Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:45 AM EDT

PDB ID	:	7KA0
Title	:	Crystal structure of the complex of M. tuberculosis PheRS with cognate precursor tRNA and phenylalanine
Authors	:	Chang, C.; Michalska, K.; Jedrzejczak, R.; Wower, J.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2020-09-29
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

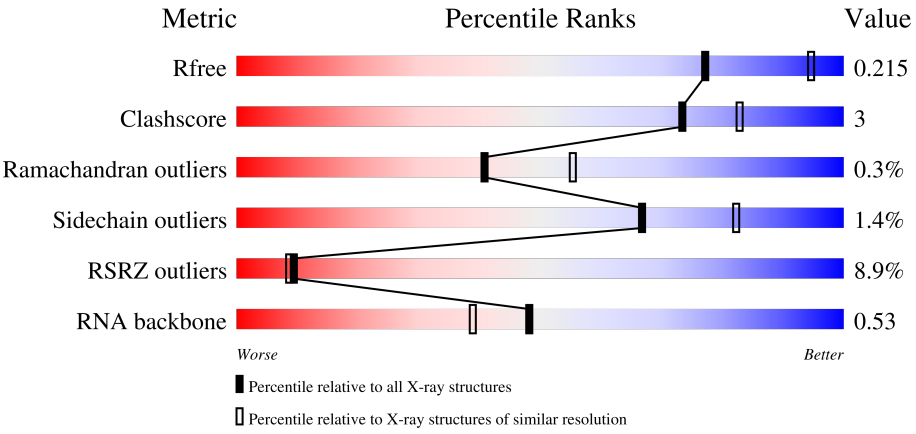
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	341	9% 87% 12% ••
1	D	341	21% 85% 13% ••
2	B	835	% 92% 8%

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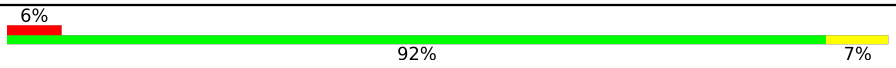
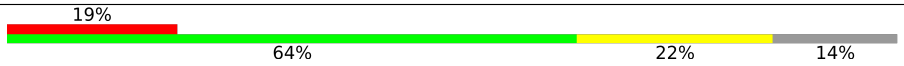
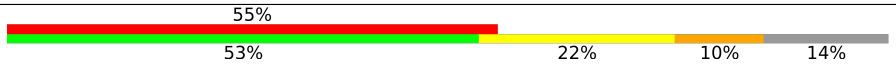
Mol	Chain	Length	Quality of chain
2	E	835	
3	C	77	
3	F	77	

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
8	MG	F	101	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21651 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	339	Total	C	N	O	S	0	2	0
			2633	1658	483	483	9			
1	D	336	Total	C	N	O	S	0	1	0
			2559	1613	463	475	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	835	Total	C	N	O	S	0	8	0
			6281	3945	1141	1173	22			
2	E	835	Total	C	N	O	S	0	5	0
			6264	3932	1138	1172	22			

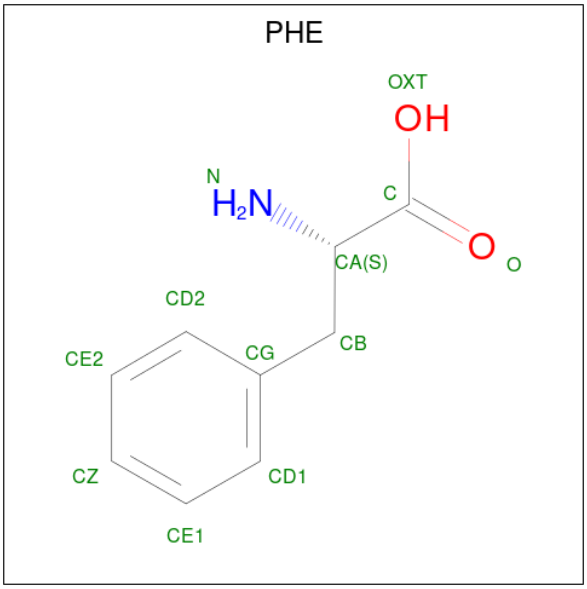
There are 8 discrepancies between the modelled and reference sequences:

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).

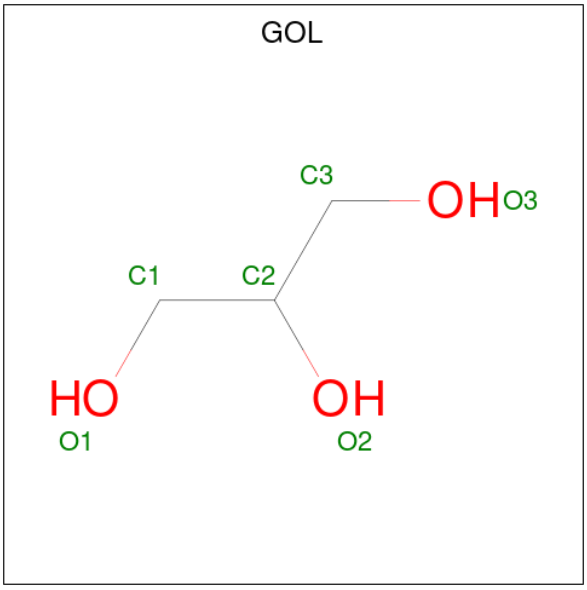
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	66	Total	C	N	O	P	0	0	0
			1413	629	256	462	66			
3	F	66	Total	C	N	O	P	0	0	0
			1413	629	256	462	66			

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



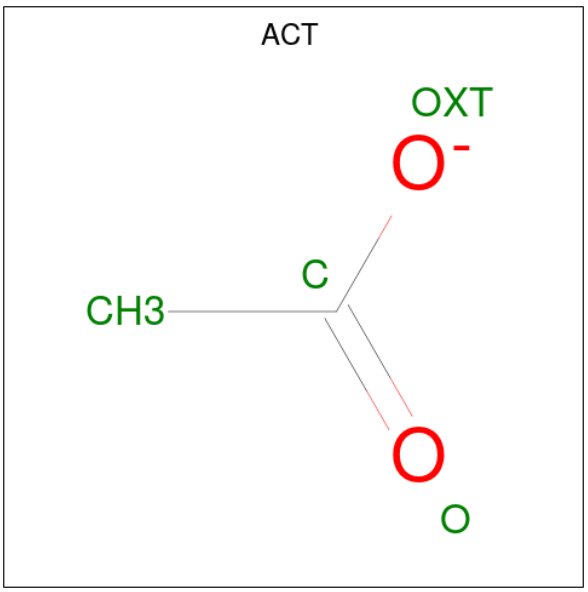
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 12 9 1 2	0	0
4	D	1	Total C N O 12 9 1 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



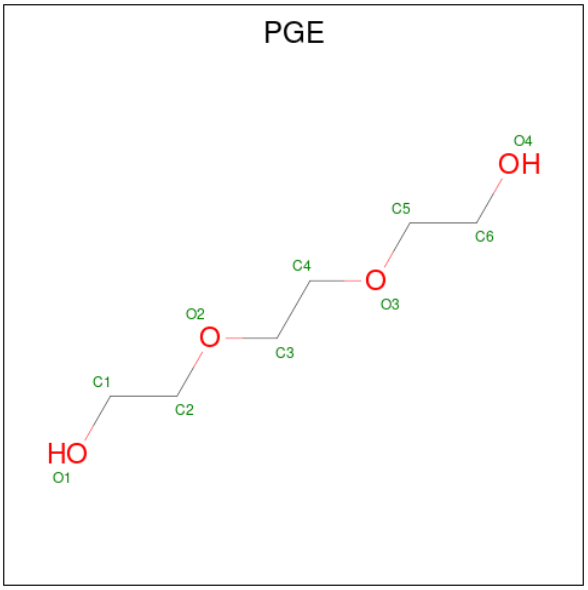
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	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	D	1	Total C O 4 2 2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 6 4	0	0
7	B	1	Total C O 10 6 4	0	0
7	E	1	Total C O 10 6 4	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Mg 2 2	0	0
8	B	1	Total Mg 1 1	0	0
8	C	3	Total Mg 3 3	0	0
8	D	2	Total Mg 2 2	0	0
8	E	2	Total Mg 2 2	0	0

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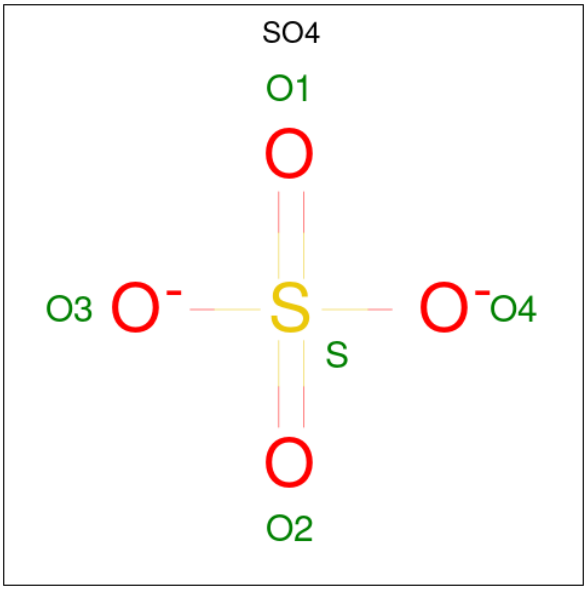
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	2	Total Mg 2 2	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	E	1	Total O S 5 4 1	0	0
9	E	1	Total O S 5 4 1	0	0
9	E	1	Total O S 5 4 1	0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total K 1 1	0	0
10	E	1	Total K 1 1	0	0

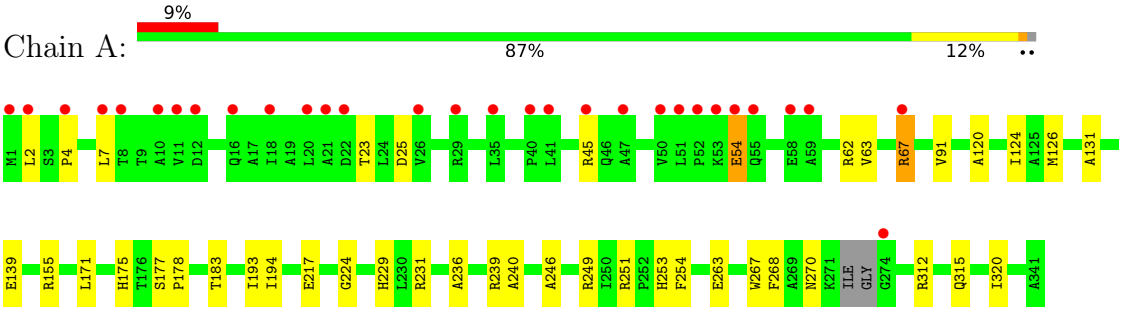
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	142	Total O 142 142	0	0
11	B	305	Total O 305 305	0	0
11	C	8	Total O 8 8	0	0
11	D	123	Total O 123 123	0	0
11	E	318	Total O 318 318	0	0
11	F	8	Total O 8 8	0	0

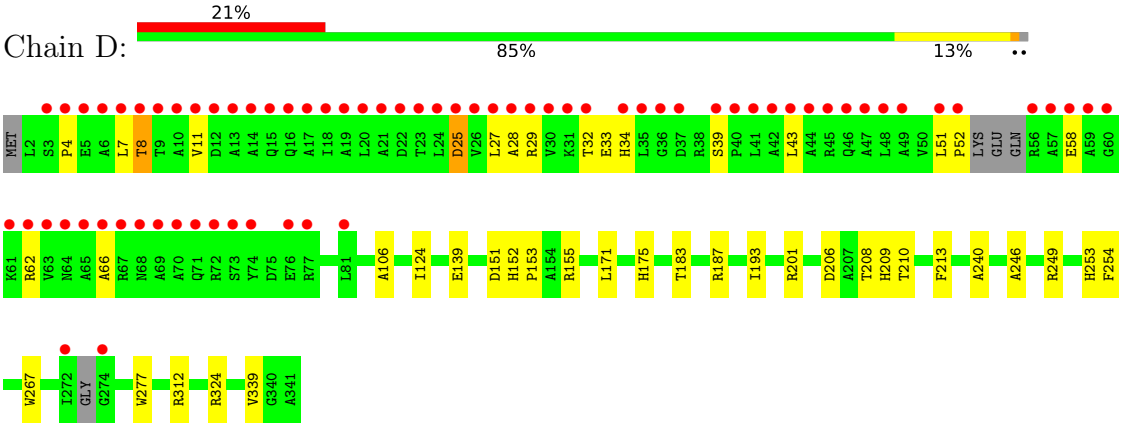
3 Residue-property plots (i)

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.

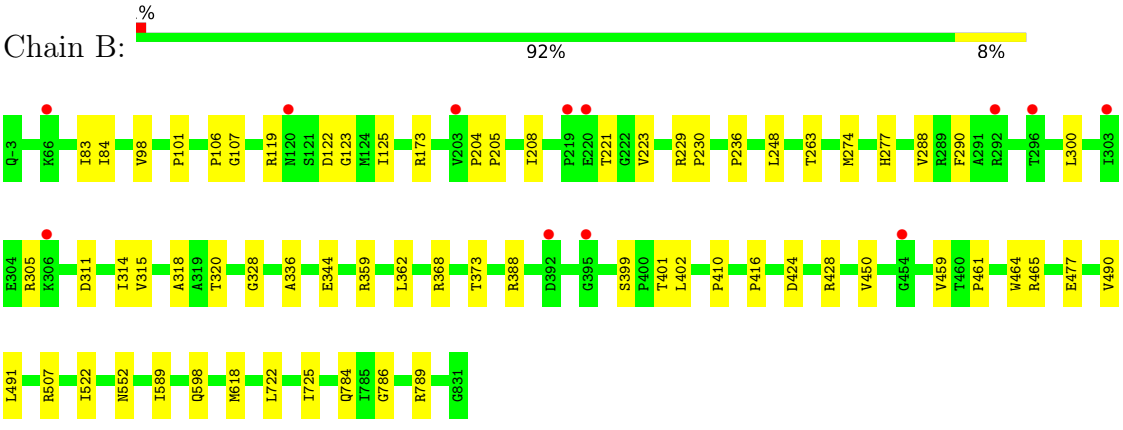
• Molecule 1: Phenylalanine–tRNA ligase alpha subunit



• Molecule 1: Phenylalanine–tRNA ligase alpha subunit

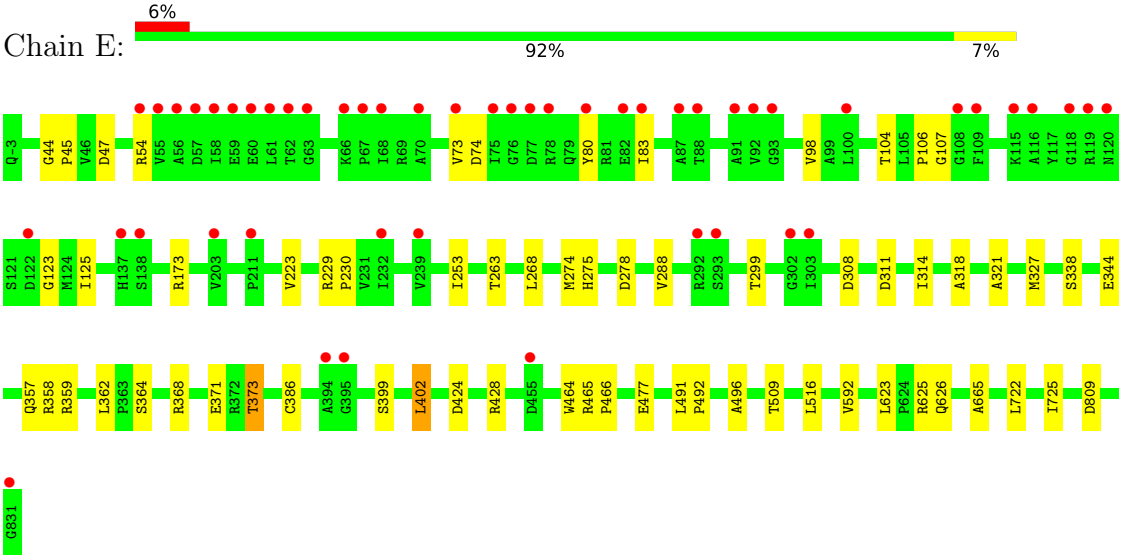


• Molecule 2: Phenylalanine–tRNA ligase beta subunit



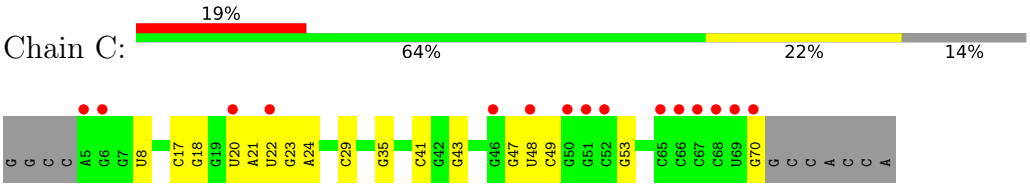
• Molecule 2: Phenylalanine–tRNA ligase beta subunit

Chain E:



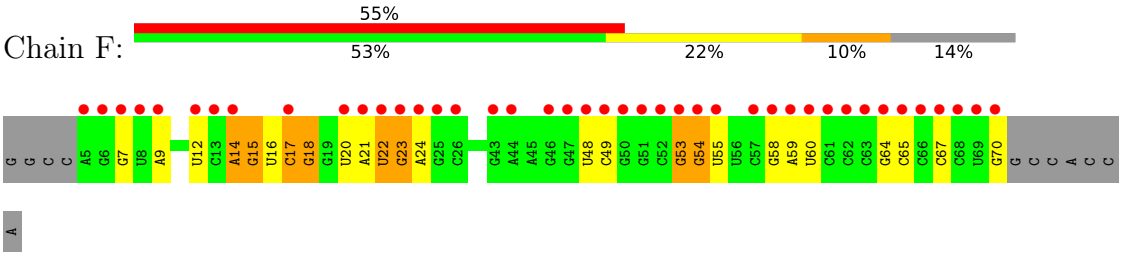
• Molecule 3: tRNA(Phe)

Chain C:



• Molecule 3: tRNA(Phe)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	292.86Å 109.98Å 127.95Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	48.04 – 2.40 48.04 – 2.36	Depositor EDS
% Data completeness (in resolution range)	91.6 (48.04-2.40) 87.8 (48.04-2.36)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.177 , 0.215 0.177 , 0.215	Depositor DCC
R_{free} test set	7191 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21651	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8489e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ACT, PGE, K, MG, SO4, GOL

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	0.28	0/2692	0.46	0/3662
1	D	0.28	0/2617	0.47	0/3565
2	B	0.28	0/6419	0.47	0/8793
2	E	0.27	0/6400	0.47	0/8765
3	C	0.18	0/1579	0.71	0/2461
3	F	0.18	0/1579	0.74	0/2461
All	All	0.26	0/21286	0.52	0/29707

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

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	2633	0	2577	25	0
1	D	2559	0	2463	25	0
2	B	6281	0	6287	34	0
2	E	6264	0	6267	37	1
3	C	1413	0	715	2	0
3	F	1413	0	715	10	1
4	A	12	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	12	0	8	0	0
5	A	30	0	40	4	0
5	B	12	0	16	1	0
5	D	24	0	32	4	0
5	E	6	0	8	0	0
6	A	4	0	3	0	0
6	D	4	0	3	0	0
7	A	10	0	14	2	0
7	B	10	0	14	1	0
7	E	10	0	14	3	0
8	A	2	0	0	0	0
8	B	1	0	0	0	0
8	C	3	0	0	0	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
9	B	15	0	0	0	0
9	D	5	0	0	0	0
9	E	15	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
11	A	142	0	0	1	0
11	B	305	0	0	0	0
11	C	8	0	0	0	0
11	D	123	0	0	0	0
11	E	318	0	0	0	0
11	F	8	0	0	0	0
All	All	21651	0	19184	128	1

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 3.

All (128) 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:373:THR:HG21	2:E:466:PRO:HG3	1.70	0.73
2:B:288:VAL:HG22	2:B:314:ILE:HG22	1.70	0.71
2:E:625:ARG:HD3	7:E:906:PGE:H2	1.73	0.70
2:E:54:ARG:NH2	2:E:74:ASP:OD2	2.28	0.67
2:B:263:THR:HB	2:B:274:MET:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HH12	5:A:407:GOL:H2	1.60	0.66
1:D:4:PRO:HA	1:D:7:LEU:HB3	1.78	0.66
1:D:312:ARG:HB2	5:D:405:GOL:H11	1.77	0.66
1:D:25:ASP:N	1:D:25:ASP:OD1	2.28	0.65
2:E:288:VAL:HG22	2:E:314:ILE:HG22	1.78	0.64
2:B:450:VAL:HG12	2:B:459:VAL:HG22	1.79	0.63
1:D:11:VAL:HG21	1:D:66:ALA:HB1	1.80	0.63
2:E:311:ASP:OD2	2:E:359:ARG:NH2	2.32	0.63
2:E:357:GLN:NE2	2:E:371:GLU:OE2	2.30	0.63
2:B:98:VAL:HG12	2:B:125:ILE:HG22	1.81	0.61
5:D:407:GOL:H2	2:E:428:ARG:HB3	1.82	0.61
3:F:7:G:H1	3:F:67:C:H42	1.49	0.61
2:B:230:PRO:HG2	2:B:399:SER:HB3	1.81	0.61
1:D:151:ASP:HA	2:E:358:ARG:HH22	1.68	0.59
2:B:173:ARG:NH2	2:B:477:GLU:OE2	2.36	0.59
7:B:908:PGE:H3	1:D:240:ALA:HB2	1.84	0.58
2:B:204[A]:PRO:O	2:B:388:ARG:NH2	2.29	0.58
2:E:98:VAL:HG12	2:E:125:ILE:HG22	1.85	0.58
1:A:23:THR:HG22	1:A:25:ASP:H	1.67	0.58
2:E:626:GLN:H	7:E:906:PGE:H4	1.67	0.58
1:A:236:ALA:HB1	7:A:405:PGE:H32	1.86	0.57
2:B:311:ASP:OD2	2:B:359:ARG:NH2	2.37	0.57
1:D:58:GLU:O	1:D:62:ARG:NH1	2.37	0.56
1:A:251[A]:ARG:NH1	1:A:263:GLU:OE1	2.31	0.56
2:E:230:PRO:HG2	2:E:399:SER:HB3	1.88	0.56
1:D:51:LEU:HD12	1:D:52:PRO:HD2	1.88	0.56
2:B:84:ILE:HD11	2:B:119:ARG:HB2	1.89	0.55
3:F:18:G:H5"	3:F:18:G:C8	2.42	0.55
2:E:229:ARG:HH11	2:E:402:LEU:HB2	1.73	0.53
3:F:18:G:N2	3:F:58:G:O6	2.29	0.53
2:E:223:VAL:HG21	2:E:288:VAL:HG11	1.90	0.52
2:E:623:LEU:HB2	7:E:906:PGE:H6	1.92	0.52
2:B:277:HIS:NE2	2:B:344:GLU:OE2	2.39	0.51
2:B:315:VAL:HG23	2:B:320:THR:HA	1.92	0.51
1:A:183:THR:HG21	1:A:193:ILE:HG12	1.93	0.51
3:F:18:G:O6	3:F:59:A:N6	2.43	0.51
2:E:491:LEU:HD12	2:E:492:PRO:HD2	1.93	0.51
2:E:173:ARG:NH2	2:E:477:GLU:OE2	2.40	0.50
2:E:278:ASP:OD2	2:E:338:SER:OG	2.22	0.50
1:A:224:GLY:HA2	5:B:902:GOL:H2	1.93	0.50
2:B:229:ARG:HH11	2:B:402:LEU:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:PRO:HB3	2:B:336:ALA:O	2.12	0.50
1:D:183:THR:HG21	1:D:193:ILE:HG12	1.94	0.50
2:E:509:THR:HG22	2:E:665:ALA:HB1	1.93	0.50
1:A:253:HIS:CG	1:A:254:PHE:H	2.30	0.50
1:A:231:ARG:HH22	5:A:408:GOL:H12	1.75	0.49
1:A:2:LEU:O	1:A:62:ARG:NH2	2.46	0.49
1:A:4:PRO:HB3	1:A:62:ARG:HD3	1.94	0.49
1:D:201:ARG:HG3	1:D:213:PHE:HE1	1.78	0.49
2:E:364:SER:O	2:E:368:ARG:HG3	2.13	0.49
3:F:14:A:H1'	3:F:23:G:N2	2.27	0.49
1:A:249:ARG:HG3	5:A:408:GOL:H11	1.95	0.48
1:A:315:GLN:HG3	1:A:320:ILE:O	2.13	0.48
2:E:308:ASP:N	2:E:311:ASP:OD2	2.43	0.48
2:B:424:ASP:O	2:B:428:ARG:HG3	2.14	0.48
1:A:246:ALA:HA	1:A:267:TRP:O	2.13	0.48
2:B:106:PRO:HA	2:B:107:GLY:HA2	1.54	0.47
2:E:263:THR:HB	2:E:274:MET:HB3	1.97	0.47
1:A:126:MET:HG2	2:E:496:ALA:HB1	1.95	0.47
3:F:15:G:N2	3:F:22:U:H3	2.13	0.47
2:B:786:GLY:HA3	2:B:789:ARG:NH1	2.29	0.47
2:B:399:SER:OG	2:B:401:THR:HG22	2.15	0.47
1:D:253:HIS:CG	1:D:254:PHE:H	2.32	0.47
2:E:253:ILE:HD12	2:E:268:LEU:HD11	1.97	0.47
2:B:786:GLY:HA3	2:B:789:ARG:HH11	1.80	0.47
2:E:424:ASP:O	2:E:428:ARG:HG3	2.15	0.47
2:B:208:ILE:HG23	2:B:402:LEU:HB3	1.95	0.46
2:B:784:GLN:HG2	3:C:35:G:OP1	2.15	0.46
3:F:53:G:N1	3:F:54:G:H1'	2.31	0.46
2:E:83:ILE:HG22	2:E:123:GLY:H	1.81	0.46
2:B:722:LEU:HD23	2:B:725:ILE:HD12	1.97	0.46
1:D:139:GLU:HG2	1:D:155:ARG:HH21	1.81	0.46
2:E:464:TRP:CD1	2:E:465:ARG:HG2	2.51	0.46
2:B:83:ILE:HG22	2:B:123:GLY:H	1.81	0.46
2:E:299:THR:HB	2:E:327:MET:HG2	1.98	0.46
2:E:106:PRO:HA	2:E:107:GLY:HA2	1.55	0.46
2:E:592:VAL:O	2:E:626:GLN:HA	2.16	0.45
1:D:8:THR:HA	1:D:11:VAL:HB	1.98	0.45
1:D:208:THR:HG23	1:D:209:HIS:ND1	2.32	0.45
2:B:223:VAL:HG21	2:B:288:VAL:HG11	1.97	0.45
3:F:14:A:H3'	3:F:15:G:C8	2.52	0.45
1:D:324:ARG:HH12	5:D:409:GOL:H12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ALA:O	1:D:32:THR:N	2.50	0.45
1:A:45:ARG:HD3	1:A:67:ARG:HE	1.81	0.45
2:B:300:LEU:HG	2:B:328:GLY:O	2.17	0.44
1:A:54:GLU:H	1:A:54:GLU:HG3	1.45	0.44
2:E:722:LEU:HD23	2:E:725:ILE:HD12	1.98	0.44
3:C:29:C:H42	3:C:43:G:H1	1.64	0.44
1:A:120:ALA:O	1:A:124:ILE:HD12	2.18	0.43
2:B:221:THR:HA	2:B:290:PHE:CZ	2.54	0.43
2:B:491:LEU:HD13	2:E:496:ALA:HB3	1.99	0.43
1:D:39:SER:O	1:D:43:LEU:HG	2.17	0.43
1:A:177:SER:N	1:A:178:PRO:HD2	2.33	0.43
1:D:29:ARG:O	1:D:32:THR:HG22	2.19	0.43
2:E:47:ASP:HB3	2:E:104:THR:OG1	2.19	0.42
2:B:204[A]:PRO:HA	2:B:205[A]:PRO:HD3	1.93	0.42
1:D:187:ARG:HE	5:D:404:GOL:C1	2.32	0.42
1:A:240:ALA:HB2	7:A:405:PGE:H1	2.01	0.42
2:E:314:ILE:HG13	2:E:321:ALA:HB3	2.01	0.42
1:D:201:ARG:HG3	1:D:213:PHE:CE1	2.55	0.42
2:E:230:PRO:HG2	2:E:399:SER:CB	2.50	0.42
1:A:194:ILE:HA	1:A:217:GLU:O	2.20	0.42
2:B:101:PRO:HD3	2:B:122:ASP:O	2.20	0.42
1:D:106:ALA:HB1	1:D:339:VAL:HG22	2.01	0.42
2:B:464:TRP:CD1	2:B:465:ARG:HG2	2.56	0.41
2:E:275:HIS:HB3	2:E:344:GLU:HG2	2.02	0.41
1:A:239:ARG:NH2	11:A:505:HOH:O	2.54	0.41
2:B:416:PRO:HD2	2:B:461:PRO:O	2.20	0.41
3:F:64:G:C6	3:F:65:C:C4	3.09	0.41
1:A:131:ALA:HB1	5:A:402:GOL:H32	2.02	0.41
1:D:246:ALA:HA	1:D:267:TRP:O	2.20	0.41
2:E:44:GLY:HA3	2:E:45:PRO:HA	1.78	0.41
3:F:53:G:O6	3:F:64:G:C6	2.74	0.41
1:A:139:GLU:HG2	1:A:155:ARG:HH21	1.86	0.41
2:E:73:VAL:HG11	2:E:98:VAL:HG11	2.02	0.41
1:A:7:LEU:HD21	1:A:63:VAL:HG22	2.02	0.41
2:B:305:ARG:NE	2:B:362:LEU:HD11	2.36	0.40
2:B:507:ARG:HG2	2:B:589:ILE:HG21	2.03	0.40
2:B:552:ASN:OD1	2:B:552:ASN:N	2.55	0.40
1:D:152:HIS:CG	1:D:153:PRO:HD2	2.56	0.40
1:A:229:HIS:HA	2:B:490:VAL:O	2.21	0.40
1:D:249:ARG:NH1	1:D:277:TRP:CD1	2.90	0.40
1:D:206:ASP:HA	1:D:324:ARG:NH2	2.37	0.40

All (1) 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)
2:E:80:TYR:OH	3:F:17:C:O2'[3_455]	2.03	0.17

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	338/341 (99%)	328 (97%)	9 (3%)	1 (0%)	41	55
1	D	331/341 (97%)	322 (97%)	9 (3%)	0	100	100
2	B	841/835 (101%)	811 (96%)	27 (3%)	3 (0%)	34	48
2	E	838/835 (100%)	807 (96%)	29 (4%)	2 (0%)	47	62
All	All	2348/2352 (100%)	2268 (97%)	74 (3%)	6 (0%)	41	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ASN
2	B	318	ALA
2	E	318	ALA
2	E	373	THR
2	B	373	THR
2	B	410	PRO

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	264/268 (98%)	257 (97%)	7 (3%)	44	65
1	D	253/268 (94%)	244 (96%)	9 (4%)	35	54
2	B	652/652 (100%)	647 (99%)	5 (1%)	81	91
2	E	650/652 (100%)	645 (99%)	5 (1%)	81	91
All	All	1819/1840 (99%)	1793 (99%)	26 (1%)	67	82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	67	ARG
1	A	91	VAL
1	A	171	LEU
1	A	175	HIS
1	A	268	PHE
1	A	312	ARG
2	B	248	LEU
2	B	368	ARG
2	B	522	ILE
2	B	598	GLN
2	B	618	MET
1	D	8	THR
1	D	25	ASP
1	D	27	LEU
1	D	33	GLU
1	D	34	HIS
1	D	124	ILE
1	D	171	LEU
1	D	175	HIS
1	D	210	THR
2	E	362	LEU
2	E	386	CYS
2	E	402	LEU
2	E	516	LEU
2	E	809	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	65/77 (84%)	14 (21%)	0
3	F	65/77 (84%)	19 (29%)	0
All	All	130/154 (84%)	33 (25%)	0

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	8	U
3	C	17	C
3	C	18	G
3	C	20	U
3	C	21	A
3	C	22	U
3	C	23	G
3	C	24	A
3	C	41	C
3	C	47	G
3	C	48	U
3	C	49	C
3	C	53	G
3	C	70	G
3	F	9	A
3	F	12	U
3	F	14	A
3	F	15	G
3	F	16	U
3	F	17	C
3	F	18	G
3	F	20	U
3	F	21	A
3	F	22	U
3	F	23	G
3	F	24	A
3	F	48	U
3	F	49	C
3	F	53	G
3	F	54	G
3	F	55	U
3	F	60	U
3	F	70	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 41 ligands modelled in this entry, 15 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
4	PHE	A	401	-	11,12,12	0.66	0	14,15,15	0.95	2 (14%)
5	GOL	B	902	-	5,5,5	0.91	0	5,5,5	0.98	0
5	GOL	A	402	-	5,5,5	0.88	0	5,5,5	1.09	0
5	GOL	A	408	-	5,5,5	0.91	0	5,5,5	0.96	0
5	GOL	D	407	-	5,5,5	0.96	0	5,5,5	0.95	0
5	GOL	D	409	-	5,5,5	0.88	0	5,5,5	0.96	0
5	GOL	B	905	-	5,5,5	0.92	0	5,5,5	0.94	0
7	PGE	A	405	-	9,9,9	0.33	0	8,8,8	0.25	0
9	SO4	D	403	-	4,4,4	0.13	0	6,6,6	0.06	0
5	GOL	D	405	-	5,5,5	0.76	0	5,5,5	0.94	0
9	SO4	E	901	-	4,4,4	0.14	0	6,6,6	0.06	0
5	GOL	A	403	-	5,5,5	1.06	0	5,5,5	0.93	0
5	GOL	D	404	-	5,5,5	0.82	0	5,5,5	1.15	0
5	GOL	A	406	-	5,5,5	0.91	0	5,5,5	0.97	0
9	SO4	B	906	-	4,4,4	0.13	0	6,6,6	0.07	0
6	ACT	D	406	-	3,3,3	1.33	0	3,3,3	1.38	0
9	SO4	E	904	-	4,4,4	0.13	0	6,6,6	0.05	0
6	ACT	A	404	-	3,3,3	1.32	0	3,3,3	1.56	0
4	PHE	D	401	-	11,12,12	0.72	1 (9%)	14,15,15	0.98	2 (14%)
9	SO4	B	903	-	4,4,4	0.15	0	6,6,6	0.06	0
5	GOL	E	905	-	5,5,5	0.82	0	5,5,5	0.98	0
9	SO4	E	908	-	4,4,4	0.15	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PGE	B	908	-	9,9,9	0.31	0	8,8,8	0.32	0
5	GOL	A	407	-	5,5,5	0.90	0	5,5,5	0.97	0
9	SO4	B	901	-	4,4,4	0.13	0	6,6,6	0.04	0
7	PGE	E	906	-	9,9,9	0.32	0	8,8,8	0.26	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
4	PHE	A	401	-	-	0/8/8/8	0/1/1/1
5	GOL	B	902	-	-	0/4/4/4	-
5	GOL	D	405	-	-	2/4/4/4	-
5	GOL	A	402	-	-	0/4/4/4	-
5	GOL	E	905	-	-	0/4/4/4	-
7	PGE	A	405	-	-	2/7/7/7	-
7	PGE	B	908	-	-	1/7/7/7	-
5	GOL	A	403	-	-	1/4/4/4	-
5	GOL	A	408	-	-	2/4/4/4	-
5	GOL	A	406	-	-	2/4/4/4	-
5	GOL	D	404	-	-	0/4/4/4	-
5	GOL	A	407	-	-	2/4/4/4	-
5	GOL	D	407	-	-	2/4/4/4	-
5	GOL	D	409	-	-	0/4/4/4	-
5	GOL	B	905	-	-	4/4/4/4	-
4	PHE	D	401	-	-	1/8/8/8	0/1/1/1
7	PGE	E	906	-	-	5/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	PHE	OXT-C	-2.12	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	PHE	OXT-C-O	-2.73	117.89	124.09
4	A	401	PHE	OXT-C-O	-2.52	118.36	124.09
4	A	401	PHE	OXT-C-CA	2.32	121.28	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	PHE	OXT-C-CA	2.26	121.09	113.38

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406	GOL	C1-C2-C3-O3
5	A	407	GOL	C1-C2-C3-O3
5	B	905	GOL	C1-C2-C3-O3
5	D	407	GOL	O1-C1-C2-C3
5	B	905	GOL	O1-C1-C2-O2
5	B	905	GOL	O2-C2-C3-O3
5	D	405	GOL	O1-C1-C2-O2
5	A	408	GOL	C1-C2-C3-O3
5	B	905	GOL	O1-C1-C2-C3
5	D	405	GOL	O1-C1-C2-C3
5	A	406	GOL	O2-C2-C3-O3
5	A	407	GOL	O2-C2-C3-O3
5	A	408	GOL	O2-C2-C3-O3
5	D	407	GOL	O1-C1-C2-O2
7	A	405	PGE	O2-C3-C4-O3
7	B	908	PGE	O1-C1-C2-O2
7	A	405	PGE	C4-C3-O2-C2
7	E	906	PGE	C3-C4-O3-C5
7	E	906	PGE	C6-C5-O3-C4
7	E	906	PGE	C1-C2-O2-C3
7	E	906	PGE	O2-C3-C4-O3
4	D	401	PHE	O-C-CA-N
5	A	403	GOL	O2-C2-C3-O3
7	E	906	PGE	C4-C3-O2-C2

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	GOL	1	0
5	A	402	GOL	1	0
5	A	408	GOL	2	0
5	D	407	GOL	1	0
5	D	409	GOL	1	0
7	A	405	PGE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	405	GOL	1	0
5	D	404	GOL	1	0
7	B	908	PGE	1	0
5	A	407	GOL	1	0
7	E	906	PGE	3	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.

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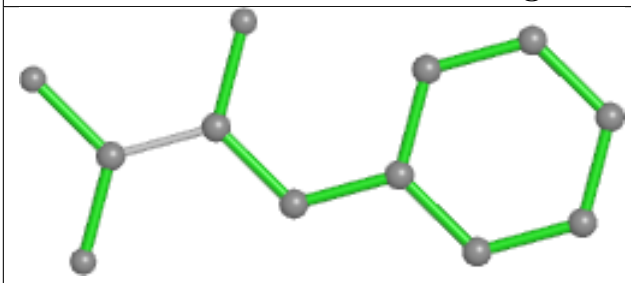
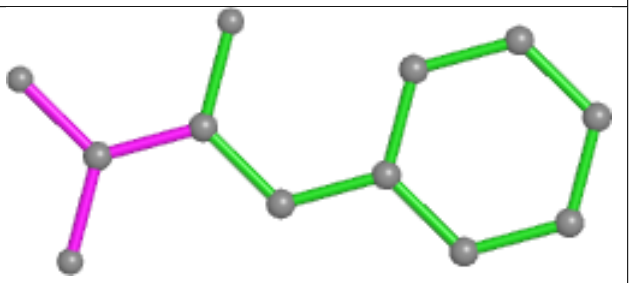
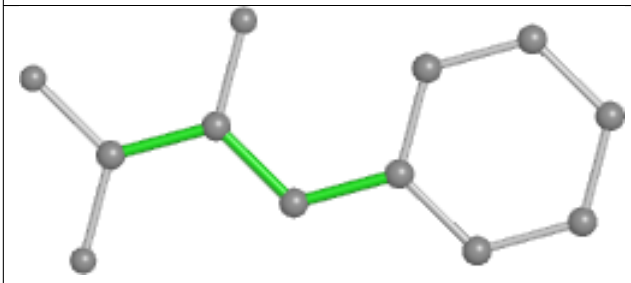


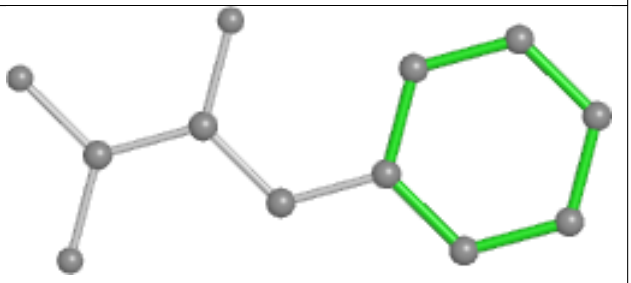
Bond lengths



Bond angles

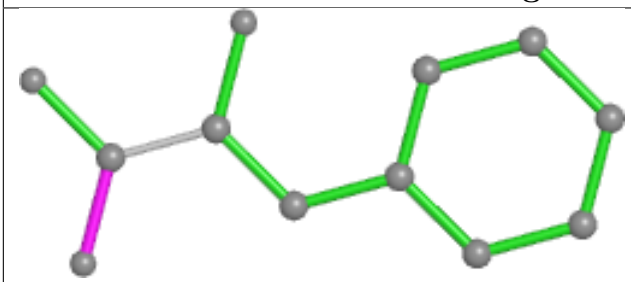


Torsions

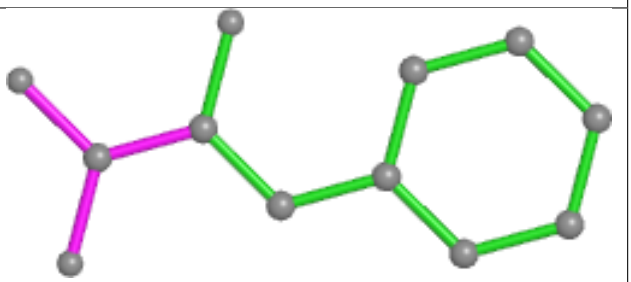


Rings

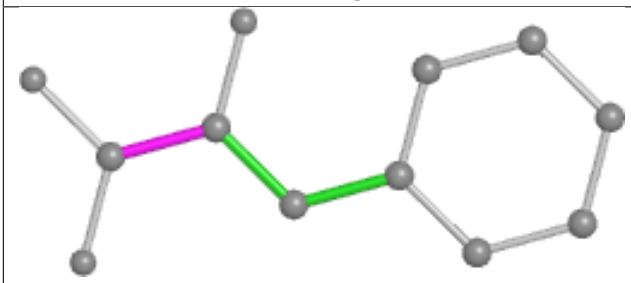
Ligand PHE D 401



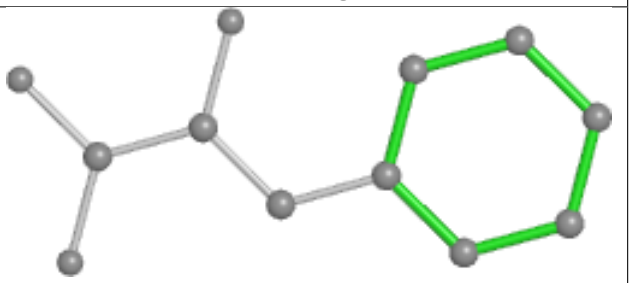
Bond lengths



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	339/341 (99%)	0.31	30 (8%)	10	9	19, 35, 103, 136	0
1	D	336/341 (98%)	1.03	71 (21%)	1	0	17, 33, 184, 257	0
2	B	835/835 (100%)	-0.13	12 (1%)	75	73	16, 46, 93, 124	0
2	E	835/835 (100%)	0.10	50 (5%)	21	20	15, 48, 114, 208	0
3	C	66/77 (85%)	1.15	15 (22%)	0	0	46, 114, 175, 240	0
3	F	66/77 (85%)	2.80	42 (63%)	0	0	45, 197, 264, 284	0
All	All	2477/2506 (98%)	0.28	220 (8%)	9	9	15, 45, 142, 284	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	66	ALA	11.4
1	D	67	ARG	11.3
1	D	51	LEU	10.5
3	F	5	A	10.0
3	F	48	U	9.4
1	D	65	ALA	8.7
3	F	70	G	8.7
1	D	63	VAL	8.3
1	D	45	ARG	8.3
2	E	78	ARG	8.0
3	C	48	U	7.8
1	D	44	ALA	7.8
1	D	10	ALA	7.7
1	D	20	LEU	7.5
3	C	70	G	7.5
1	D	47	ALA	7.4
1	D	62	ARG	7.2
3	F	66	C	6.6
1	D	41	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	59	ALA	6.4
1	D	14	ALA	6.3
3	F	67	C	6.2
1	D	27	LEU	6.2
3	F	65	C	6.2
3	F	20	U	6.1
1	D	69	ALA	5.9
3	F	6	G	5.8
1	D	70	ALA	5.8
1	D	11	VAL	5.8
3	F	22	U	5.8
3	F	49	C	5.7
1	D	49	ALA	5.7
2	E	54	ARG	5.7
1	D	58	GLU	5.7
1	D	52	PRO	5.6
1	D	30	VAL	5.6
1	D	6	ALA	5.5
1	D	7	LEU	5.5
2	E	76	GLY	5.5
2	E	80	TYR	5.3
1	D	56	ARG	5.3
1	D	9	THR	5.1
1	D	48	LEU	5.1
1	D	42	ALA	5.0
1	D	57	ALA	5.0
2	E	92	VAL	5.0
1	D	21	ALA	5.0
3	F	62	C	5.0
2	E	91	ALA	5.0
1	D	23	THR	4.9
1	D	72	ARG	4.9
2	E	203	VAL	4.7
3	F	17	C	4.7
1	D	74	TYR	4.7
1	D	4	PRO	4.6
1	D	61	LYS	4.6
1	D	272	ILE	4.6
2	E	77	ASP	4.6
3	C	20	U	4.6
3	C	22	U	4.6
2	E	56	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
3	C	5	A	4.6
3	F	63	C	4.5
1	D	12	ASP	4.5
1	D	8	THR	4.5
1	D	13	ALA	4.5
1	D	39	SER	4.4
1	D	73	SER	4.4
1	D	35	LEU	4.4
1	D	5	GLU	4.4
3	F	7	G	4.3
1	D	68	ASN	4.2
3	F	8	U	4.2
3	F	64	G	4.2
1	D	22	ASP	4.2
3	F	54	G	4.2
1	D	26	VAL	4.1
3	F	53	G	4.1
3	C	66	C	4.1
1	D	19	ALA	4.0
3	F	52	C	4.0
3	F	68	C	4.0
3	F	21	A	4.0
2	E	58	ILE	4.0
3	C	50	G	3.9
3	F	50	G	3.9
3	F	13	C	3.9
3	F	12	U	3.8
1	D	46	GLN	3.8
1	D	43	LEU	3.8
1	A	41	LEU	3.7
2	E	831	GLY	3.7
3	C	67	C	3.6
1	D	3	SER	3.6
3	F	61	C	3.6
1	A	274	GLY	3.6
1	D	274	GLY	3.6
2	E	119	ARG	3.5
1	D	29	ARG	3.5
3	C	6	G	3.5
3	F	47	G	3.5
1	D	28	ALA	3.4
2	E	293	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	15	GLN	3.4
1	A	59	ALA	3.4
3	F	46	G	3.4
2	E	61	LEU	3.4
1	D	17	ALA	3.3
1	A	40	PRO	3.3
2	E	83	ILE	3.3
1	A	47	ALA	3.3
3	F	25	G	3.3
1	D	24	LEU	3.2
2	E	302	GLY	3.2
3	F	58	G	3.2
2	E	75	ILE	3.2
2	E	109	PHE	3.2
3	F	69	U	3.1
1	D	18	ILE	3.0
2	E	62	THR	3.0
1	D	37	ASP	3.0
2	E	87	ALA	3.0
3	F	51	G	3.0
2	E	68	ILE	3.0
1	D	64	ASN	3.0
3	F	24	A	3.0
3	C	68	C	2.9
1	D	36	GLY	2.9
2	B	219	PRO	2.9
2	E	93	GLY	2.9
2	E	116	ALA	2.9
1	A	58	GLU	2.9
1	A	1	MET	2.9
1	A	29	ARG	2.9
1	D	40	PRO	2.9
3	C	65	C	2.8
3	C	69	U	2.8
2	E	394	ALA	2.8
1	A	50	VAL	2.8
2	B	303	ILE	2.8
1	A	20	LEU	2.8
1	D	71	GLN	2.8
1	D	60	GLY	2.8
1	D	76	GLU	2.8
1	A	12	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	67	PRO	2.8
2	B	66	LYS	2.7
3	C	51	G	2.7
1	D	16	GLN	2.7
3	F	9	A	2.7
1	A	4	PRO	2.7
2	E	59	GLU	2.7
2	E	239	VAL	2.7
2	E	232	ILE	2.7
1	A	45	ARG	2.7
1	A	26	VAL	2.7
3	F	23	G	2.7
2	E	60	GLU	2.6
1	A	55	GLN	2.6
2	E	55	VAL	2.6
2	E	303	ILE	2.6
2	E	137	HIS	2.6
1	A	67	ARG	2.6
2	E	73	VAL	2.6
1	D	81	LEU	2.5
2	E	118	GLY	2.5
2	B	203[A]	VAL	2.5
1	A	10	ALA	2.5
1	A	21	ALA	2.5
2	B	454	GLY	2.5
3	F	43	G	2.5
1	D	32	THR	2.5
3	F	60	U	2.4
2	E	138	SER	2.4
2	E	122	ASP	2.4
2	E	63	GLY	2.4
3	F	57	C	2.4
2	E	115	LYS	2.4
1	A	18	ILE	2.4
2	E	57	ASP	2.4
1	A	11	VAL	2.4
2	B	395	GLY	2.3
2	E	108	GLY	2.3
2	E	100	LEU	2.3
2	E	66	LYS	2.3
2	E	82	GLU	2.3
1	D	77	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	54	GLU	2.3
2	E	70	ALA	2.3
2	E	120	ASN	2.2
2	B	296	THR	2.2
1	A	7	LEU	2.2
1	D	31	LYS	2.2
2	B	306	LYS	2.2
3	F	14	A	2.2
1	A	35	LEU	2.2
2	E	211	PRO	2.2
3	F	55	U	2.2
1	A	8	THR	2.2
2	E	395	GLY	2.2
1	A	16	GLN	2.1
1	D	25	ASP	2.1
1	A	51	LEU	2.1
2	B	120	ASN	2.1
3	F	59	A	2.1
2	E	88	THR	2.1
1	D	34	HIS	2.1
1	A	53	LYS	2.1
2	E	455	ASP	2.1
3	F	44	A	2.1
3	C	46	G	2.0
2	B	392	ASP	2.0
1	A	52	PRO	2.0
2	B	292	ARG	2.0
2	E	292	ARG	2.0
3	C	52	C	2.0
3	F	26	C	2.0
1	A	2	LEU	2.0
1	A	22	ASP	2.0
2	B	220	GLU	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, 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
5	GOL	A	408	6/6	0.73	0.27	73,76,80,81	0
8	MG	C	102	1/1	0.76	0.22	86,86,86,86	0
8	MG	F	101	1/1	0.77	0.41	93,93,93,93	0
7	PGE	E	906	10/10	0.80	0.30	50,57,61,67	10
8	MG	F	102	1/1	0.82	0.91	96,96,96,96	0
5	GOL	A	402	6/6	0.83	0.18	64,67,69,70	0
5	GOL	D	407	6/6	0.84	0.22	59,66,69,71	0
10	K	B	904	1/1	0.84	0.33	122,122,122,122	0
5	GOL	D	405	6/6	0.85	0.23	49,54,60,66	0
5	GOL	A	407	6/6	0.85	0.24	72,74,75,76	0
5	GOL	B	902	6/6	0.85	0.21	57,65,68,69	0
9	SO4	B	906	5/5	0.85	0.25	70,75,80,84	5
8	MG	C	101	1/1	0.85	0.39	93,93,93,93	0
5	GOL	E	905	6/6	0.86	0.17	54,67,68,74	0
5	GOL	A	406	6/6	0.86	0.30	63,65,73,77	0
5	GOL	B	905	6/6	0.87	0.15	68,73,75,76	0
5	GOL	D	404	6/6	0.88	0.20	55,60,63,66	0
7	PGE	A	405	10/10	0.89	0.21	61,73,79,81	0
7	PGE	B	908	10/10	0.89	0.20	75,82,85,86	0
9	SO4	E	901	5/5	0.89	0.31	73,75,77,79	5
5	GOL	A	403	6/6	0.89	0.20	57,69,76,79	0
6	ACT	A	404	4/4	0.90	0.14	57,60,62,66	0
8	MG	B	907	1/1	0.90	0.19	68,68,68,68	0
9	SO4	E	908	5/5	0.90	0.27	61,70,73,74	5
9	SO4	B	901	5/5	0.90	0.26	70,71,75,78	5
8	MG	C	103	1/1	0.92	0.23	63,63,63,63	0
8	MG	A	409	1/1	0.92	0.07	34,34,34,34	0
5	GOL	D	409	6/6	0.93	0.29	64,67,69,74	0
9	SO4	E	904	5/5	0.94	0.18	91,98,101,103	0
9	SO4	D	403	5/5	0.94	0.33	104,108,110,111	0
9	SO4	B	903	5/5	0.94	0.13	92,97,99,102	0
10	K	E	907	1/1	0.95	0.13	65,65,65,65	0
8	MG	D	410	1/1	0.96	0.09	31,31,31,31	0
6	ACT	D	406	4/4	0.96	0.09	67,69,69,70	0
8	MG	A	410	1/1	0.96	0.15	59,59,59,59	0
8	MG	E	902	1/1	0.97	0.38	71,71,71,71	0
4	PHE	A	401	12/12	0.97	0.20	32,32,43,47	0

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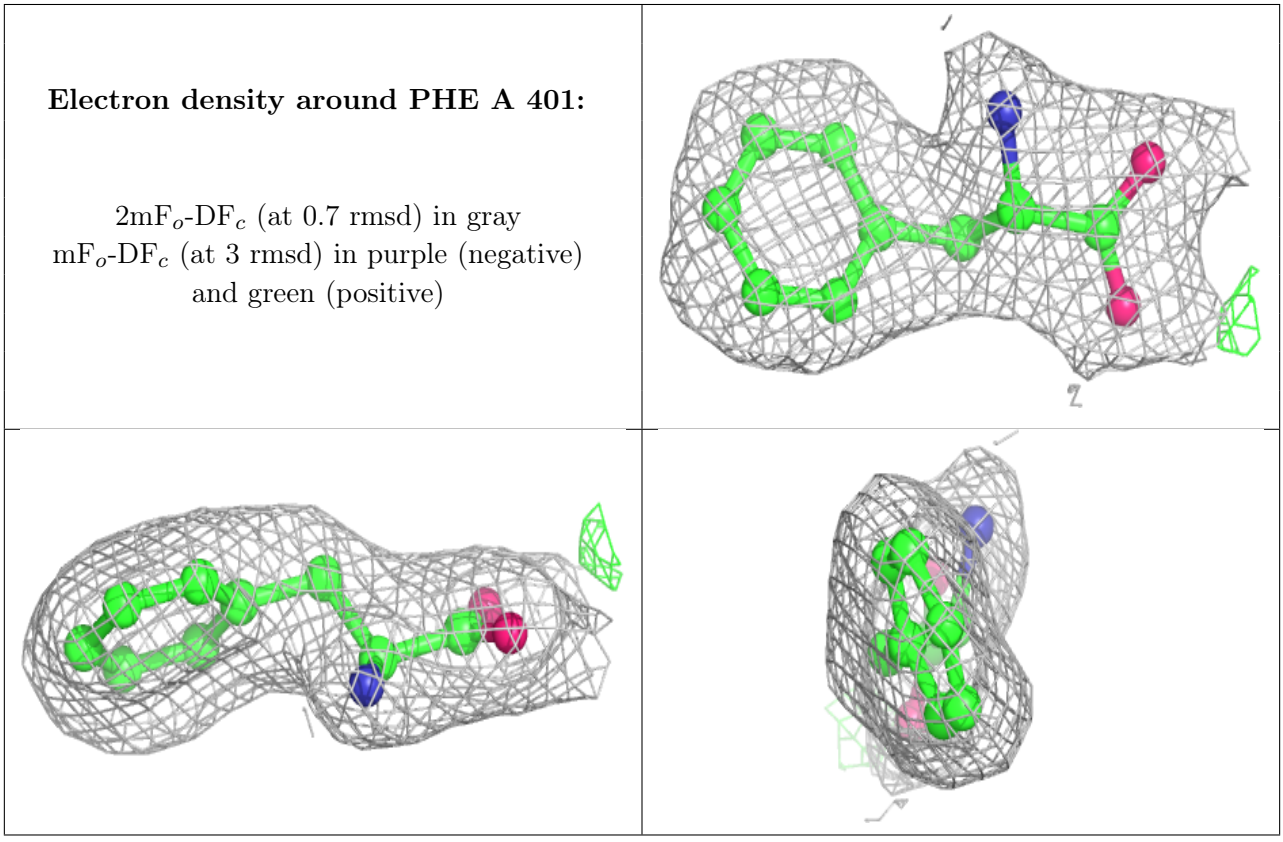
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PHE	D	401	12/12	0.97	0.19	22,29,32,37	0
10	K	D	408	1/1	0.98	0.16	75,75,75,75	0
8	MG	D	402	1/1	0.98	0.08	41,41,41,41	0
8	MG	E	903	1/1	0.99	0.30	54,54,54,54	0

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.

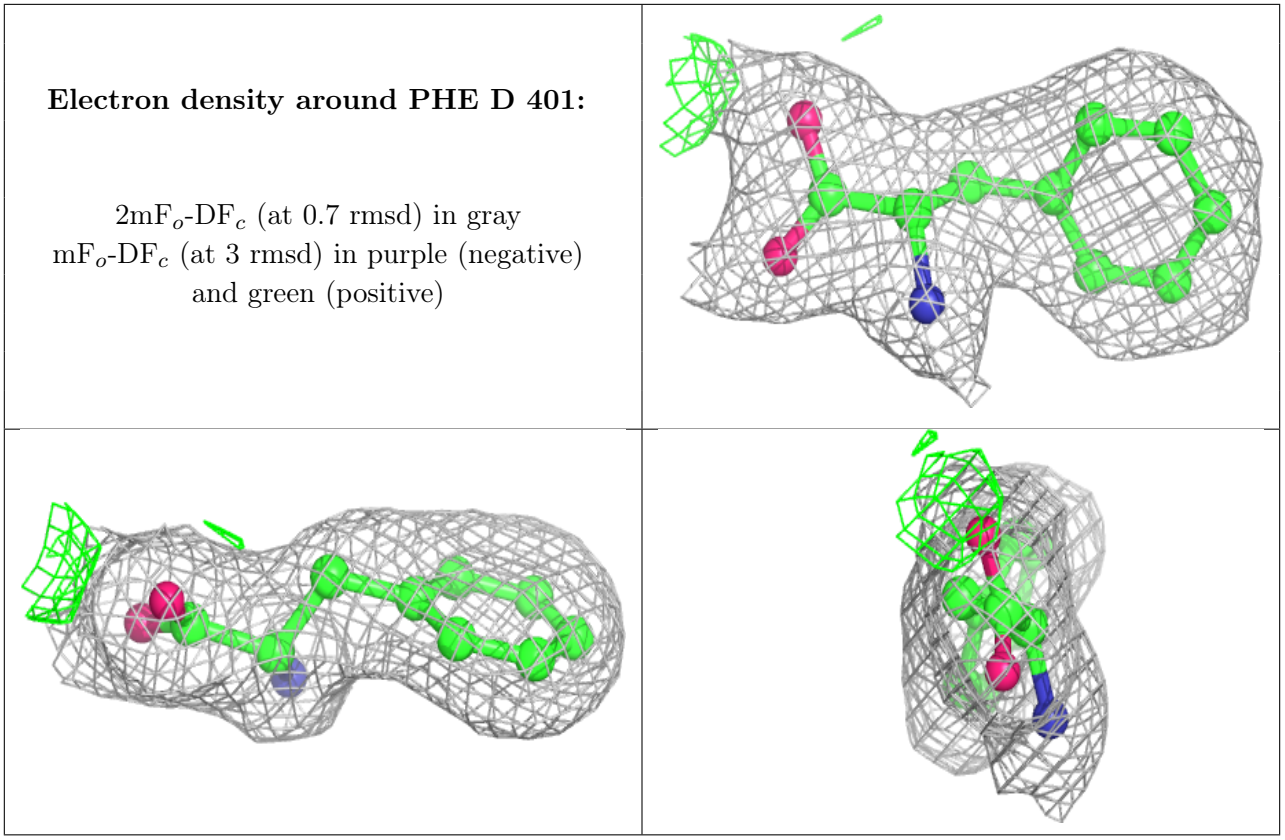
Electron density around PHE A 401:

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



Electron density around PHE 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)



6.5 Other polymers (i)

There are no such residues in this entry.