wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2025 – 02:08 PM EST

PDB ID	:	9DRV
Title	:	Crystal structure of M. tuberculosis PheRS-tRNA complex bound to inhibitor D-004
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	:	2.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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:

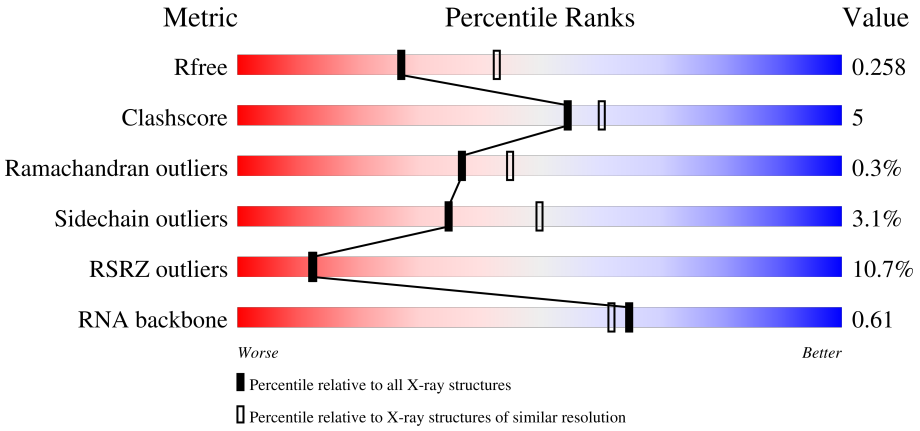
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.46 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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)
RNA backbone	3690	1040 (2.76-2.16)

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 <=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	350	19% 80% 16%
1	D	350	12% 80% 18%
2	B	835	2% 90% 9%
2	E	835	13% 82% 15%

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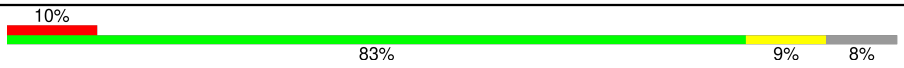
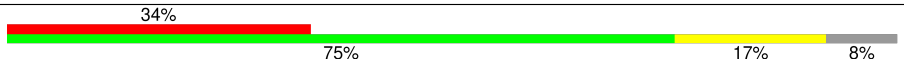
Mol	Chain	Length	Quality of chain
3	C	77	
3	F	77	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21397 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	341	Total	C	N	O	S	0	0	0
			2598	1640	465	484	9			
1	D	344	Total	C	N	O	S	0	0	0
			2640	1662	477	492	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLU	-	expression tag	UNP P9WFU3
A	-7	ASN	-	expression tag	UNP P9WFU3
A	-6	LEU	-	expression tag	UNP P9WFU3
A	-5	TYR	-	expression tag	UNP P9WFU3
A	-4	PHE	-	expression tag	UNP P9WFU3
A	-3	GLN	-	expression tag	UNP P9WFU3
A	-2	SER	-	expression tag	UNP P9WFU3
A	-1	ASN	-	expression tag	UNP P9WFU3
A	0	ALA	-	expression tag	UNP P9WFU3
D	-8	GLU	-	expression tag	UNP P9WFU3
D	-7	ASN	-	expression tag	UNP P9WFU3
D	-6	LEU	-	expression tag	UNP P9WFU3
D	-5	TYR	-	expression tag	UNP P9WFU3
D	-4	PHE	-	expression tag	UNP P9WFU3
D	-3	GLN	-	expression tag	UNP P9WFU3
D	-2	SER	-	expression tag	UNP P9WFU3
D	-1	ASN	-	expression tag	UNP P9WFU3
D	0	ALA	-	expression tag	UNP P9WFU3

- 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	0	0
			6222	3908	1127	1166	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	816	Total	C	N	O	S	0	0	0
			5992	3762	1089	1121	20			

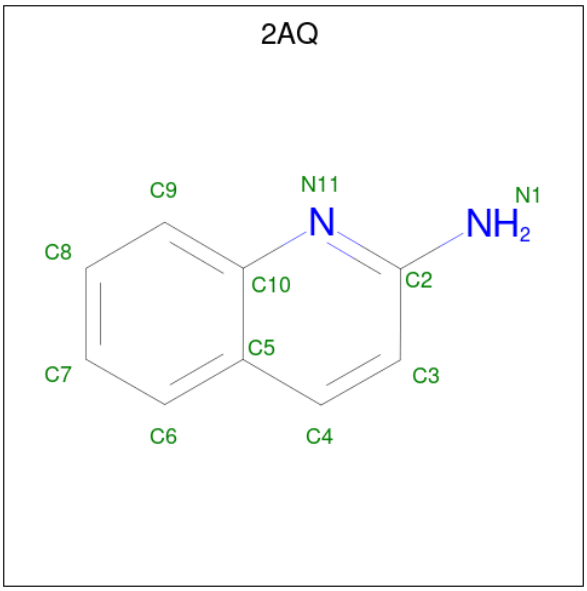
There are 8 discrepancies between the modelled and reference sequences:

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 QUINOLIN-2-AMINE (three-letter code: 2AQ) (formula: $C_9H_8N_2$) (labeled as "Ligand of Interest" by depositor).

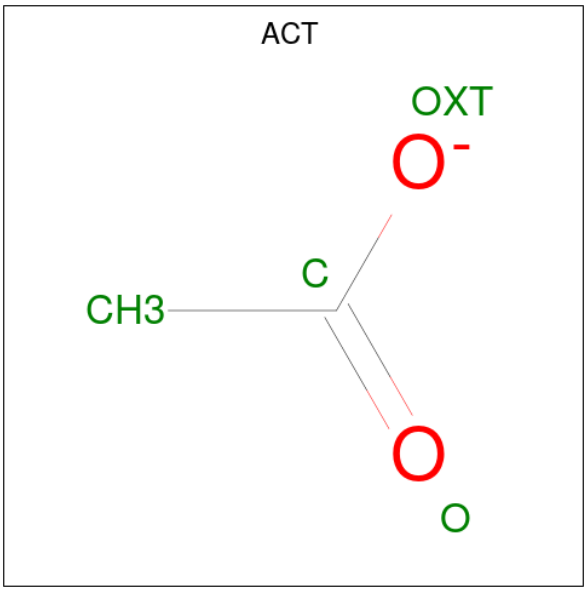


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 11 9 2	0	0
4	D	1	Total C N 11 9 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

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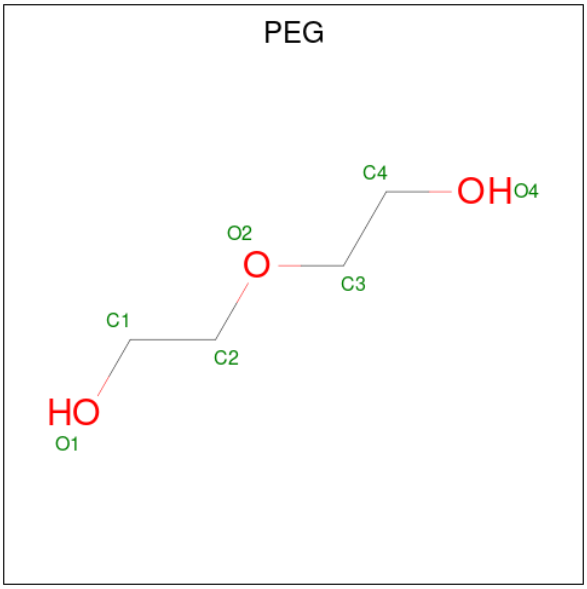
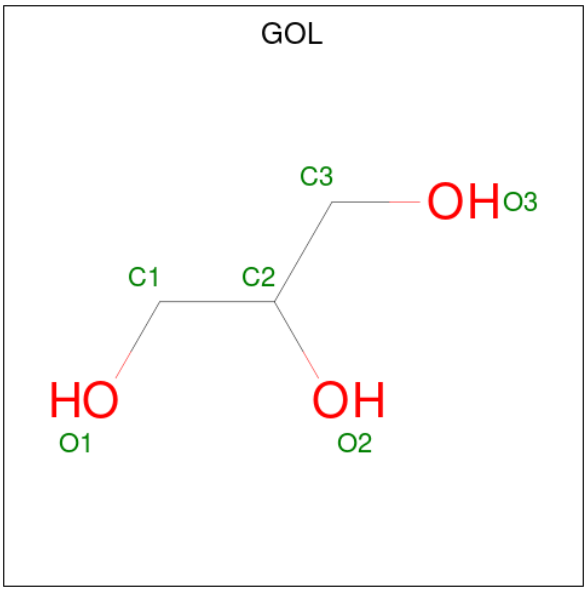
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



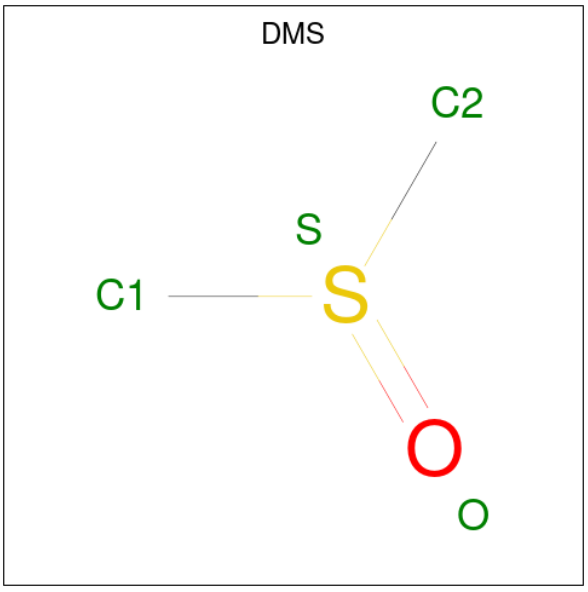
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	E	1	Total C O 7 4 3	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



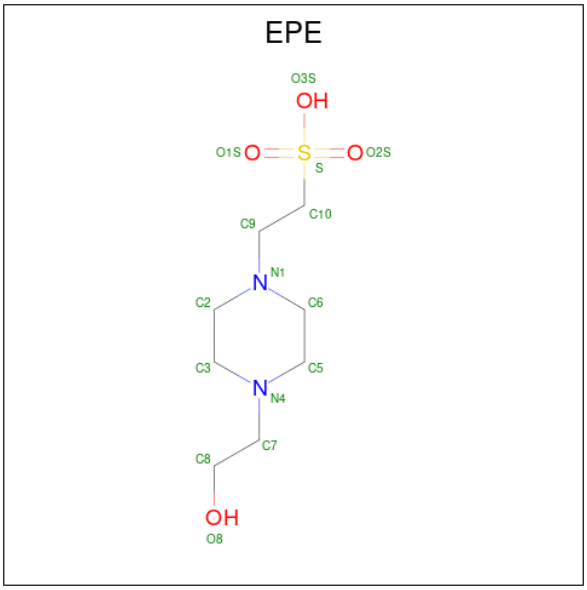
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	E	1	Total C O 6 3 3	0	0

- Molecule 9 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



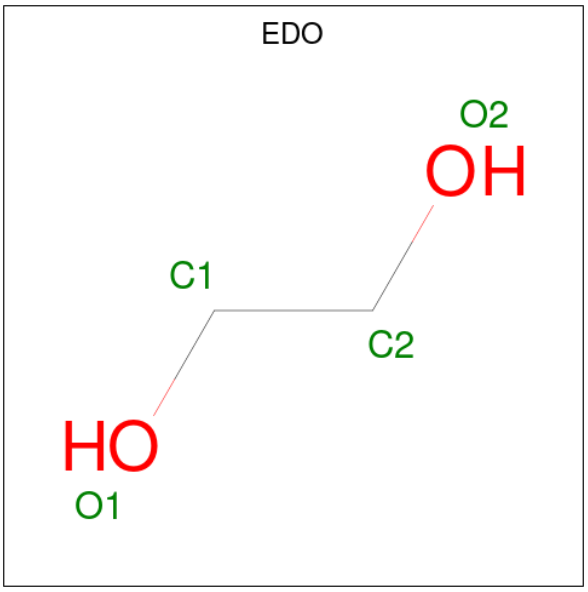
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O S 4 2 1 1	0	0

- Molecule 10 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 12 is water.

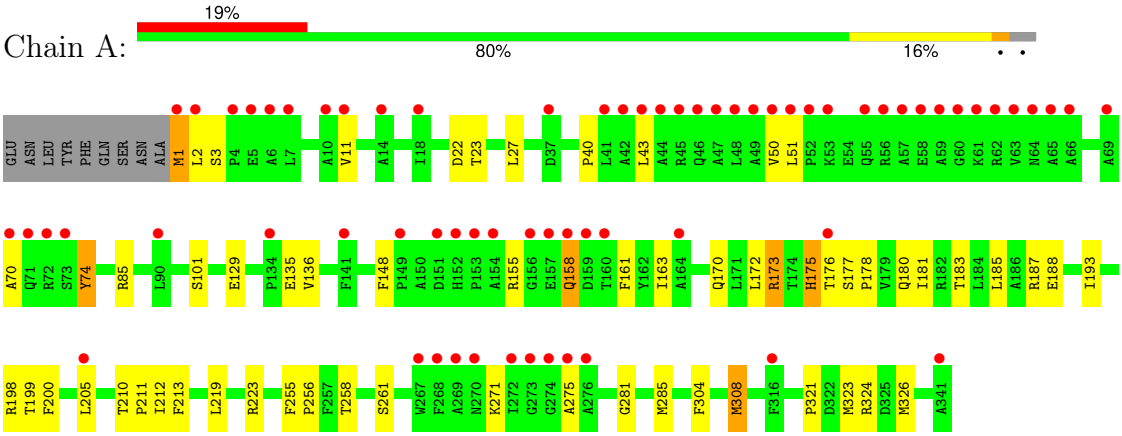
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	72	Total O 72 72	0	0
12	B	329	Total O 329 329	0	0
12	C	50	Total O 50 50	0	0
12	D	56	Total O 56 56	0	0
12	E	208	Total O 208 208	0	0
12	F	33	Total O 33 33	0	0

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.

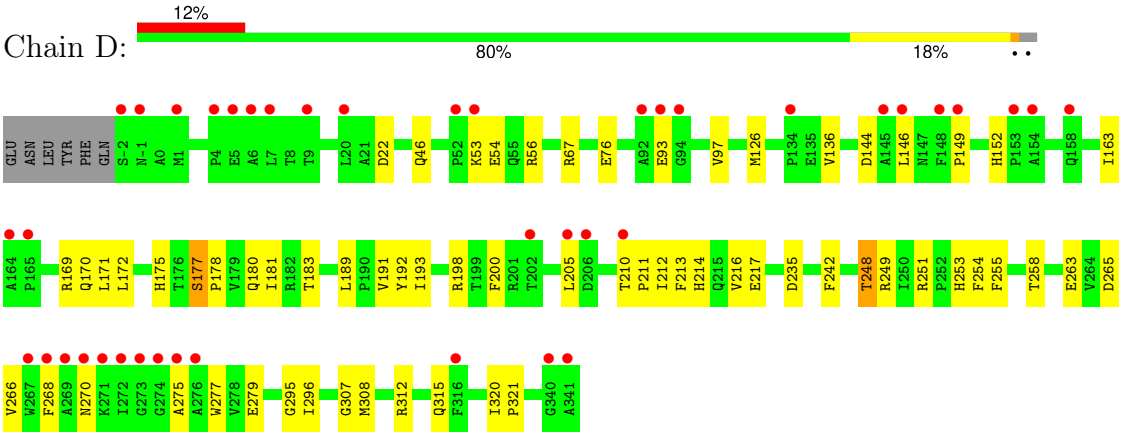
• Molecule 1: Phenylalanine–tRNA ligase alpha subunit

Chain A:



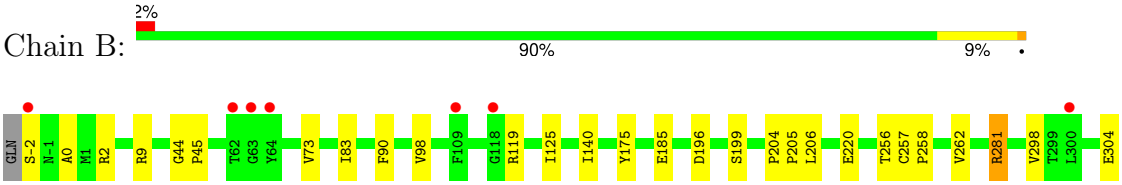
• Molecule 1: Phenylalanine–tRNA ligase alpha subunit

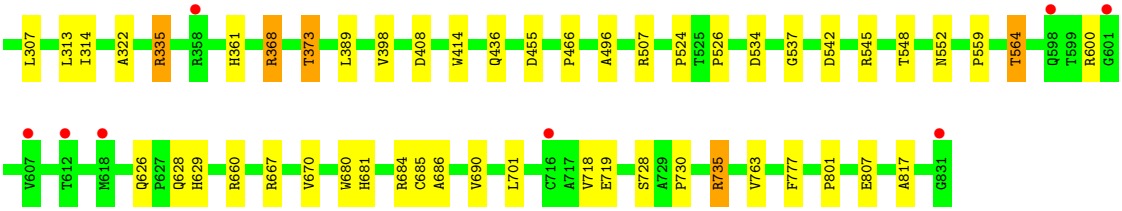
Chain D:



• Molecule 2: Phenylalanine–tRNA ligase beta subunit

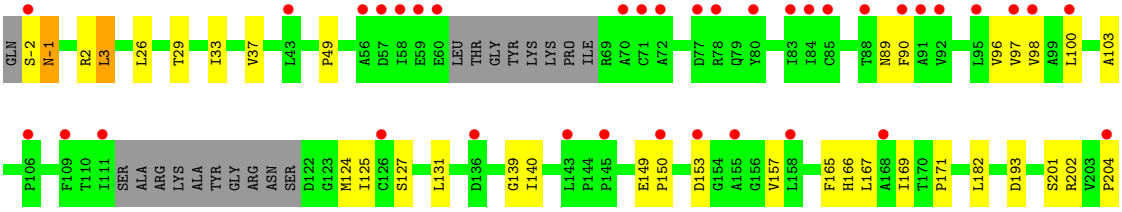
Chain B:





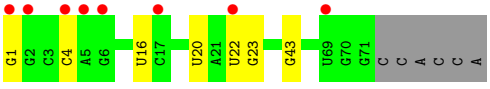
• Molecule 2: Phenylalanine–tRNA ligase beta subunit

Chain E:



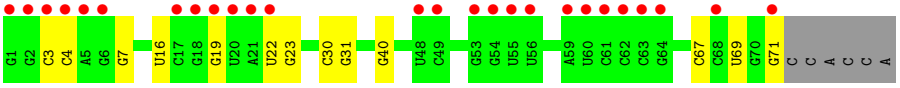
• Molecule 3: tRNA(phe)

Chain C:



• Molecule 3: tRNA(phe)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	147.09Å 64.39Å 188.78Å 90.00° 111.10° 90.00°	Depositor
Resolution (Å)	48.75 – 2.46 48.75 – 2.46	Depositor EDS
% Data completeness (in resolution range)	60.7 (48.75-2.46) 89.6 (48.75-2.46)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.210 , 0.260 0.211 , 0.258	Depositor DCC
R_{free} test set	5917 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	21397	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DMS, EPE, MG, GOL, PEG, ACT, EDO, 2AQ

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	0.24	0/2658	0.50	0/3623
1	D	0.24	0/2700	0.50	0/3676
2	B	0.24	0/6358	0.51	0/8710
2	E	0.24	0/6122	0.52	0/8397
3	C	0.28	1/1702 (0.1%)	0.66	0/2652
3	F	0.12	0/1701	0.67	0/2652
All	All	0.24	1/21241 (0.0%)	0.54	0/29710

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	G	OP3-P	-10.53	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2524	33	0
1	D	2640	0	2581	41	0
2	B	6222	0	6233	44	0
2	E	5992	0	5924	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1523	0	770	1	0
3	F	1522	0	770	3	0
4	A	11	0	8	0	0
4	D	11	0	8	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	A	4	0	3	0	0
6	B	16	0	12	2	0
6	D	8	0	6	0	0
6	E	12	0	9	0	0
7	A	7	0	10	0	0
7	B	7	0	10	0	0
7	E	7	0	10	0	0
8	B	18	0	24	0	0
8	E	6	0	8	0	0
9	B	4	0	6	0	0
10	B	30	0	34	0	0
11	B	4	0	6	0	0
11	E	4	0	6	0	0
12	A	72	0	0	0	0
12	B	329	0	0	0	0
12	C	50	0	0	0	0
12	D	56	0	0	0	0
12	E	208	0	0	1	0
12	F	33	0	0	0	0
All	All	21397	0	18962	181	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.

The worst 5 of 181 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)
2:E:3:LEU:HD21	2:E:182:LEU:HD23	1.68	0.74
2:B:507:ARG:HD3	2:B:628:GLN:HE21	1.52	0.74
2:E:171:PRO:HA	2:E:372:ARG:HH11	1.54	0.71
2:E:421:MET:HG3	2:E:471:PRO:HB3	1.77	0.66
2:E:275:HIS:CE1	2:E:328:GLY:HA3	2.31	0.65

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/350 (97%)	322 (95%)	16 (5%)	1 (0%)	37	45
1	D	342/350 (98%)	327 (96%)	13 (4%)	2 (1%)	22	28
2	B	832/835 (100%)	812 (98%)	18 (2%)	2 (0%)	44	54
2	E	810/835 (97%)	776 (96%)	32 (4%)	2 (0%)	44	54
All	All	2323/2370 (98%)	2237 (96%)	79 (3%)	7 (0%)	37	45

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	89	ASN
2	B	373	THR
1	D	275	ALA
1	A	321	PRO
2	E	324	GLY

5.3.2 Protein sidechains (i)

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	260/276 (94%)	248 (95%)	12 (5%)	23	33
1	D	267/276 (97%)	260 (97%)	7 (3%)	41	57
2	B	647/652 (99%)	628 (97%)	19 (3%)	37	52
2	E	608/652 (93%)	591 (97%)	17 (3%)	38	54
All	All	1782/1856 (96%)	1727 (97%)	55 (3%)	35	50

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	718	VAL
1	D	279	GLU
2	E	564	THR
2	E	344	GLU
2	B	728	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	628	GLN
1	D	142	ASN
2	E	275	HIS
1	A	175	HIS
1	A	170	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	70/77 (90%)	5 (7%)	0
3	F	70/77 (90%)	8 (11%)	0
All	All	140/154 (90%)	13 (9%)	0

5 of 13 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	4	C
3	C	16	U
3	C	22	U
3	C	23	G
3	C	43	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
8	GOL	B	912	-	5,5,5	0.96	0	5,5,5	1.05	0
6	ACT	D	402	-	3,3,3	1.35	0	3,3,3	1.37	0
6	ACT	D	403	-	3,3,3	1.39	1 (33%)	3,3,3	1.37	0
6	ACT	E	906	-	3,3,3	1.31	0	3,3,3	1.37	0
4	2AQ	A	401	-	12,12,12	1.73	2 (16%)	15,16,16	1.15	1 (6%)
8	GOL	B	905	-	5,5,5	0.92	0	5,5,5	1.08	0
8	GOL	B	904	-	5,5,5	0.92	0	5,5,5	1.12	0
6	ACT	B	901	-	3,3,3	1.37	0	3,3,3	1.35	0
6	ACT	B	910	-	3,3,3	1.36	0	3,3,3	1.38	0
10	EPE	B	907	-	15,15,15	0.83	1 (6%)	19,20,20	1.85	5 (26%)
11	EDO	B	909	-	3,3,3	0.42	0	2,2,2	0.39	0
7	PEG	A	404	-	6,6,6	0.12	0	5,5,5	0.09	0
6	ACT	E	904	-	3,3,3	1.36	0	3,3,3	1.36	0
6	ACT	A	403	-	3,3,3	1.35	0	3,3,3	1.37	0
9	DMS	B	906	-	3,3,3	0.66	0	3,3,3	0.52	0
11	EDO	E	905	-	3,3,3	0.42	0	2,2,2	0.36	0
7	PEG	E	901	-	6,6,6	0.11	0	5,5,5	0.08	0
4	2AQ	D	401	-	12,12,12	1.71	2 (16%)	15,16,16	1.09	0
6	ACT	B	902	-	3,3,3	1.34	0	3,3,3	1.36	0
6	ACT	B	911	-	3,3,3	1.39	0	3,3,3	1.37	0
6	ACT	E	903	-	3,3,3	1.36	0	3,3,3	1.36	0
7	PEG	B	903	-	6,6,6	0.12	0	5,5,5	0.09	0
8	GOL	E	907	-	5,5,5	0.94	0	5,5,5	1.06	0
10	EPE	B	908	-	15,15,15	0.84	1 (6%)	19,20,20	1.67	3 (15%)

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
8	GOL	B	912	-	-	1/4/4/4	-
11	EDO	E	905	-	-	0/1/1/1	-
4	2AQ	A	401	-	-	-	0/2/2/2
10	EPE	B	907	-	-	4/9/19/19	0/1/1/1
7	PEG	E	901	-	-	1/4/4/4	-
4	2AQ	D	401	-	-	-	0/2/2/2
8	GOL	B	905	-	-	0/4/4/4	-
8	GOL	E	907	-	-	1/4/4/4	-
7	PEG	B	903	-	-	1/4/4/4	-
11	EDO	B	909	-	-	0/1/1/1	-
8	GOL	B	904	-	-	0/4/4/4	-
7	PEG	A	404	-	-	1/4/4/4	-
10	EPE	B	908	-	-	6/9/19/19	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	2AQ	C5-C10	-3.68	1.36	1.42
4	A	401	2AQ	C2-N1	3.63	1.45	1.35
4	D	401	2AQ	C2-N1	3.58	1.45	1.35
4	D	401	2AQ	C5-C10	-3.56	1.36	1.42
10	B	908	EPE	C10-S	2.90	1.81	1.77

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	908	EPE	C5-N4-C3	4.40	118.31	108.84
10	B	907	EPE	C5-N4-C3	4.33	118.17	108.84
10	B	907	EPE	C7-N4-C5	3.60	120.84	111.24
10	B	907	EPE	C7-N4-C3	3.44	120.40	111.24
10	B	908	EPE	C7-N4-C5	2.60	118.16	111.24

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	908	EPE	C10-C9-N1-C2
10	B	908	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
8	E	907	GOL	O1-C1-C2-C3
10	B	908	EPE	C9-C10-S-O3S
10	B	907	EPE	C8-C7-N4-C5

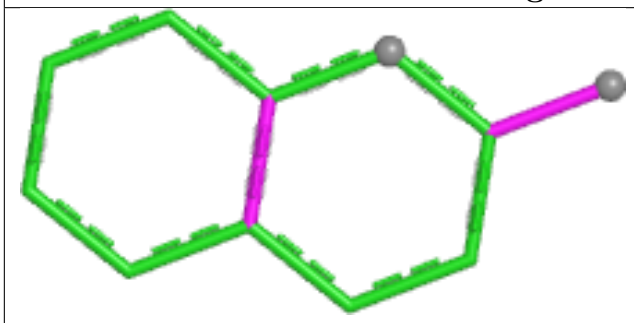
There are no ring outliers.

2 monomers are involved in 2 short contacts:

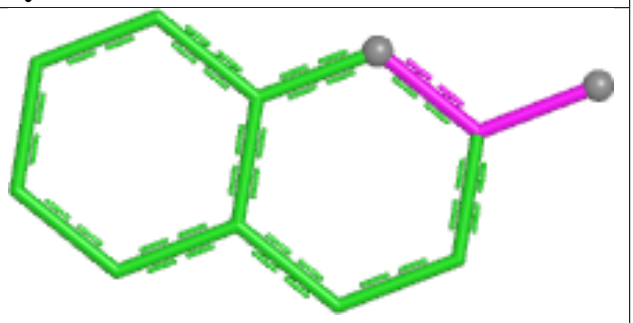
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	901	ACT	1	0
6	B	910	ACT	1	0

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 then 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.

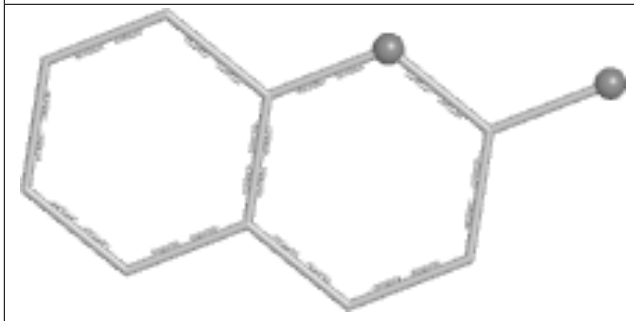
Ligand 2AQ A 401



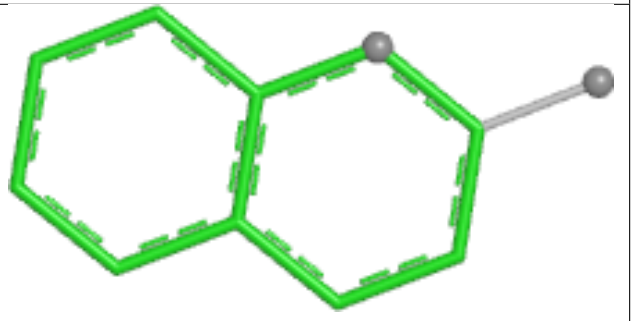
Bond lengths



Bond angles

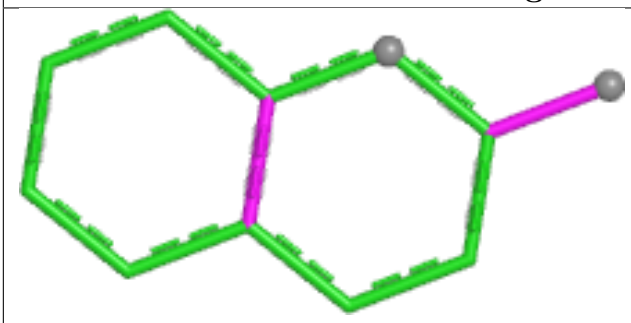


Torsions

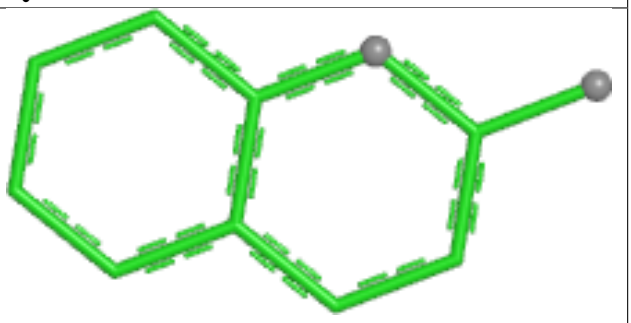


Rings

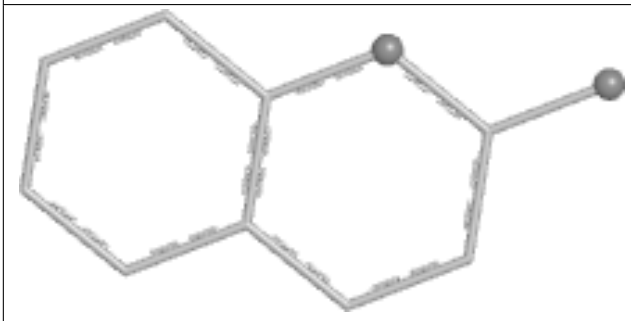
Ligand 2AQ D 401



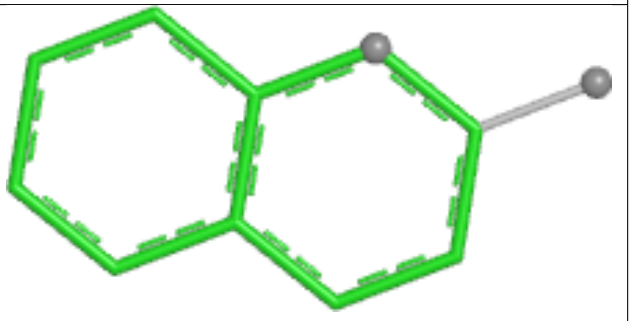
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	341/350 (97%)	0.90	68 (19%) 3 3	25, 51, 121, 153	0
1	D	344/350 (98%)	0.79	41 (11%) 10 10	27, 55, 101, 186	0
2	B	834/835 (99%)	-0.04	15 (1%) 67 69	20, 33, 64, 127	0
2	E	816/835 (97%)	0.70	106 (12%) 9 8	23, 52, 109, 174	0
3	C	71/77 (92%)	0.47	8 (11%) 11 11	30, 54, 174, 201	0
3	F	71/77 (92%)	1.37	26 (36%) 1 0	34, 78, 191, 205	0
All	All	2477/2524 (98%)	0.51	264 (10%) 12 12	20, 43, 111, 205	0

The worst 5 of 264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	341	ALA	8.2
2	E	100	LEU	5.4
2	E	85	CYS	5.3
1	A	62	ARG	5.1
1	A	57	ALA	5.0

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

There are no monosaccharides in this entry.

6.4 Ligands (i)

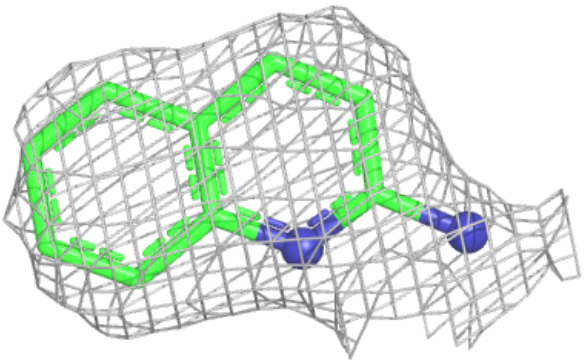
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

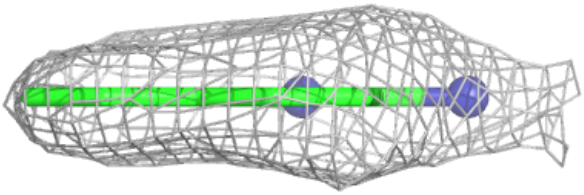
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PEG	E	901	7/7	0.70	0.22	49,56,69,78	0
6	ACT	E	903	4/4	0.74	0.15	42,56,56,66	0
7	PEG	A	404	7/7	0.75	0.17	44,54,61,63	0
8	GOL	E	907	6/6	0.79	0.17	51,59,64,67	0
6	ACT	D	403	4/4	0.80	0.18	38,53,57,61	0
8	GOL	B	905	6/6	0.81	0.14	52,61,65,69	0
6	ACT	B	910	4/4	0.81	0.18	41,45,49,50	0
11	EDO	B	909	4/4	0.82	0.16	47,48,49,50	0
6	ACT	E	906	4/4	0.83	0.20	63,68,69,70	0
7	PEG	B	903	7/7	0.84	0.25	30,38,50,51	0
8	GOL	B	904	6/6	0.85	0.16	27,34,37,39	0
10	EPE	B	908	15/15	0.86	0.14	48,57,73,86	0
11	EDO	E	905	4/4	0.86	0.22	42,48,51,68	0
10	EPE	B	907	15/15	0.87	0.14	52,60,67,77	0
6	ACT	B	901	4/4	0.87	0.11	46,46,47,49	0
6	ACT	B	911	4/4	0.88	0.14	40,42,48,55	0
5	MG	C	400	1/1	0.89	0.09	47,47,47,47	0
6	ACT	D	402	4/4	0.90	0.14	33,37,38,41	0
8	GOL	B	912	6/6	0.91	0.10	34,45,51,52	0
4	2AQ	D	401	11/11	0.91	0.12	42,50,52,54	0
6	ACT	E	904	4/4	0.92	0.11	39,42,47,52	0
6	ACT	A	403	4/4	0.93	0.14	30,32,40,42	0
4	2AQ	A	401	11/11	0.94	0.09	34,38,41,43	0
5	MG	E	902	1/1	0.95	0.06	42,42,42,42	0
6	ACT	B	902	4/4	0.96	0.08	28,32,33,34	0
9	DMS	B	906	4/4	0.96	0.12	37,43,47,47	0
5	MG	A	402	1/1	1.00	0.01	30,30,30,30	0

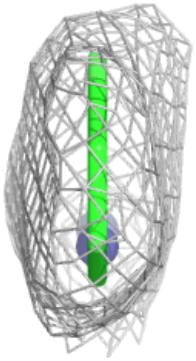
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2AQ D 401:

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

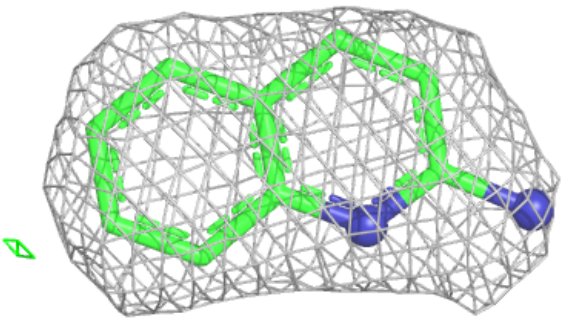


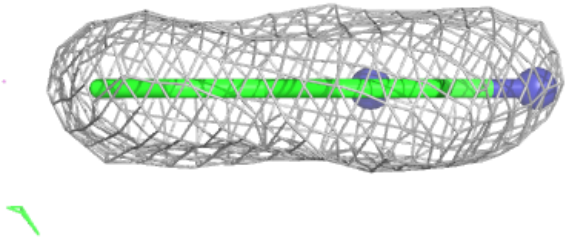


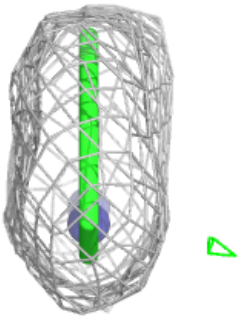


Electron density around 2AQ A 401:

$2mF_o$-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 (i)

There are no such residues in this entry.