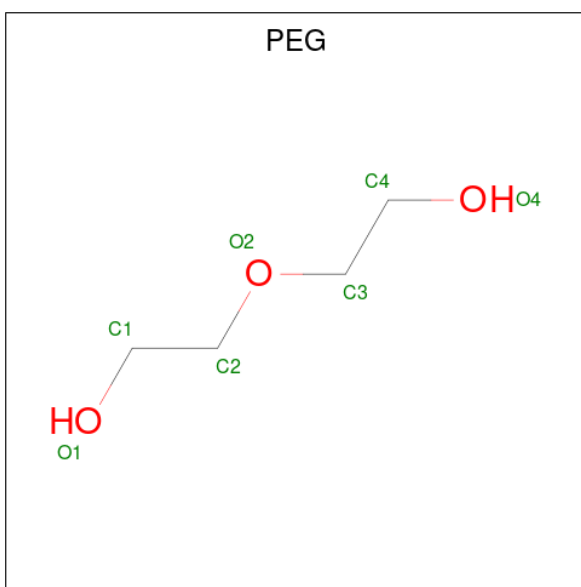
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



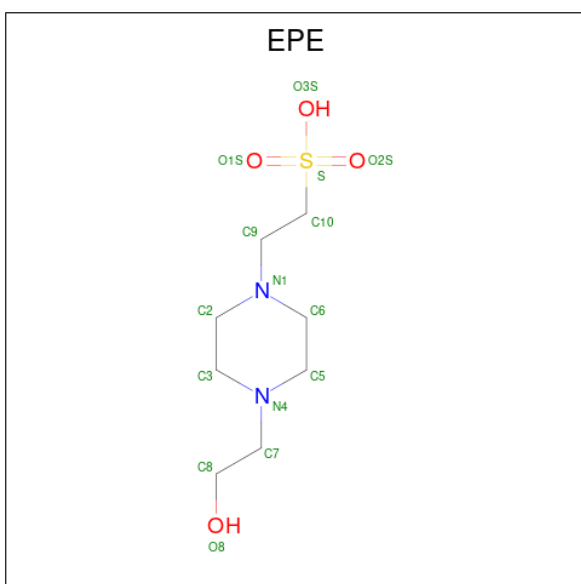
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



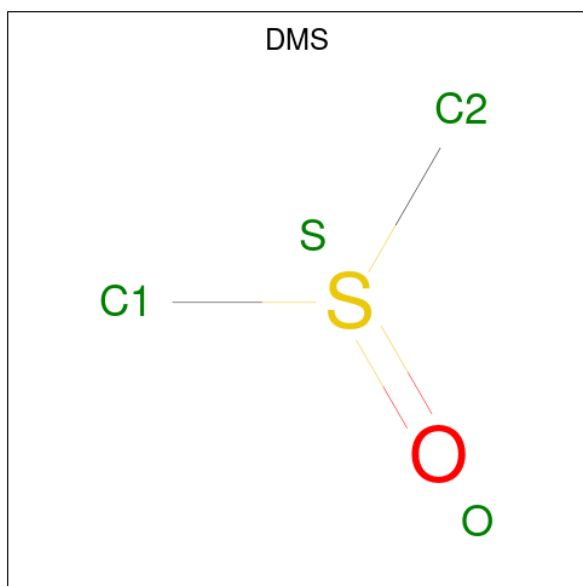
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	E	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 10 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	O	S	0	0
			4	2	1	1		

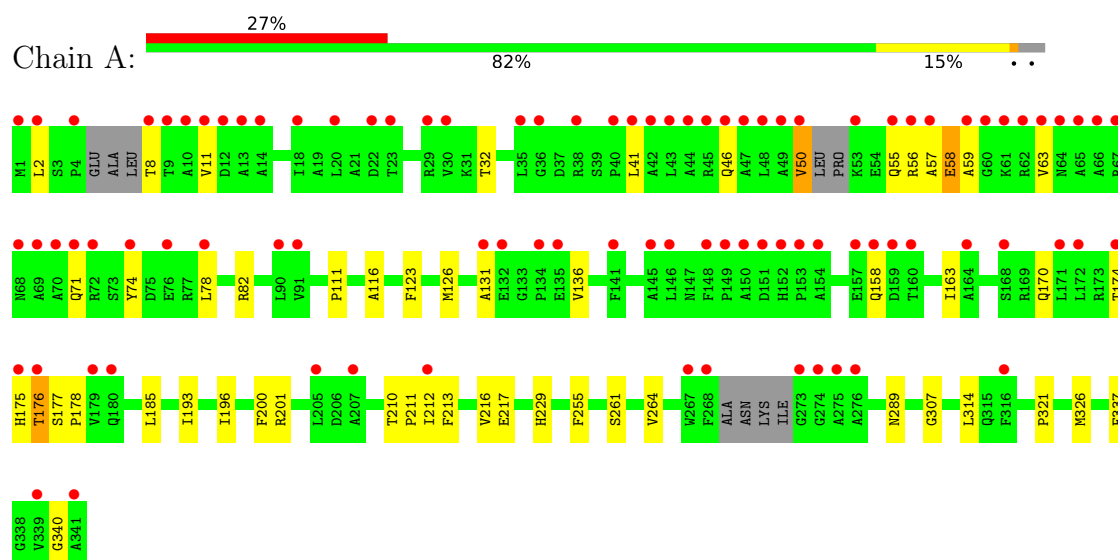
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	65	Total	O	0	0
			65	65		
11	B	327	Total	O	0	0
			327	327		
11	C	80	Total	O	0	0
			80	80		
11	D	59	Total	O	0	0
			59	59		
11	E	166	Total	O	0	0
			166	166		
11	F	25	Total	O	0	0
			25	25		

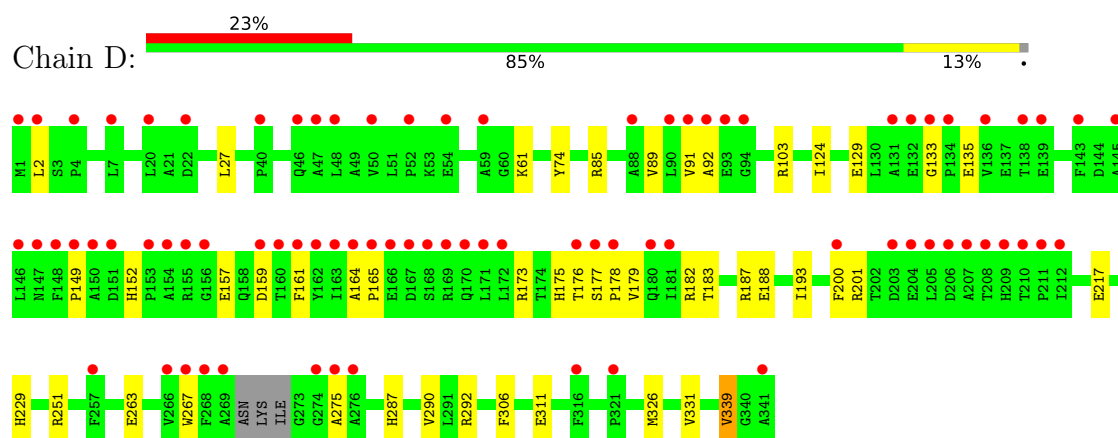
3 Residue-property plots

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: Phenylalanine-tRNA ligase alpha subunit

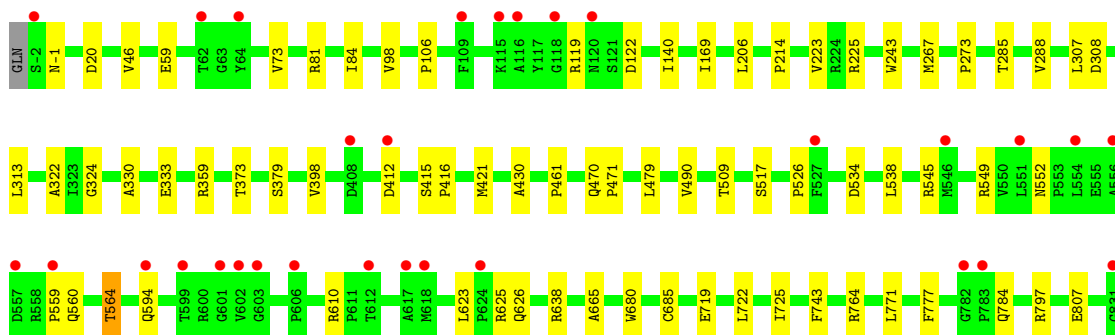


• Molecule 1: Phenylalanine-tRNA ligase alpha subunit

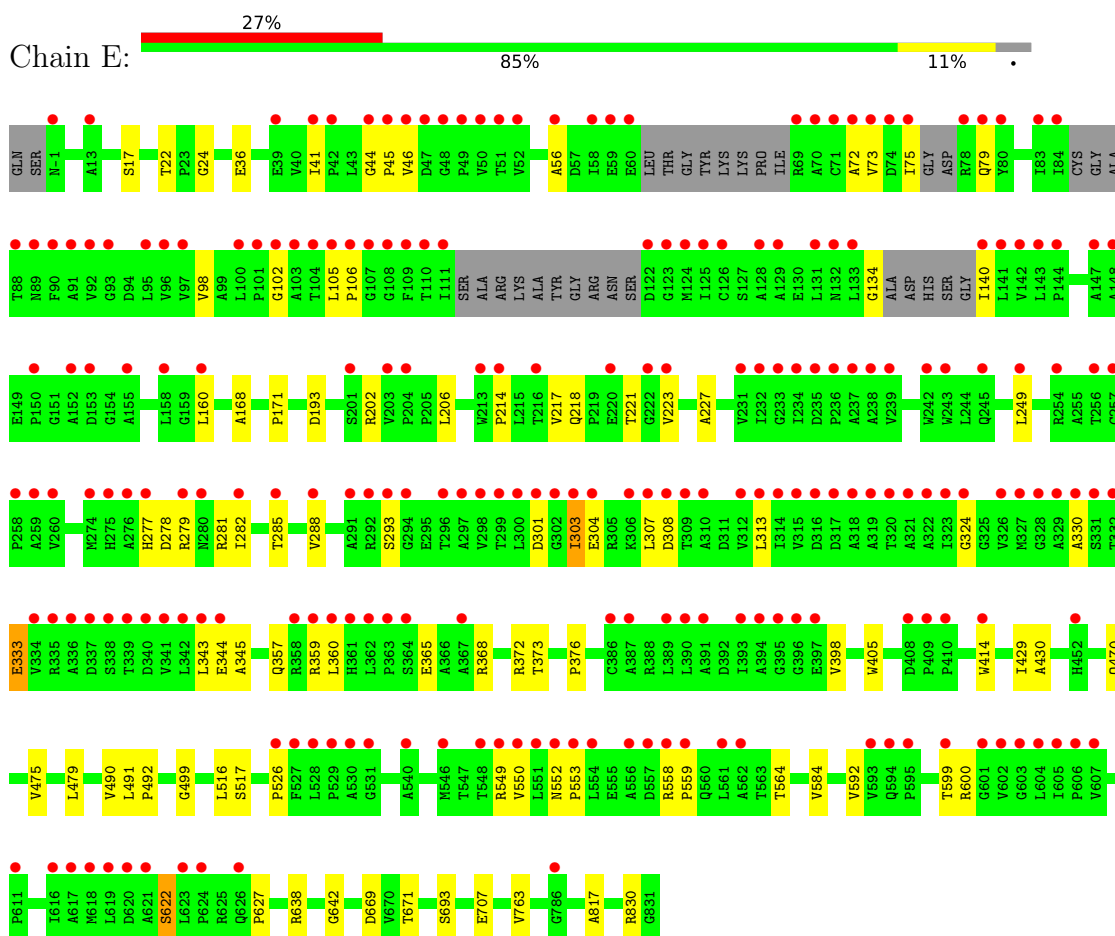


• Molecule 2: Phenylalanine-tRNA ligase beta subunit

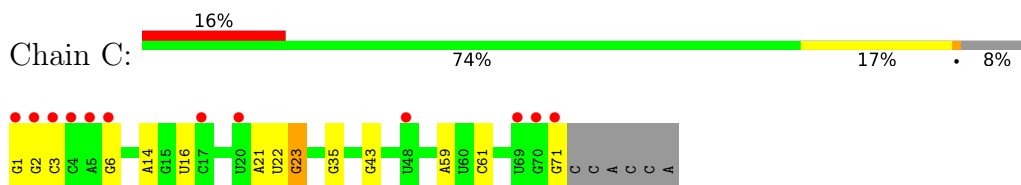




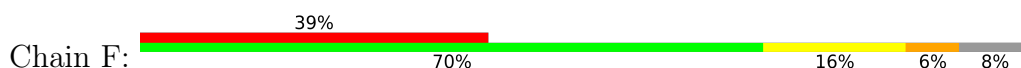
• Molecule 2: Phenylalanine-tRNA ligase beta subunit

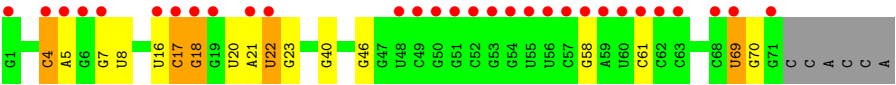


• Molecule 3: tRNA(Phe)



• Molecule 3: tRNA(Phe)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.68Å 64.11Å 188.33Å 90.00° 111.21° 90.00°	Depositor
Resolution (Å)	46.77 – 2.35 46.77 – 2.35	Depositor EDS
% Data completeness (in resolution range)	76.8 (46.77-2.35) 93.3 (46.77-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.201 , 0.250 0.201 , 0.250	Depositor DCC
R_{free} test set	6383 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21276	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, MG, AX7, DMS, ACT, EPE

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	0.09	0/2587	0.25	0/3520
1	D	0.09	0/2660	0.25	0/3620
2	B	0.09	0/6390	0.25	0/8750
2	E	0.11	0/6088	0.25	0/8345
3	C	0.08	0/1702	0.20	0/2652
3	F	0.06	0/1701	0.15	0/2652
All	All	0.09	0/21128	0.24	0/29539

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2531	0	2446	33	0
1	D	2598	0	2536	34	0
2	B	6247	0	6271	43	0
2	E	5963	0	5955	55	0
3	C	1523	0	770	6	0
3	F	1522	0	770	10	0
4	A	10	0	7	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	10	0	7	0	0
5	A	1	0	0	0	0
5	C	4	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	8	0	6	0	0
6	B	36	0	27	0	0
6	C	4	0	3	0	0
6	D	4	0	3	0	0
6	E	12	0	9	0	0
7	B	12	0	18	1	0
7	C	4	0	6	2	0
7	E	16	0	24	2	0
8	B	21	0	30	1	0
8	E	7	0	10	0	0
9	B	15	0	17	2	0
10	D	4	0	6	0	0
11	A	65	0	0	0	0
11	B	327	0	0	1	0
11	C	80	0	0	0	0
11	D	59	0	0	0	0
11	E	166	0	0	0	0
11	F	25	0	0	0	0
All	All	21276	0	18921	163	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 4.

All (163) 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:D:135:GLU:HA	1:D:173:ARG:HD3	1.61	0.81
1:D:183:THR:HG23	1:D:187:ARG:HD3	1.62	0.80
2:B:267:MET:HG3	2:B:273:PRO:HA	1.64	0.80
1:D:173:ARG:HH21	1:D:176:THR:HG22	1.48	0.78
1:A:174:THR:HB	1:A:201:ARG:HH11	1.49	0.76
3:C:3:C:H42	3:C:71:G:H1	1.34	0.73
1:D:183:THR:HG21	1:D:193:ILE:HG12	1.74	0.70
1:A:46:GLN:HG2	3:F:20:U:H5''	1.73	0.70
1:D:251:ARG:NH1	1:D:263:GLU:OE1	2.27	0.68
1:A:217:GLU:OE2	4:A:401:AX7:NAG	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:G:N7	2:E:830:ARG:NH2	2.38	0.65
1:D:311:GLU:HA	1:D:326:MET:HE1	1.77	0.65
2:E:217:VAL:HG22	2:E:288:VAL:HB	1.79	0.64
2:E:206:LEU:HD13	2:E:398:VAL:HG11	1.80	0.64
2:B:308:ASP:HB2	2:B:359:ARG:HH12	1.63	0.64
1:D:200:PHE:HE2	2:E:526:PRO:HG3	1.64	0.63
3:C:23:G:H21	7:C:101:EDO:H11	1.63	0.63
2:E:227:ALA:HB3	2:E:345:ALA:HB3	1.80	0.63
2:B:206:LEU:HD13	2:B:398:VAL:HG11	1.81	0.62
2:B:81:ARG:NH1	2:B:122:ASP:OD2	2.32	0.62
1:A:314:LEU:HD23	1:A:326:MET:HE2	1.83	0.61
2:E:279:ARG:HA	2:E:282:ILE:HD12	1.83	0.61
1:D:27:LEU:HD21	1:D:74:TYR:HE1	1.66	0.60
1:A:174:THR:HB	1:A:201:ARG:NH1	2.16	0.59
1:A:196:ILE:HG12	1:A:216:VAL:HG22	1.86	0.57
2:E:553:PRO:HG3	2:E:559:PRO:HB3	1.86	0.57
2:B:322:ALA:HB1	8:B:905:PEG:H42	1.86	0.57
2:E:36:GLU:HB3	2:E:168:ALA:HB3	1.87	0.56
2:B:538:LEU:O	2:B:545:ARG:NH1	2.38	0.56
2:E:277:HIS:CE1	2:E:344:GLU:HG2	2.41	0.56
2:E:278:ASP:HB3	2:E:281:ARG:HB2	1.87	0.56
1:D:159:ASP:OD2	1:D:201:ARG:NH2	2.38	0.55
2:E:73:VAL:HG11	2:E:98:VAL:HG21	1.88	0.55
2:B:421:MET:HG3	2:B:471:PRO:HB3	1.89	0.54
2:B:594:GLN:NE2	11:B:1008:HOH:O	2.38	0.54
1:A:123:PHE:HA	1:A:126:MET:HE2	1.90	0.54
2:E:365:GLU:OE2	2:E:368:ARG:NH1	2.42	0.53
2:B:534:ASP:OD1	2:B:545:ARG:NH2	2.41	0.53
2:E:105:LEU:HG	2:E:106:PRO:HD2	1.91	0.53
2:B:623:LEU:O	2:B:625:ARG:NH2	2.37	0.53
2:E:75:ILE:HD11	2:E:79:GLN:HB3	1.91	0.53
2:E:223:VAL:HG12	2:E:405:TRP:HZ3	1.74	0.53
1:D:91:VAL:HG12	1:D:92:ALA:H	1.75	0.52
1:D:177:SER:N	1:D:178:PRO:HD2	2.25	0.52
1:D:292:ARG:NH2	2:E:470:GLN:OE1	2.42	0.51
3:F:4:C:H2'	3:F:5:A:C8	2.45	0.51
3:F:69:U:H2'	3:F:70:G:H8	1.76	0.51
2:E:600:ARG:HE	2:E:622:SER:HB2	1.77	0.50
1:D:157:GLU:O	2:E:552:ASN:ND2	2.44	0.50
1:A:163:ILE:HB	1:A:170:GLN:HB3	1.94	0.50
2:E:218:GLN:O	2:E:221:THR:OG1	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PRO:HD2	1:D:152:HIS:HD2	1.77	0.50
3:C:14:A:H1'	7:C:101:EDO:H12	1.93	0.50
3:C:59:A:O2'	3:C:61:C:OP2	2.27	0.49
2:E:491:LEU:HD23	2:E:492:PRO:HD2	1.94	0.49
2:B:223:VAL:HG21	2:B:288:VAL:HG11	1.95	0.49
1:A:131:ALA:HB2	1:A:193:ILE:HG12	1.95	0.49
2:E:223:VAL:HG12	2:E:405:TRP:CZ3	2.48	0.49
2:E:517:SER:O	2:E:638:ARG:NH2	2.45	0.49
1:D:164:ALA:HB2	2:E:549:ARG:HB2	1.95	0.49
1:A:200:PHE:HE2	2:B:526:PRO:HG3	1.76	0.49
1:A:32:THR:OG1	3:F:46:G:OP1	2.29	0.49
2:B:59:GLU:OE1	2:B:119:ARG:NH2	2.42	0.48
1:A:158:GLN:OE1	1:A:201:ARG:NH2	2.42	0.48
2:E:669:ASP:HB2	7:E:908:EDO:H12	1.95	0.48
2:B:549:ARG:HG3	2:B:560:GLN:HG2	1.95	0.48
2:E:45:PRO:HA	2:E:160:LEU:HD23	1.95	0.48
1:D:173:ARG:NH2	1:D:176:THR:HG22	2.25	0.48
1:A:55:GLN:C	1:A:57:ALA:H	2.22	0.47
1:A:229:HIS:HA	2:B:490:VAL:O	2.14	0.47
3:F:69:U:H2'	3:F:70:G:C8	2.49	0.47
2:E:171:PRO:HA	2:E:372:ARG:HE	1.80	0.47
3:F:17:C:O2'	3:F:61:C:O2'	2.32	0.47
2:B:46:VAL:HG12	2:B:106:PRO:HD3	1.96	0.47
2:E:376:PRO:HG2	2:E:414:TRP:HB3	1.96	0.47
2:B:243:TRP:CG	9:B:915:EPE:H32	2.49	0.47
2:E:134:GLY:HA3	2:E:249:LEU:HD11	1.96	0.47
2:B:416:PRO:HB2	2:B:461:PRO:HG2	1.96	0.47
1:D:149:PRO:HD2	1:D:152:HIS:CD2	2.50	0.46
2:B:412:ASP:OD1	2:B:412:ASP:N	2.40	0.46
3:C:1:G:H2'	3:C:2:G:C8	2.50	0.46
1:D:217:GLU:HG3	1:D:306:PHE:O	2.15	0.46
2:E:359:ARG:HG2	2:E:360:LEU:HD23	1.98	0.46
1:D:129:GLU:OE1	1:D:187:ARG:NH2	2.42	0.46
2:E:558:ARG:N	2:E:559:PRO:HD3	2.31	0.46
1:D:165:PRO:HG2	2:E:599:THR:HB	1.98	0.45
2:E:22:THR:HG22	2:E:24:GLY:H	1.82	0.45
3:F:8:U:O2'	3:F:21:A:N1	2.34	0.45
2:B:564:THR:OG1	2:B:719:GLU:OE1	2.29	0.45
1:D:135:GLU:HG2	1:D:200:PHE:CE1	2.52	0.45
2:E:214:PRO:HG2	2:E:285:THR:HA	1.98	0.44
1:D:175:HIS:CE1	1:D:177:SER:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:277:HIS:NE2	2:E:344:GLU:HG2	2.32	0.44
1:D:177:SER:OG	1:D:217:GLU:OE1	2.28	0.44
2:E:552:ASN:OD1	2:E:552:ASN:N	2.51	0.44
3:F:21:A:H3'	3:F:22:U:H5''	1.99	0.44
2:B:214:PRO:HB2	2:B:285:THR:HG23	1.99	0.44
2:E:429:ILE:HD12	2:E:475:VAL:HG21	2.00	0.44
2:B:84:ILE:HD11	2:B:119:ARG:HB2	1.99	0.44
2:E:308:ASP:HB2	2:E:359:ARG:HH12	1.83	0.44
2:B:517:SER:O	2:B:638:ARG:NH2	2.49	0.44
1:D:229:HIS:HA	2:E:490:VAL:O	2.16	0.44
1:A:185:LEU:O	2:B:610:ARG:NH2	2.50	0.44
1:A:255:PHE:HD2	1:A:261:SER:HB3	1.81	0.44
2:B:722:LEU:HD23	2:B:725:ILE:HD12	2.00	0.44
1:A:55:GLN:O	1:A:56:ARG:HB3	2.18	0.43
2:B:73:VAL:HG11	2:B:98:VAL:HG21	1.99	0.43
3:F:18:G:O2'	3:F:58:G:N2	2.46	0.43
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.83	0.43
1:A:177:SER:N	1:A:178:PRO:HD2	2.33	0.43
2:B:307:LEU:HD13	2:B:313:LEU:HD11	2.00	0.43
2:B:807:GLU:HG2	3:F:40:G:P	2.57	0.43
2:E:592:VAL:HG23	2:E:627:PRO:HD2	2.00	0.43
2:E:56:ALA:N	2:E:72:ALA:O	2.47	0.43
2:E:330:ALA:HA	2:E:333:GLU:HB3	1.99	0.43
2:E:671:THR:HB	7:E:906:EDO:H22	2.00	0.43
1:A:116:ALA:HB1	1:A:196:ILE:HG21	2.00	0.43
2:B:680:TRP:HB3	2:B:685:CYS:HB2	2.00	0.43
1:A:210:THR:HG23	1:A:213:PHE:HB3	2.01	0.43
2:B:330:ALA:O	2:B:333:GLU:HG2	2.19	0.43
2:E:202:ARG:HE	2:E:202:ARG:HB3	1.63	0.43
2:E:430:ALA:HB2	2:E:479:LEU:HD11	2.01	0.43
2:E:763:VAL:HG13	2:E:817:ALA:HB1	2.00	0.43
1:D:133:GLY:HA3	1:D:179:VAL:HG22	2.01	0.43
2:E:308:ASP:HB2	2:E:359:ARG:NH1	2.34	0.43
1:D:161:PHE:HD2	2:E:550:VAL:HG11	1.83	0.42
2:E:307:LEU:HD13	2:E:313:LEU:HD11	2.00	0.42
2:B:777:PHE:HA	2:E:642:GLY:HA2	2.01	0.42
1:D:267:TRP:HE1	1:D:275:ALA:HA	1.84	0.42
2:E:171:PRO:HA	2:E:372:ARG:NE	2.34	0.42
2:B:-1:ASN:HB2	2:B:169:ILE:O	2.19	0.42
2:B:119:ARG:HD2	2:B:119:ARG:HA	1.85	0.42
2:B:430:ALA:HB2	2:B:479:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LYS:HB2	1:D:61:LYS:HE2	1.71	0.42
1:D:124:ILE:HD12	2:E:499:GLY:HA2	2.02	0.42
2:B:225:ARG:HD3	2:B:379:SER:HB2	2.02	0.42
1:D:182:ARG:HG2	1:D:182:ARG:NH1	2.35	0.42
1:A:111:PRO:HG3	1:A:337:PHE:CD1	2.55	0.42
1:D:339:VAL:HG11	2:E:516:LEU:HD23	2.02	0.42
1:A:216:VAL:O	1:A:307:GLY:HA2	2.20	0.42
2:B:743:PHE:CE1	2:B:797:ARG:HG3	2.55	0.42
1:A:50:VAL:HG22	1:A:56:ARG:NH1	2.35	0.41
1:A:58:GLU:HB3	1:A:59:ALA:H	1.64	0.41
1:D:85:ARG:O	1:D:89:VAL:HG13	2.20	0.41
2:E:44:GLY:HA3	2:E:45:PRO:HA	1.81	0.41
2:B:509:THR:HG22	2:B:665:ALA:HB1	2.01	0.41
1:A:55:GLN:HG2	1:A:56:ARG:N	2.35	0.41
2:E:46:VAL:HG22	2:E:160:LEU:HD22	2.03	0.41
2:B:552:ASN:OD1	2:B:552:ASN:N	2.54	0.41
1:D:287:HIS:HB3	1:D:290:VAL:HG23	2.02	0.41
1:A:78:LEU:O	1:A:82:ARG:HB2	2.21	0.41
2:B:20:ASP:H	7:B:914:EDO:H11	1.86	0.41
2:B:140:ILE:H	2:B:140:ILE:HG13	1.71	0.41
1:A:8:THR:HG22	1:A:11:VAL:HG23	2.04	0.40
1:A:71:GLN:O	1:A:74:TYR:N	2.54	0.40
1:A:289:ASN:CG	2:B:470:GLN:HE22	2.28	0.40
1:D:182:ARG:HG2	1:D:182:ARG:HH11	1.86	0.40
1:A:211:PRO:C	1:A:212:ILE:HD13	2.46	0.40
1:A:136:VAL:H	2:B:626:GLN:HE22	1.69	0.40
1:A:176:THR:OG1	1:A:217:GLU:OE1	2.28	0.40
2:B:764:ARG:HG2	2:B:771:LEU:HD23	2.04	0.40
9:B:915:EPE:H61	9:B:915:EPE:H102	1.66	0.40
2:E:303:ILE:HG13	2:E:304:GLU:N	2.35	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	324/341 (95%)	310 (96%)	11 (3%)	3 (1%)	14	14
1	D	335/341 (98%)	324 (97%)	11 (3%)	0	100	100
2	B	834/835 (100%)	810 (97%)	21 (2%)	3 (0%)	30	34
2	E	793/835 (95%)	762 (96%)	28 (4%)	3 (0%)	30	34
All	All	2286/2352 (97%)	2206 (96%)	71 (3%)	9 (0%)	30	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
2	B	373	THR
2	E	324	GLY
2	E	373	THR
1	A	321	PRO
2	B	559	PRO
2	B	324	GLY
1	A	340	GLY
2	E	102	GLY

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	253/268 (94%)	247 (98%)	6 (2%)	43	57
1	D	261/268 (97%)	255 (98%)	6 (2%)	44	58
2	B	651/652 (100%)	648 (100%)	3 (0%)	81	89
2	E	616/652 (94%)	601 (98%)	15 (2%)	43	57
All	All	1781/1840 (97%)	1751 (98%)	30 (2%)	55	68

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	50	VAL
1	A	63	VAL
1	A	175	HIS
1	A	176	THR
1	A	264	VAL
2	B	415	SER
2	B	564	THR
2	B	784	GLN
1	D	2	LEU
1	D	103[A]	ARG
1	D	103[B]	ARG
1	D	188	GLU
1	D	331	VAL
1	D	339	VAL
2	E	17	SER
2	E	41	ILE
2	E	140	ILE
2	E	193	ASP
2	E	293	SER
2	E	301	ASP
2	E	303	ILE
2	E	333	GLU
2	E	343	LEU
2	E	357	GLN
2	E	564	THR
2	E	584	VAL
2	E	622	SER
2	E	693	SER
2	E	707	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	28	GLN
2	B	35	HIS
2	B	452	HIS
2	B	505	GLN
1	D	142	ASN
1	D	215	GLN
2	E	166	HIS
2	E	200	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	245	GLN
2	E	277	HIS
2	E	594	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	70/77 (90%)	6 (8%)	0
3	F	70/77 (90%)	8 (11%)	0
All	All	140/154 (90%)	14 (10%)	0

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	6	G
3	C	16	U
3	C	21	A
3	C	22	U
3	C	23	G
3	C	43	G
3	F	4	C
3	F	7	G
3	F	16	U
3	F	17	C
3	F	18	G
3	F	22	U
3	F	23	G
3	F	69	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 7 are monoatomic - leaving 32 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	$\# Z > 2$
6	ACT	E	905	-	3,3,3	1.36	0	3,3,3	1.38	0
6	ACT	B	901	-	3,3,3	1.36	0	3,3,3	1.36	0
6	ACT	B	904	-	3,3,3	1.35	0	3,3,3	1.36	0
6	ACT	A	403	-	3,3,3	1.32	0	3,3,3	1.35	0
8	PEG	B	916	-	6,6,6	0.10	0	5,5,5	0.10	0
9	EPE	B	915	-	15,15,15	0.80	1 (6%)	19,20,20	1.65	4 (21%)
6	ACT	B	912	-	3,3,3	1.38	0	3,3,3	1.36	0
6	ACT	B	903	-	3,3,3	1.37	0	3,3,3	1.37	0
7	EDO	C	101	-	3,3,3	0.42	0	2,2,2	0.42	0
7	EDO	B	913	-	3,3,3	0.42	0	2,2,2	0.37	0
7	EDO	E	908	-	3,3,3	0.42	0	2,2,2	0.38	0
7	EDO	E	906	-	3,3,3	0.43	0	2,2,2	0.38	0
8	PEG	B	906	-	6,6,6	0.11	0	5,5,5	0.12	0
10	DMS	D	404	-	3,3,3	0.67	0	3,3,3	0.52	0
6	ACT	B	908	-	3,3,3	1.37	0	3,3,3	1.36	0
4	AX7	A	401	-	11,11,11	4.24	6 (54%)	15,15,15	3.60	6 (40%)
6	ACT	A	404	-	3,3,3	1.38	0	3,3,3	1.36	0
7	EDO	B	914	-	3,3,3	0.41	0	2,2,2	0.40	0
8	PEG	B	905	-	6,6,6	0.10	0	5,5,5	0.13	0
6	ACT	B	910	-	3,3,3	1.36	0	3,3,3	1.35	0
6	ACT	E	903	-	3,3,3	1.38	0	3,3,3	1.36	0
6	ACT	B	911	-	3,3,3	1.38	0	3,3,3	1.37	0
6	ACT	B	909	-	3,3,3	1.37	0	3,3,3	1.38	0
6	ACT	D	403	-	3,3,3	1.37	0	3,3,3	1.33	0
6	ACT	E	904	-	3,3,3	1.37	0	3,3,3	1.36	0
7	EDO	E	907	-	3,3,3	0.42	0	2,2,2	0.40	0
6	ACT	B	907	-	3,3,3	1.38	0	3,3,3	1.37	0
6	ACT	C	102	-	3,3,3	1.36	0	3,3,3	1.36	0
7	EDO	E	901	-	3,3,3	0.43	0	2,2,2	0.37	0
7	EDO	B	902	-	3,3,3	0.42	0	2,2,2	0.39	0
4	AX7	D	401	-	11,11,11	4.21	6 (54%)	15,15,15	3.56	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PEG	E	902	-	6,6,6	0.11	0	5,5,5	0.11	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
7	EDO	B	913	-	-	0/1/1/1	-
7	EDO	E	908	-	-	0/1/1/1	-
7	EDO	E	906	-	-	0/1/1/1	-
8	PEG	B	906	-	-	1/4/4/4	-
7	EDO	E	901	-	-	0/1/1/1	-
8	PEG	B	916	-	-	2/4/4/4	-
7	EDO	B	902	-	-	0/1/1/1	-
8	PEG	B	905	-	-	1/4/4/4	-
8	PEG	E	902	-	-	2/4/4/4	-
7	EDO	B	914	-	-	0/1/1/1	-
9	EPE	B	915	-	-	6/9/19/19	0/1/1/1
4	AX7	A	401	-	-	-	0/2/2/2
4	AX7	D	401	-	-	-	0/2/2/2
7	EDO	C	101	-	-	0/1/1/1	-
7	EDO	E	907	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	AX7	CAI-NAF	9.10	1.55	1.38
4	D	401	AX7	CAI-NAF	9.09	1.55	1.38
4	A	401	AX7	CAJ-NAG	-7.14	1.25	1.39
4	D	401	AX7	CAJ-NAG	-7.00	1.25	1.39
4	A	401	AX7	CAH-NAG	-5.25	1.25	1.34
4	D	401	AX7	CAH-NAG	-5.15	1.25	1.34
4	D	401	AX7	CAH-NAA	4.85	1.45	1.34
4	A	401	AX7	CAH-NAA	4.73	1.45	1.34
9	B	915	EPE	C10-S	2.61	1.81	1.77
4	A	401	AX7	CAI-CAJ	2.56	1.43	1.40
4	D	401	AX7	CAI-CAJ	2.49	1.43	1.40
4	A	401	AX7	CAE-CAJ	-2.11	1.36	1.40
4	D	401	AX7	CAE-CAJ	-2.01	1.36	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	AX7	CAJ-NAG-CAH	10.75	122.17	104.19
4	D	401	AX7	CAJ-NAG-CAH	10.75	122.16	104.19
4	A	401	AX7	CAI-CAJ-NAG	-5.66	101.67	109.42
4	D	401	AX7	CAI-CAJ-NAG	-5.63	101.71	109.42
9	B	915	EPE	C5-N4-C3	4.23	117.96	108.84
4	A	401	AX7	CAI-NAF-CAH	-4.05	99.98	107.39
4	D	401	AX7	CAI-NAF-CAH	-3.93	100.20	107.39
9	B	915	EPE	C7-N4-C3	3.11	119.52	111.24
4	D	401	AX7	CAE-CAJ-NAG	3.08	136.94	128.21
4	A	401	AX7	CAE-CAJ-NAG	3.00	136.73	128.21
4	A	401	AX7	CAD-CAI-CAJ	-2.89	118.93	122.10
4	D	401	AX7	CAD-CAI-CAJ	-2.70	119.14	122.10
9	B	915	EPE	C7-N4-C5	2.31	117.39	111.24
9	B	915	EPE	O3S-S-C10	2.30	110.50	106.00
4	A	401	AX7	NAA-CAH-NAF	2.03	125.73	122.70

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	915	EPE	C9-C10-S-O1S
9	B	915	EPE	C9-C10-S-O2S
9	B	915	EPE	C9-C10-S-O3S
8	E	902	PEG	O2-C3-C4-O4
9	B	915	EPE	N4-C7-C8-O8
9	B	915	EPE	C8-C7-N4-C3
8	E	902	PEG	O1-C1-C2-O2
9	B	915	EPE	S-C10-C9-N1
8	B	916	PEG	O2-C3-C4-O4
8	B	906	PEG	C4-C3-O2-C2
8	B	905	PEG	C1-C2-O2-C3
8	B	916	PEG	C4-C3-O2-C2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

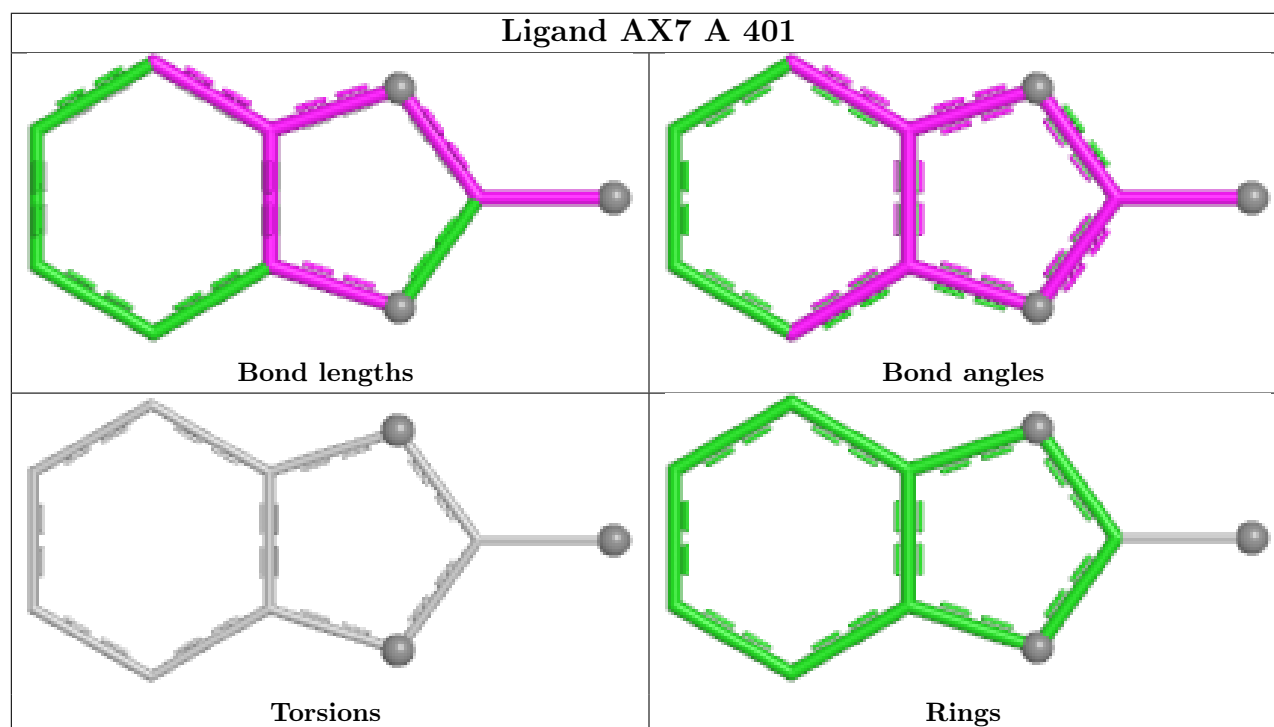
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	915	EPE	2	0
7	C	101	EDO	2	0
7	E	908	EDO	1	0
7	E	906	EDO	1	0
4	A	401	AX7	1	0

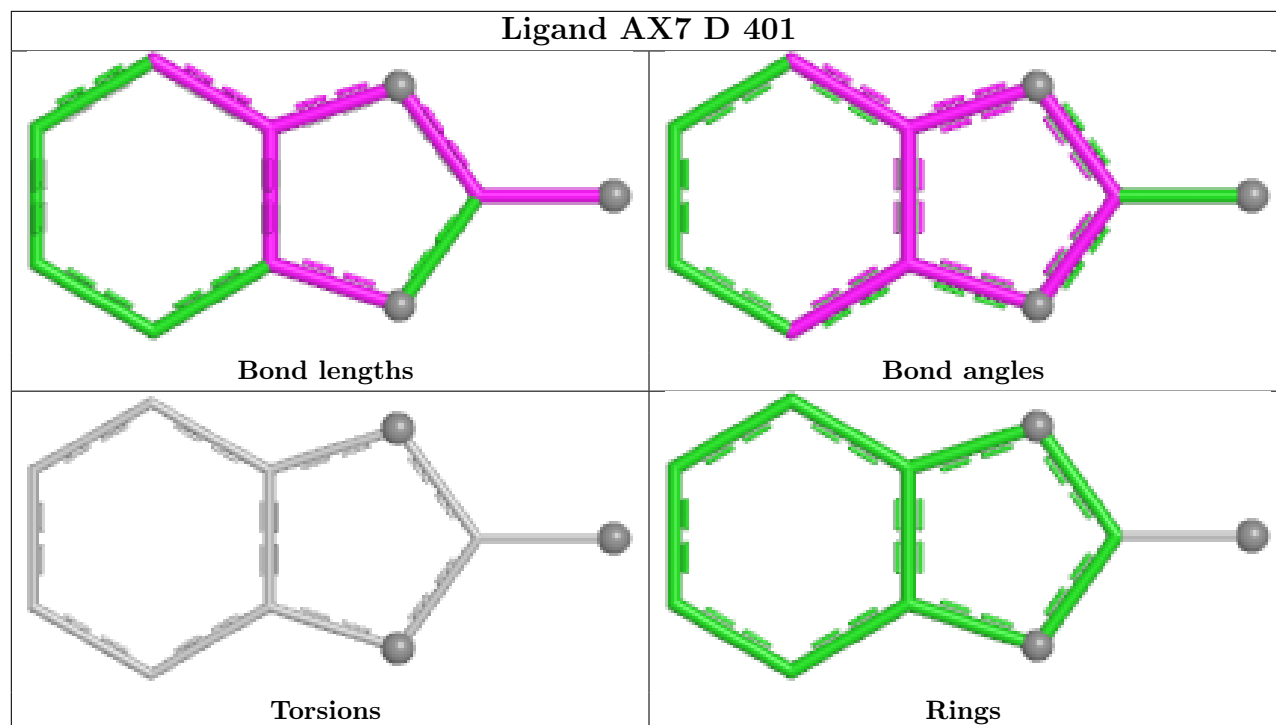
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	914	EDO	1	0
8	B	905	PEG	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.





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	332/341 (97%)	1.12	92 (27%)	1 1	19, 51, 112, 159	0
1	D	338/341 (99%)	1.12	80 (23%)	2 1	20, 54, 105, 144	1 (0%)
2	B	834/835 (99%)	-0.04	30 (3%)	46 52	16, 30, 71, 111	2 (0%)
2	E	805/835 (96%)	1.06	226 (28%)	1 1	16, 51, 119, 215	0
3	C	71/77 (92%)	0.34	12 (16%)	4 4	22, 49, 165, 172	0
3	F	71/77 (92%)	1.41	30 (42%)	0 0	30, 75, 177, 205	0
All	All	2451/2506 (97%)	0.69	470 (19%)	3 3	16, 40, 112, 215	3 (0%)

All (470) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	HIS	6.8
2	E	554	LEU	6.7
1	A	341	ALA	6.6
2	E	557	ASP	6.1
1	A	59	ALA	5.8
1	D	341	ALA	5.5
2	E	319	ALA	5.5
2	E	78	ARG	5.5
1	D	145	ALA	5.4
2	E	103	ALA	5.3
2	B	599	THR	5.3
1	A	149	PRO	5.3
2	E	102	GLY	5.3
1	D	136	VAL	5.2
1	D	275	ALA	5.2
2	E	234	ILE	5.1
2	E	527	PHE	5.0
1	D	269	ALA	5.0
1	D	92	ALA	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	259	ALA	4.9
2	E	334	VAL	4.9
1	D	146	LEU	4.8
1	A	65	ALA	4.8
2	E	243	TRP	4.8
1	A	44	ALA	4.7
2	E	315	VAL	4.7
2	E	301	ASP	4.7
1	D	276	ALA	4.7
1	D	267	TRP	4.7
2	E	58	ILE	4.7
1	A	180	GLN	4.6
1	A	41	LEU	4.6
1	A	47	ALA	4.6
2	E	316	ASP	4.6
2	E	141	LEU	4.5
1	A	268	PHE	4.5
2	E	318	ALA	4.5
2	E	104	THR	4.5
2	E	300	LEU	4.5
1	D	164	ALA	4.5
2	E	607	VAL	4.4
2	E	394	ALA	4.4
2	E	84	ILE	4.3
2	E	336	ALA	4.3
2	E	362	LEU	4.2
1	A	50	VAL	4.2
1	A	42	ALA	4.2
1	A	158	GLN	4.2
2	E	326	VAL	4.2
1	D	1	MET	4.1
1	D	148	PHE	4.1
2	E	619	LEU	4.1
2	E	548	THR	4.1
2	E	126	CYS	4.1
1	A	35	LEU	4.1
2	E	90	PHE	4.1
2	E	294	GLY	4.1
2	E	71	CYS	4.1
1	D	134	PRO	4.1
2	E	363	PRO	4.1
2	E	313	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	142	VAL	4.1
2	E	160	LEU	4.0
2	E	599	THR	4.0
1	D	316	PHE	4.0
1	A	205	LEU	4.0
1	D	132	GLU	4.0
2	E	70	ALA	4.0
2	E	216	THR	4.0
1	A	48	LEU	4.0
1	D	274	GLY	3.9
2	E	80	TYR	3.9
3	F	17	C	3.9
1	D	257	PHE	3.9
2	E	109	PHE	3.9
2	E	75	ILE	3.9
1	A	43	LEU	3.9
2	E	275	HIS	3.9
2	E	393	ILE	3.9
2	E	100	LEU	3.9
3	C	17	C	3.9
1	A	150	ALA	3.9
1	A	276	ALA	3.9
1	A	63	VAL	3.8
2	E	236	PRO	3.8
2	E	391	ALA	3.8
2	B	783	PRO	3.8
2	E	49	PRO	3.8
1	D	205	LEU	3.8
2	E	105	LEU	3.8
1	A	49	ALA	3.7
2	E	232	ILE	3.7
2	E	245	GLN	3.7
2	E	111	ILE	3.7
2	E	341	VAL	3.7
1	A	157	GLU	3.6
2	E	360	LEU	3.6
2	E	337	ASP	3.6
1	D	161	PHE	3.6
1	D	163	ILE	3.6
1	D	212	ILE	3.6
1	D	4	PRO	3.6
2	E	553	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	93	GLU	3.6
1	D	268	PHE	3.6
1	A	40	PRO	3.6
2	B	-2	SER	3.6
2	E	95	LEU	3.6
1	A	267	TRP	3.6
2	E	291	ALA	3.6
3	F	61	C	3.5
1	A	146	LEU	3.5
1	D	91	VAL	3.5
1	A	275	ALA	3.5
2	E	152	ALA	3.5
2	E	237	ALA	3.5
2	E	330	ALA	3.5
1	D	151	ASP	3.5
2	E	45	PRO	3.5
2	E	358	ARG	3.5
2	E	338	SER	3.5
1	A	153	PRO	3.5
2	E	239	VAL	3.5
2	E	618	MET	3.5
2	E	123	GLY	3.5
1	D	165	PRO	3.4
2	E	320	THR	3.4
1	A	2	LEU	3.4
2	E	303	ILE	3.4
2	B	109	PHE	3.4
2	E	302	GLY	3.4
2	E	131	LEU	3.4
3	F	71	G	3.4
1	A	69	ALA	3.4
2	E	222	GLY	3.4
1	D	176	THR	3.3
1	D	154	ALA	3.3
2	E	556	ALA	3.3
1	D	133	GLY	3.3
2	E	132	ASN	3.3
2	E	327	MET	3.3
2	E	106	PRO	3.3
2	E	144	PRO	3.3
2	E	258	PRO	3.3
2	E	606	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	57	C	3.3
1	A	316	PHE	3.3
2	E	546	MET	3.3
2	B	551	LEU	3.3
2	E	293	SER	3.3
2	E	203	VAL	3.3
1	D	172	LEU	3.3
1	A	11	VAL	3.3
2	E	550	VAL	3.3
2	E	593	VAL	3.3
2	E	143	LEU	3.2
1	A	76	GLU	3.2
1	D	149	PRO	3.2
2	E	204	PRO	3.2
2	E	559	PRO	3.2
3	C	1	G	3.2
3	F	1	G	3.2
2	E	344	GLU	3.2
2	E	101	PRO	3.2
2	E	617	ALA	3.2
3	F	48	U	3.2
2	E	307	LEU	3.2
2	E	526	PRO	3.2
1	A	154	ALA	3.2
1	D	207	ALA	3.2
2	E	260	VAL	3.2
1	D	155	ARG	3.1
2	E	359	ARG	3.1
2	B	601	GLY	3.1
2	E	233	GLY	3.1
2	E	395	GLY	3.1
1	D	153	PRO	3.1
2	E	323	ILE	3.1
1	A	176	THR	3.1
2	B	603	GLY	3.1
2	B	116	ALA	3.1
2	E	329	ALA	3.1
2	E	125	ILE	3.1
2	E	235	ASP	3.1
2	E	92	VAL	3.1
2	E	561	LEU	3.1
1	A	159	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	530	ALA	3.1
1	A	179	VAL	3.1
1	A	60	GLY	3.0
2	E	552	ASN	3.0
2	E	46	VAL	3.0
1	D	147	ASN	3.0
1	A	57	ALA	3.0
1	A	70	ALA	3.0
2	E	624	PRO	3.0
2	E	551	LEU	3.0
1	A	274	GLY	3.0
1	D	200	PHE	3.0
1	A	4	PRO	3.0
1	A	66	ALA	3.0
1	D	210	THR	3.0
2	B	120	ASN	3.0
2	E	317	ASP	3.0
3	F	19	G	3.0
1	D	159	ASP	2.9
3	F	18	G	2.9
2	E	213	TRP	2.9
2	E	242	TRP	2.9
2	E	56	ALA	2.9
2	B	115	LYS	2.9
1	A	151	ASP	2.9
2	B	412	ASP	2.9
2	E	328	GLY	2.9
2	E	150	PRO	2.9
1	A	207	ALA	2.9
1	D	2	LEU	2.9
1	D	59	ALA	2.9
2	E	72	ALA	2.9
2	E	155	ALA	2.9
2	E	528	LEU	2.9
2	E	594	GLN	2.9
3	F	69	U	2.9
1	D	206	ASP	2.9
2	E	-1	ASN	2.9
1	A	55	GLN	2.9
3	C	4	C	2.9
2	E	73	VAL	2.9
3	F	56	U	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	557	ASP	2.9
1	A	36	GLY	2.8
1	A	61	LYS	2.8
2	E	361	HIS	2.8
2	B	554	LEU	2.8
2	E	310	ALA	2.8
2	E	321	ALA	2.8
2	E	51	THR	2.8
2	E	339	THR	2.8
1	A	175	HIS	2.8
3	F	5	A	2.8
2	E	298	VAL	2.8
3	F	7	G	2.8
1	A	160	THR	2.8
2	B	62	THR	2.8
2	E	88	THR	2.8
2	E	390	LEU	2.8
1	D	143	PHE	2.8
2	E	83	ILE	2.8
2	E	332	THR	2.8
1	A	64	ASN	2.8
2	E	601	GLY	2.8
2	E	60	GLU	2.8
1	A	62	ARG	2.8
3	F	22	U	2.8
2	E	256	THR	2.7
1	D	203	ASP	2.7
2	E	79	GLN	2.7
2	E	340	ASP	2.7
1	D	204	GLU	2.7
1	D	20	LEU	2.7
2	E	322	ALA	2.7
1	D	180	GLN	2.7
2	E	296	THR	2.7
2	E	279	ARG	2.7
2	E	335	ARG	2.7
2	B	118	GLY	2.7
2	E	531	GLY	2.7
2	E	409	PRO	2.7
2	E	238	ALA	2.7
1	A	141	PHE	2.7
3	C	3	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	38	ARG	2.7
2	E	558	ARG	2.7
3	F	51	G	2.7
1	A	20	LEU	2.7
3	F	55	U	2.6
2	E	562	ALA	2.6
1	A	74	TYR	2.6
1	D	162	TYR	2.6
2	E	47	ASP	2.6
2	E	280	ASN	2.6
2	E	107	GLY	2.6
1	D	150	ALA	2.6
1	A	22	ASP	2.6
2	B	527	PHE	2.6
1	A	56	ARG	2.6
2	E	396	GLY	2.6
2	E	410	PRO	2.6
2	E	386	CYS	2.6
1	D	139	GLU	2.6
1	A	145	ALA	2.6
2	E	148	ALA	2.6
2	E	292	ARG	2.6
1	D	208	THR	2.6
2	E	140	ILE	2.6
3	F	4	C	2.6
1	A	78	LEU	2.6
3	C	5	A	2.6
3	C	48	U	2.6
2	E	387	ALA	2.6
1	A	9	THR	2.6
2	E	285	THR	2.6
1	A	91	VAL	2.6
2	E	288	VAL	2.6
2	E	331	SER	2.6
2	E	452	HIS	2.6
1	D	166	GLU	2.5
3	F	16	U	2.5
3	F	54	G	2.5
1	A	10	ALA	2.5
1	A	134	PRO	2.5
1	D	211	PRO	2.5
2	E	282	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	71	GLN	2.5
1	D	170	GLN	2.5
3	F	62	C	2.5
1	A	172	LEU	2.5
2	E	89	ASN	2.5
2	B	831	GLY	2.5
1	A	148	PHE	2.5
1	D	54	GLU	2.5
2	E	59	GLU	2.5
3	C	20	U	2.5
2	E	13	ALA	2.5
2	E	129	ALA	2.5
2	E	277	HIS	2.5
2	E	108	GLY	2.5
2	E	603	GLY	2.5
3	C	2	G	2.5
1	D	50	VAL	2.4
3	C	69	U	2.4
2	E	249	LEU	2.4
2	E	153	ASP	2.4
2	E	308	ASP	2.4
2	E	276	ALA	2.4
2	E	529	PRO	2.4
1	D	138	THR	2.4
3	F	58	G	2.4
2	E	274	MET	2.4
3	F	52	C	2.4
1	A	45	ARG	2.4
1	A	72	ARG	2.4
1	D	46	GLN	2.4
2	E	74	ASP	2.4
2	B	559	PRO	2.4
1	D	156	GLY	2.4
1	A	174	THR	2.4
2	E	309	THR	2.4
3	C	6	G	2.4
3	C	71	G	2.4
2	E	97	VAL	2.4
1	D	48	LEU	2.4
1	D	22	ASP	2.4
1	A	131	ALA	2.4
1	A	53	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	201	SER	2.4
2	B	546	MET	2.4
1	A	68	ASN	2.3
1	D	40	PRO	2.3
1	D	52	PRO	2.3
1	D	321	PRO	2.3
2	E	42	PRO	2.3
2	E	128	ALA	2.3
2	E	147	ALA	2.3
1	D	160	THR	2.3
2	B	594	GLN	2.3
2	E	158	LEU	2.3
2	E	214	PRO	2.3
2	E	611	PRO	2.3
1	D	94	GLY	2.3
2	B	782	GLY	2.3
1	A	13	ALA	2.3
2	E	254	ARG	2.3
1	D	266	VAL	2.3
2	E	96	VAL	2.3
1	D	171	LEU	2.3
3	F	50	G	2.3
1	A	12	ASP	2.3
1	D	167	ASP	2.3
3	F	49	C	2.3
2	E	414	TRP	2.3
1	A	14	ALA	2.3
2	E	297	ALA	2.3
1	D	177	SER	2.3
2	E	549	ARG	2.3
2	E	220	GLU	2.3
2	B	602	VAL	2.3
1	A	90	LEU	2.3
1	D	7	LEU	2.3
2	E	133	LEU	2.3
2	E	122	ASP	2.3
2	E	620	ASP	2.3
2	E	48	GLY	2.3
3	F	59	A	2.3
2	B	612	THR	2.3
2	B	606	PRO	2.2
1	A	1	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	29	ARG	2.2
2	E	306	LYS	2.2
2	E	343	LEU	2.2
2	E	124	MET	2.2
2	E	44	GLY	2.2
2	E	324	GLY	2.2
1	D	47	ALA	2.2
1	D	131	ALA	2.2
2	E	342	LEU	2.2
2	E	786	GLY	2.2
3	F	6	G	2.2
1	A	135	GLU	2.2
1	D	88	ALA	2.2
1	A	168	SER	2.2
1	A	18	ILE	2.2
2	E	52	VAL	2.2
2	E	231	VAL	2.2
2	B	618	MET	2.2
2	E	257	CYS	2.2
3	F	53	G	2.2
1	A	164	ALA	2.2
2	E	364	SER	2.2
2	E	621	ALA	2.2
1	D	181	ILE	2.1
2	B	408	ASP	2.1
2	E	312	VAL	2.1
1	A	46	GLN	2.1
1	A	23	THR	2.1
2	B	556	ALA	2.1
1	A	67	ARG	2.1
2	E	604	LEU	2.1
2	E	397	GLU	2.1
2	E	408	ASP	2.1
1	A	339	VAL	2.1
1	A	273	GLY	2.1
3	C	70	G	2.1
2	B	617	ALA	2.1
1	A	171	LEU	2.1
2	E	605	ILE	2.1
1	D	178	PRO	2.1
2	B	624	PRO	2.1
2	E	50	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	223	VAL	2.1
2	E	93	GLY	2.1
3	F	60	U	2.1
1	D	168	SER	2.1
2	E	110	THR	2.1
3	F	68	C	2.1
2	E	367	ALA	2.1
2	E	39	GLU	2.1
1	D	90	LEU	2.1
1	D	209	HIS	2.1
2	E	299	THR	2.0
1	A	132	GLU	2.0
2	E	91	ALA	2.0
2	E	389	LEU	2.0
2	E	623	LEU	2.0
1	A	212	ILE	2.0
2	E	41	ILE	2.0
2	B	64	TYR	2.0
1	A	30	VAL	2.0
2	E	602	VAL	2.0
1	A	8	THR	2.0
2	E	304	GLU	2.0
2	E	540	ALA	2.0
3	F	21	A	2.0
3	F	63	C	2.0
2	E	626	GLN	2.0
1	D	169	ARG	2.0
2	E	69	ARG	2.0
2	E	314	ILE	2.0
2	E	595	PRO	2.0
2	E	616	ILE	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 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
5	MG	F	101	1/1	0.74	0.14	56,56,56,56	0
8	PEG	E	902	7/7	0.78	0.29	41,47,53,54	0
6	ACT	B	909	4/4	0.80	0.17	43,43,49,54	0
9	EPE	B	915	15/15	0.81	0.22	65,74,84,92	0
7	EDO	B	914	4/4	0.83	0.14	41,43,45,47	0
6	ACT	B	907	4/4	0.85	0.17	49,51,52,59	0
8	PEG	B	905	7/7	0.85	0.14	30,36,48,48	0
8	PEG	B	906	7/7	0.86	0.14	45,57,63,63	0
6	ACT	E	904	4/4	0.87	0.16	44,53,54,57	0
7	EDO	E	907	4/4	0.87	0.13	43,45,48,48	0
5	MG	C	106	1/1	0.88	0.09	52,52,52,52	0
7	EDO	B	902	4/4	0.88	0.14	40,47,49,49	0
7	EDO	C	101	4/4	0.89	0.15	39,48,49,51	0
8	PEG	B	916	7/7	0.89	0.16	29,42,58,60	0
7	EDO	B	913	4/4	0.90	0.14	36,38,50,52	0
6	ACT	E	903	4/4	0.91	0.11	41,43,43,45	0
5	MG	C	105	1/1	0.91	0.08	50,50,50,50	0
7	EDO	E	906	4/4	0.91	0.14	39,46,46,47	0
6	ACT	C	102	4/4	0.92	0.12	18,23,25,38	0
6	ACT	E	905	4/4	0.92	0.10	37,41,43,50	0
7	EDO	E	908	4/4	0.92	0.10	41,41,44,50	0
6	ACT	B	903	4/4	0.92	0.09	26,40,42,53	0
6	ACT	B	904	4/4	0.93	0.12	18,28,28,36	0
4	AX7	A	401	10/10	0.93	0.10	32,43,50,52	0
5	MG	C	103	1/1	0.93	0.08	47,47,47,47	0
6	ACT	B	911	4/4	0.93	0.09	24,30,38,43	0
7	EDO	E	901	4/4	0.94	0.10	36,37,39,56	0
4	AX7	D	401	10/10	0.94	0.08	32,43,48,57	0
6	ACT	B	912	4/4	0.94	0.08	37,38,41,45	0
6	ACT	B	910	4/4	0.95	0.09	29,33,33,39	0
5	MG	C	104	1/1	0.95	0.05	47,47,47,47	0
6	ACT	B	908	4/4	0.95	0.09	40,42,44,50	0
6	ACT	A	404	4/4	0.95	0.10	32,34,37,45	0
6	ACT	D	403	4/4	0.96	0.11	13,23,31,34	0
10	DMS	D	404	4/4	0.96	0.10	52,57,62,64	0
6	ACT	B	901	4/4	0.97	0.08	24,25,32,35	0
6	ACT	A	403	4/4	0.98	0.08	11,20,26,38	0

Continued on next page...

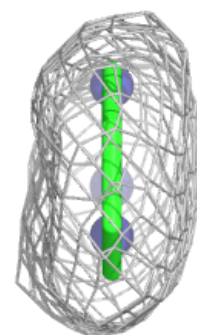
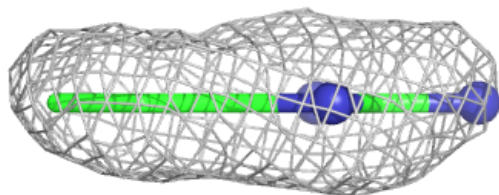
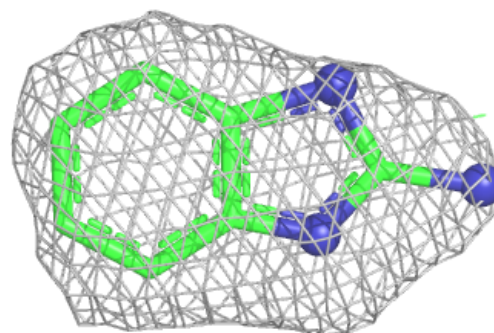
Continued from previous page...

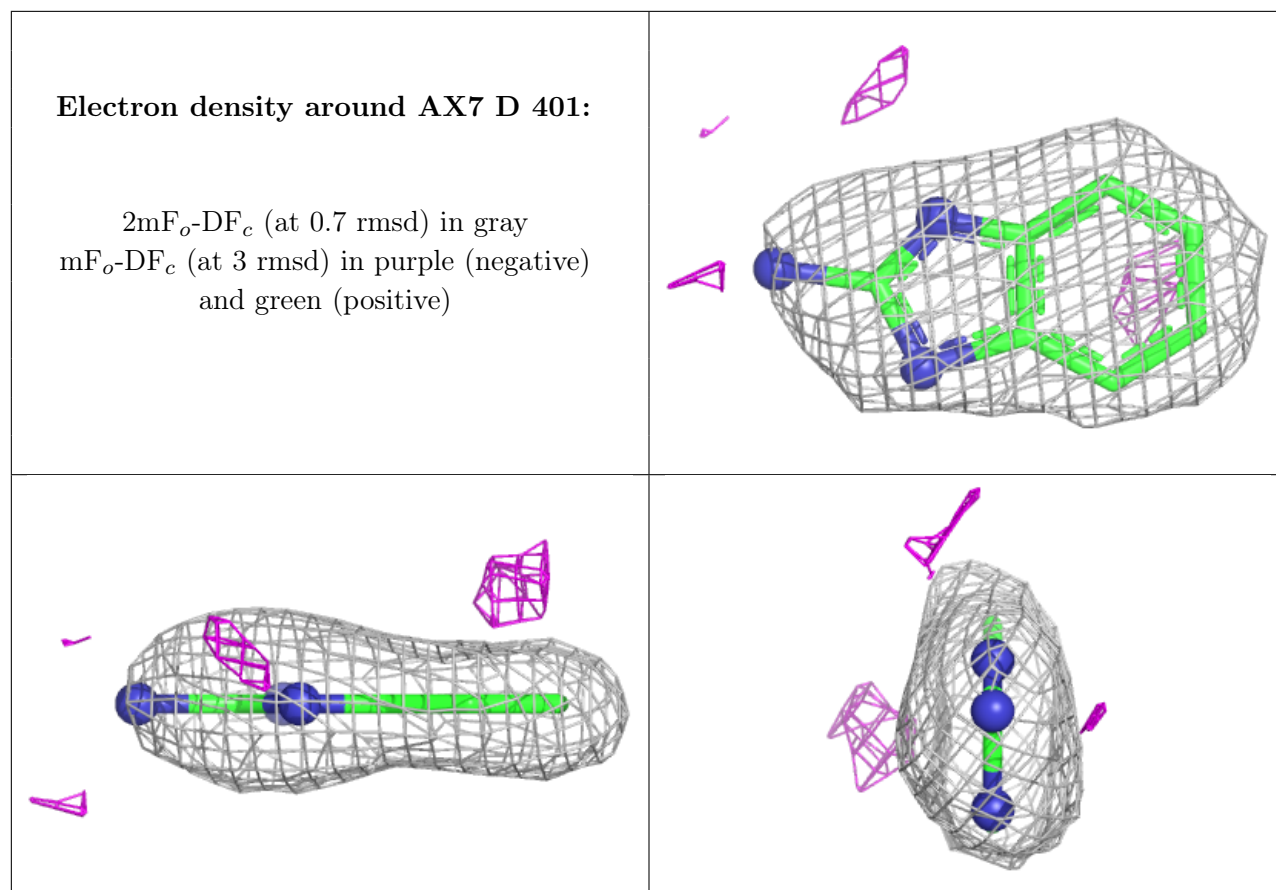
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	402	1/1	0.99	0.03	33,33,33,33	0
5	MG	A	402	1/1	0.99	0.02	20,20,20,20	0

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 AX7 A 401:

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 ⓘ

There are no such residues in this entry.